Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2N0A
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Title	:	Atomic-resolution structure of alpha-synuclein fibrils
Authors	:	Tuttle, M.D.; Comellas, G.; Nieuwkoop, A.J.; Covell, D.J.; Berthold, D.A.; Kloepper, K.D.; Courtney, J.M.; Kim, J.K.; Schwieters, C.D.; Lee, V.M.; George, J.M.; Rienstra, C.M.
Deposited on	:	2015-03-04

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

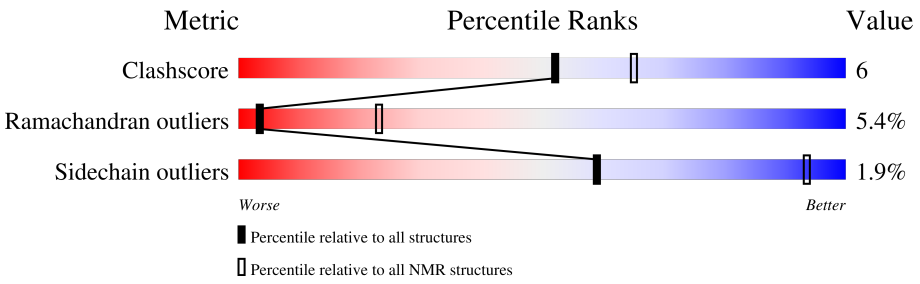
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 2%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	140	83% 16% • •
1	B	140	88% 11% •
1	C	140	82% 17% •
1	D	140	82% 15% •
1	E	140	84% 16%
1	F	140	82% 16% •
1	G	140	74% 23% •
1	H	140	86% 14%

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Mol	Chain	Length	Quality of chain
1	I	140	86% 14%
1	J	140	91% 9%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 20160 atoms, of which 10030 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Alpha-synuclein.

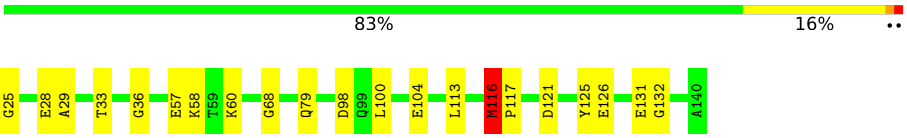
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	140	2016	627	1003	166	216	4	0
1	B	140	2016	627	1003	166	216	4	0
1	C	140	2016	627	1003	166	216	4	0
1	D	140	2016	627	1003	166	216	4	0
1	E	140	2016	627	1003	166	216	4	0
1	F	140	2016	627	1003	166	216	4	0
1	G	140	2016	627	1003	166	216	4	0
1	H	140	2016	627	1003	166	216	4	0
1	I	140	2016	627	1003	166	216	4	0
1	J	140	2016	627	1003	166	216	4	0

4 Residue-property plots (i)

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.

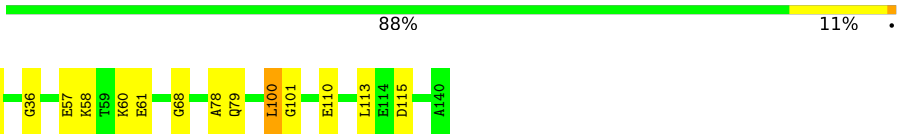
- Molecule 1: Alpha-synuclein

Chain A:



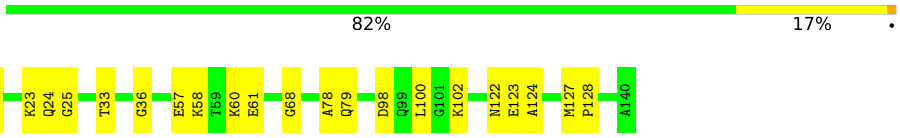
- Molecule 1: Alpha-synuclein

Chain B:



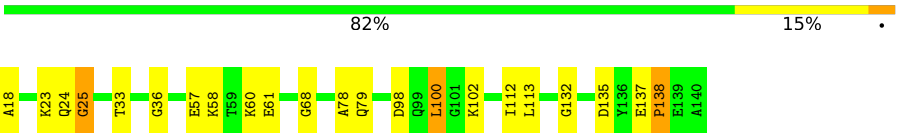
- Molecule 1: Alpha-synuclein

Chain C:



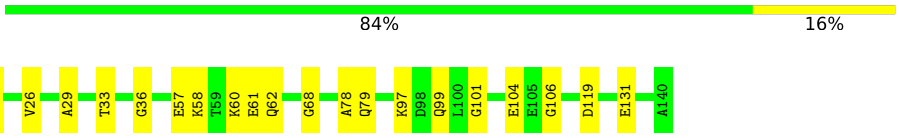
- Molecule 1: Alpha-synuclein

Chain D:



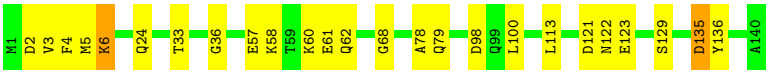
- Molecule 1: Alpha-synuclein

Chain E:



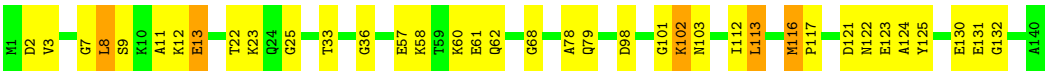
- Molecule 1: Alpha-synuclein

Chain F:



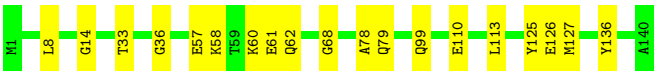
• Molecule 1: Alpha-synuclein

Chain G:



• Molecule 1: Alpha-synuclein

Chain H:

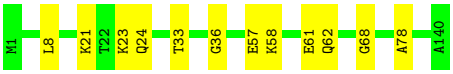


• Molecule 1: Alpha-synuclein

Chain I:

• Molecule 1: Alpha-synuclein

Chain J:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 256 calculated structures, 1 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
X-PLOR NIH	geometry optimization	2.33.4
X-PLOR NIH	refinement	2.33.4
X-PLOR NIH	structure solution	2.33.4

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	277
Number of shifts mapped to atoms	277
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	2%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1013	1003	1003	17
1	B	1013	1003	1003	11
1	C	1013	1003	1003	16
1	D	1013	1003	1003	19
1	E	1013	1003	1003	14
1	F	1013	1003	1003	15
1	G	1013	1003	1003	23
1	H	1013	1003	1003	12
1	I	1013	1003	1003	11
1	J	1013	1003	1003	7
All	All	10130	10030	10030	114

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:G:116:MET:N	1:G:117:PRO:CD	0.59	2.65
1:D:137:GLU:N	1:D:138:PRO:CD	0.59	2.66
1:D:100:LEU:HD23	1:D:100:LEU:N	0.57	2.15
1:C:5:MET:N	1:C:5:MET:SD	0.56	2.77
1:D:100:LEU:N	1:D:100:LEU:CD2	0.54	2.71
1:H:8:LEU:HD12	1:H:8:LEU:N	0.53	2.18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:C:23:LYS:O	1:C:25:GLY:N	0.53	2.41
1:F:2:ASP:O	1:F:4:PHE:N	0.53	2.42
1:A:116:MET:N	1:A:117:PRO:CD	0.52	2.72
1:I:28:GLU:N	1:I:28:GLU:OE1	0.52	2.42
1:F:121:ASP:O	1:F:123:GLU:N	0.52	2.43
1:G:2:ASP:OD1	1:G:3:VAL:N	0.52	2.43
1:H:125:TYR:O	1:H:125:TYR:CD2	0.52	2.63
1:D:102:LYS:NZ	1:E:101:GLY:O	0.51	2.42
1:E:119:ASP:N	1:E:119:ASP:OD1	0.51	2.42
1:J:24:GLN:N	1:J:24:GLN:OE1	0.51	2.44
1:A:116:MET:H	1:A:117:PRO:CD	0.50	2.19
1:D:113:LEU:HD12	1:D:113:LEU:N	0.50	2.22
1:E:97:LYS:NZ	1:E:99:GLN:CG	0.50	2.75
1:H:136:TYR:CD1	1:H:136:TYR:O	0.49	2.65
1:D:8:LEU:N	1:D:8:LEU:HD22	0.49	2.23
1:J:8:LEU:CD2	1:J:8:LEU:N	0.48	2.76
1:E:131:GLU:OE1	1:E:131:GLU:N	0.48	2.46
1:C:3:VAL:HG12	1:C:4:PHE:N	0.48	2.23
1:J:8:LEU:N	1:J:8:LEU:HD22	0.48	2.22
1:B:12:LYS:N	1:B:12:LYS:CD	0.48	2.76
1:C:100:LEU:N	1:D:98:ASP:CG	0.48	2.67
1:C:122:ASN:C	1:C:124:ALA:N	0.48	2.67
1:H:8:LEU:N	1:H:8:LEU:CD1	0.48	2.76
1:B:100:LEU:HD13	1:B:101:GLY:N	0.48	2.24
1:C:122:ASN:O	1:C:124:ALA:N	0.48	2.47
1:D:8:LEU:N	1:D:8:LEU:CD2	0.48	2.77
1:G:130:GLU:N	1:G:130:GLU:OE1	0.47	2.48
1:A:100:LEU:N	1:A:100:LEU:HD12	0.47	2.24
1:C:127:MET:N	1:C:128:PRO:CD	0.47	2.78
1:D:23:LYS:O	1:D:25:GLY:N	0.47	2.47
1:I:58:LYS:O	1:J:58:LYS:CB	0.47	2.63
1:F:6:LYS:NZ	1:F:6:LYS:CB	0.47	2.78
1:B:113:LEU:HD11	1:B:115:ASP:OD2	0.46	2.10
1:A:28:GLU:O	1:A:29:ALA:HB3	0.46	2.10
1:H:58:LYS:O	1:I:58:LYS:CB	0.46	2.64
1:A:60:LYS:O	1:B:61:GLU:O	0.46	2.34
1:G:58:LYS:O	1:H:58:LYS:CB	0.46	2.64
1:B:60:LYS:O	1:C:61:GLU:O	0.46	2.34
1:F:58:LYS:O	1:G:58:LYS:CB	0.46	2.64
1:H:60:LYS:O	1:I:61:GLU:O	0.46	2.34
1:E:58:LYS:O	1:F:58:LYS:CB	0.46	2.64
1:G:11:ALA:O	1:G:13:GLU:N	0.46	2.49

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:I:60:LYS:O	1:J:61:GLU:O	0.46	2.34
1:G:8:LEU:N	1:G:8:LEU:HD12	0.46	2.26
1:C:60:LYS:O	1:D:61:GLU:O	0.46	2.33
1:G:60:LYS:O	1:H:61:GLU:O	0.46	2.34
1:I:18:ALA:O	1:I:19:ALA:HB3	0.45	2.11
1:G:131:GLU:CD	1:G:132:GLY:N	0.45	2.70
1:D:58:LYS:O	1:E:58:LYS:CB	0.45	2.64
1:F:60:LYS:O	1:G:61:GLU:O	0.45	2.35
1:G:7:GLY:C	1:G:9:SER:N	0.45	2.70
1:A:8:LEU:HD12	1:A:8:LEU:N	0.45	2.26
1:A:79:GLN:O	1:B:78:ALA:O	0.45	2.34
1:A:8:LEU:C	1:A:10:LYS:H	0.45	2.15
1:B:1:MET:SD	1:B:1:MET:N	0.45	2.90
1:D:60:LYS:O	1:E:61:GLU:O	0.45	2.34
1:E:60:LYS:O	1:F:61:GLU:O	0.45	2.34
1:B:110:GLU:OE1	1:B:110:GLU:N	0.45	2.45
1:A:8:LEU:N	1:A:8:LEU:CD1	0.45	2.80
1:A:58:LYS:O	1:B:58:LYS:CB	0.45	2.65
1:D:100:LEU:HD23	1:D:100:LEU:H	0.45	1.69
1:I:79:GLN:O	1:J:78:ALA:O	0.45	2.35
1:J:21:LYS:CB	1:J:21:LYS:NZ	0.45	2.80
1:B:58:LYS:O	1:C:58:LYS:CB	0.44	2.65
1:C:58:LYS:O	1:D:58:LYS:CB	0.44	2.65
1:F:24:GLN:N	1:F:24:GLN:CD	0.44	2.71
1:H:79:GLN:O	1:I:78:ALA:O	0.44	2.35
1:F:79:GLN:O	1:G:78:ALA:O	0.44	2.35
1:B:79:GLN:O	1:C:78:ALA:O	0.44	2.35
1:G:79:GLN:O	1:H:78:ALA:O	0.44	2.35
1:E:79:GLN:O	1:F:78:ALA:O	0.44	2.35
1:A:131:GLU:OE1	1:A:132:GLY:O	0.44	2.35
1:C:79:GLN:O	1:D:78:ALA:O	0.44	2.35
1:D:79:GLN:O	1:E:78:ALA:O	0.44	2.35
1:G:7:GLY:O	1:G:9:SER:N	0.43	2.51
1:A:24:GLN:CD	1:A:25:GLY:N	0.43	2.71
1:G:103:ASN:O	1:G:103:ASN:OD1	0.43	2.37
1:C:100:LEU:N	1:D:98:ASP:OD2	0.43	2.49
1:I:123:GLU:O	1:I:126:GLU:O	0.43	2.36
1:C:2:ASP:O	1:C:3:VAL:O	0.43	2.37
1:D:14:GLY:O	1:D:15:VAL:O	0.42	2.37
1:G:101:GLY:O	1:G:102:LYS:O	0.42	2.36
1:I:24:GLN:N	1:I:24:GLN:CD	0.42	2.72
1:G:122:ASN:O	1:G:124:ALA:N	0.42	2.52

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:98:ASP:OD1	1:A:98:ASP:O	0.42	2.38
1:C:122:ASN:C	1:C:124:ALA:H	0.42	2.17
1:G:23:LYS:C	1:G:25:GLY:N	0.42	2.73
1:G:23:LYS:C	1:G:25:GLY:H	0.42	2.18
1:G:112:ILE:O	1:G:113:LEU:O	0.42	2.38
1:F:98:ASP:OD2	1:G:98:ASP:O	0.42	2.37
1:F:100:LEU:C	1:F:100:LEU:HD23	0.42	2.36
1:F:135:ASP:OD1	1:F:136:TYR:N	0.41	2.52
1:A:125:TYR:CG	1:A:126:GLU:N	0.41	2.88
1:E:131:GLU:H	1:E:131:GLU:CD	0.41	2.18
1:G:2:ASP:OD1	1:G:2:ASP:N	0.41	2.54
1:E:21:LYS:C	1:E:23:LYS:N	0.41	2.74
1:H:125:TYR:O	1:H:127:MET:N	0.41	2.53
1:F:135:ASP:CG	1:F:136:TYR:N	0.41	2.73
1:H:125:TYR:O	1:H:125:TYR:CG	0.41	2.73
1:A:100:LEU:N	1:A:100:LEU:CD1	0.40	2.85
1:A:121:ASP:OD1	1:A:121:ASP:O	0.40	2.38
1:D:113:LEU:N	1:D:113:LEU:CD1	0.40	2.84
1:G:121:ASP:O	1:G:125:TYR:CB	0.40	2.70
1:A:8:LEU:C	1:A:10:LYS:N	0.40	2.75
1:E:21:LYS:O	1:E:23:LYS:N	0.40	2.55
1:E:104:GLU:C	1:E:106:GLY:N	0.40	2.74
1:F:4:PHE:CE2	1:F:5:MET:O	0.40	2.74
1:I:2:ASP:O	1:I:4:PHE:CE2	0.40	2.75

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	138/140 (99%)	112 (81%)	21 (15%)	5 (4%)	6 34
1	B	138/140 (99%)	118 (86%)	17 (12%)	3 (2%)	10 49
1	C	138/140 (99%)	110 (80%)	19 (14%)	9 (7%)	2 18
1	D	138/140 (99%)	104 (75%)	23 (17%)	11 (8%)	2 14
1	E	138/140 (99%)	113 (82%)	18 (13%)	7 (5%)	4 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	138/140 (99%)	110 (80%)	18 (13%)	10 (7%)	2	16
1	G	138/140 (99%)	113 (82%)	15 (11%)	10 (7%)	2	16
1	H	138/140 (99%)	118 (86%)	12 (9%)	8 (6%)	3	21
1	I	138/140 (99%)	114 (83%)	18 (13%)	6 (4%)	5	29
1	J	138/140 (99%)	118 (86%)	15 (11%)	5 (4%)	6	34
All	All	1380/1400 (99%)	1130 (82%)	176 (13%)	74 (5%)	3	23

All 74 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	36	GLY
1	A	57	GLU
1	A	68	GLY
1	A	104	GLU
1	A	116	MET
1	B	36	GLY
1	B	57	GLU
1	B	68	GLY
1	C	3	VAL
1	C	11	ALA
1	C	24	GLN
1	C	36	GLY
1	C	57	GLU
1	C	68	GLY
1	C	98	ASP
1	C	102	LYS
1	C	123	GLU
1	D	15	VAL
1	D	18	ALA
1	D	24	GLN
1	D	25	GLY
1	D	36	GLY
1	D	57	GLU
1	D	68	GLY
1	D	112	ILE
1	D	132	GLY
1	D	135	ASP
1	D	138	PRO
1	E	18	ALA

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Mol	Chain	Res	Type
1	E	26	VAL
1	E	29	ALA
1	E	36	GLY
1	E	57	GLU
1	E	62	GLN
1	E	68	GLY
1	F	3	VAL
1	F	6	LYS
1	F	36	GLY
1	F	57	GLU
1	F	62	GLN
1	F	68	GLY
1	F	113	LEU
1	F	122	ASN
1	F	129	SER
1	F	135	ASP
1	G	8	LEU
1	G	12	LYS
1	G	13	GLU
1	G	36	GLY
1	G	57	GLU
1	G	62	GLN
1	G	68	GLY
1	G	102	LYS
1	G	113	LEU
1	G	123	GLU
1	H	14	GLY
1	H	36	GLY
1	H	57	GLU
1	H	62	GLN
1	H	68	GLY
1	H	99	GLN
1	H	110	GLU
1	H	126	GLU
1	I	21	LYS
1	I	36	GLY
1	I	57	GLU
1	I	62	GLN
1	I	68	GLY
1	I	111	GLY
1	J	23	LYS
1	J	36	GLY

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Mol	Chain	Res	Type
1	J	57	GLU
1	J	62	GLN
1	J	68	GLY

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	99 (96%)	4 (4%)	36	84
1	B	103/103 (100%)	99 (96%)	4 (4%)	36	84
1	C	103/103 (100%)	102 (99%)	1 (1%)	77	96
1	D	103/103 (100%)	101 (98%)	2 (2%)	59	93
1	E	103/103 (100%)	102 (99%)	1 (1%)	77	96
1	F	103/103 (100%)	102 (99%)	1 (1%)	77	96
1	G	103/103 (100%)	100 (97%)	3 (3%)	45	89
1	H	103/103 (100%)	101 (98%)	2 (2%)	59	93
1	I	103/103 (100%)	102 (99%)	1 (1%)	77	96
1	J	103/103 (100%)	102 (99%)	1 (1%)	77	96
All	All	1030/1030 (100%)	1010 (98%)	20 (2%)	59	93

All 20 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	24	GLN
1	A	33	THR
1	A	113	LEU
1	A	116	MET
1	B	1	MET
1	B	22	THR
1	B	33	THR
1	B	100	LEU
1	C	33	THR
1	D	33	THR

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Mol	Chain	Res	Type
1	D	100	LEU
1	E	33	THR
1	F	33	THR
1	G	22	THR
1	G	33	THR
1	G	116	MET
1	H	33	THR
1	H	113	LEU
1	I	33	THR
1	J	33	THR

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 2% for the well-defined parts and 2% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	277
Number of shifts mapped to atoms	277
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	66	0.04 ± 0.25	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	47	-0.72 ± 0.22	Should be checked
$^{13}C'$	55	0.57 ± 0.22	Should be applied
^{15}N	63	-2.62 ± 0.46	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 277 atoms were assigned a chemical shift out of a possible 17190. 0 out of 230 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	230/7080 (3%)	46/2930 (2%)	121/2800 (4%)	63/1350 (5%)
Sidechain	47/9480 (0%)	0/6160 (0%)	47/3080 (2%)	0/240 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/630 (0%)	0/300 (0%)	0/320 (0%)	0/10 (0%)
Overall	277/17190 (2%)	46/9390 (0%)	168/6200 (3%)	63/1600 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 2%, i.e. 277 atoms were assigned a chemical shift out of a possible 17190. 0 out of 230 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	230/7080 (3%)	46/2930 (2%)	121/2800 (4%)	63/1350 (5%)
Sidechain	47/9480 (0%)	0/6160 (0%)	47/3080 (2%)	0/240 (0%)
Aromatic	0/630 (0%)	0/300 (0%)	0/320 (0%)	0/10 (0%)
Overall	277/17190 (2%)	46/9390 (0%)	168/6200 (3%)	63/1600 (4%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

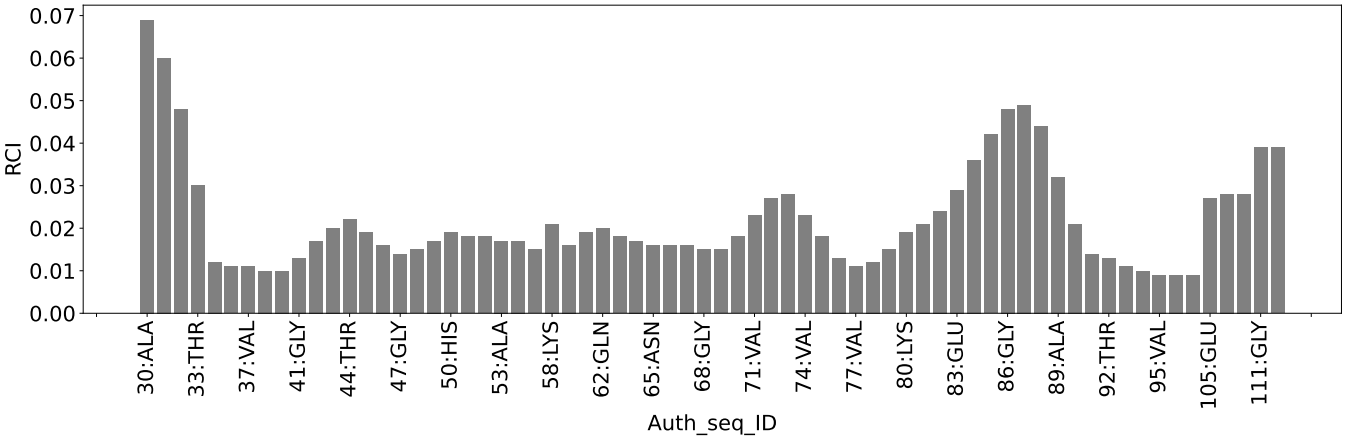
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
30:ALA
33:THR
37:VAL
41:GLY
44:THR
47:GLY
50:HIS
53:ALA
58:LYS
62:GLN
65:ASN
68:GLY
71:VAL
74:VAL
77:VAL
80:LYS
83:GLU
86:GLY
89:ALA
92:THR
95:VAL
105:GLU
111:GLY
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	375
Intra-residue (|i-j|=0)	24
Sequential (|i-j|=1)	14
Medium range (|i-j|>1 and |i-j|<5)	67
Long range (|i-j|≥5)	270
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	90
Number of unmapped restraints	0
Number of restraints per residue	0.3
Number of long range restraints per residue[1]	0.2

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

8.2 Residual restraint violations (i)

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 (i)

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)	None	None
0.2-0.5 (Medium)	2.0	0.31
>0.5 (Large)	45.0	2.34

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

Dihedral-angle violations less than 1° are not included in the calculation.

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	2.0	4.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

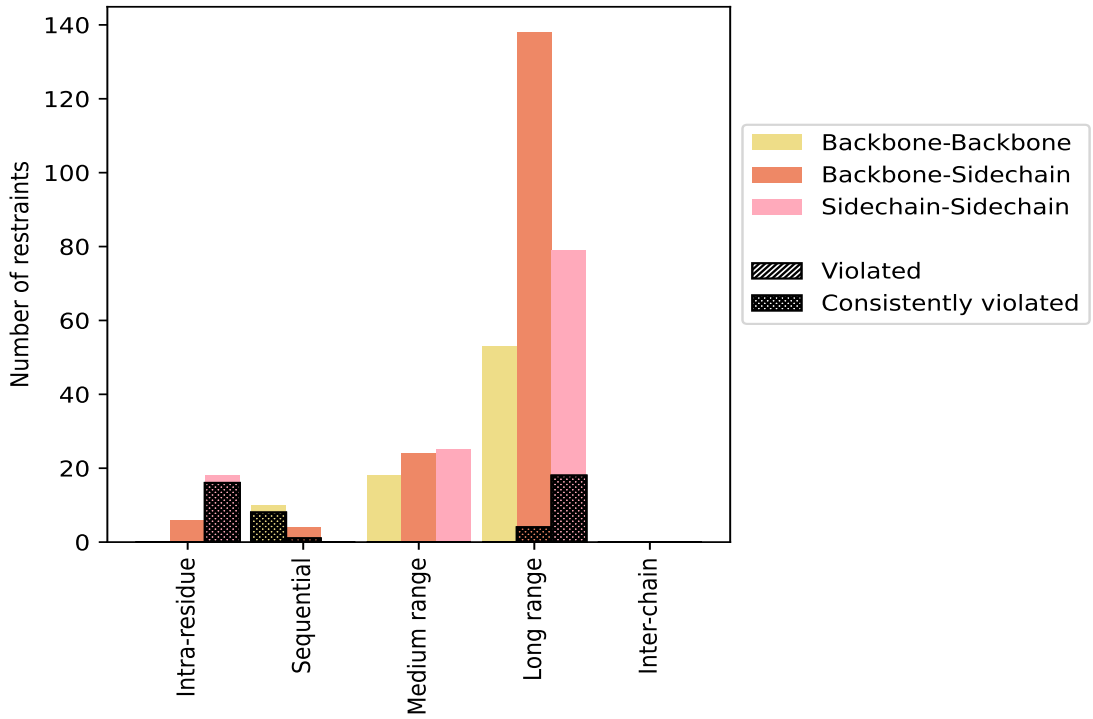
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	24	6.4	16	66.7	4.3	16	66.7	4.3
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	6	1.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	18	4.8	16	88.9	4.3	16	88.9	4.3
Sequential (|i-j|=1)	14	3.7	9	64.3	2.4	9	64.3	2.4
Backbone-Backbone	10	2.7	8	80.0	2.1	8	80.0	2.1
Backbone-Sidechain	4	1.1	1	25.0	0.3	1	25.0	0.3
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	67	17.9	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	18	4.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	24	6.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	25	6.7	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	270	72.0	22	8.1	5.9	22	8.1	5.9
Backbone-Backbone	53	14.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	138	36.8	4	2.9	1.1	4	2.9	1.1
Sidechain-Sidechain	79	21.1	18	22.8	4.8	18	22.8	4.8
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	375	100.0	47	12.5	12.5	47	12.5	12.5
Backbone-Backbone	81	21.6	8	9.9	2.1	8	9.9	2.1
Backbone-Sidechain	172	45.9	5	2.9	1.3	5	2.9	1.3
Sidechain-Sidechain	122	32.5	34	27.9	9.1	34	27.9	9.1

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

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



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

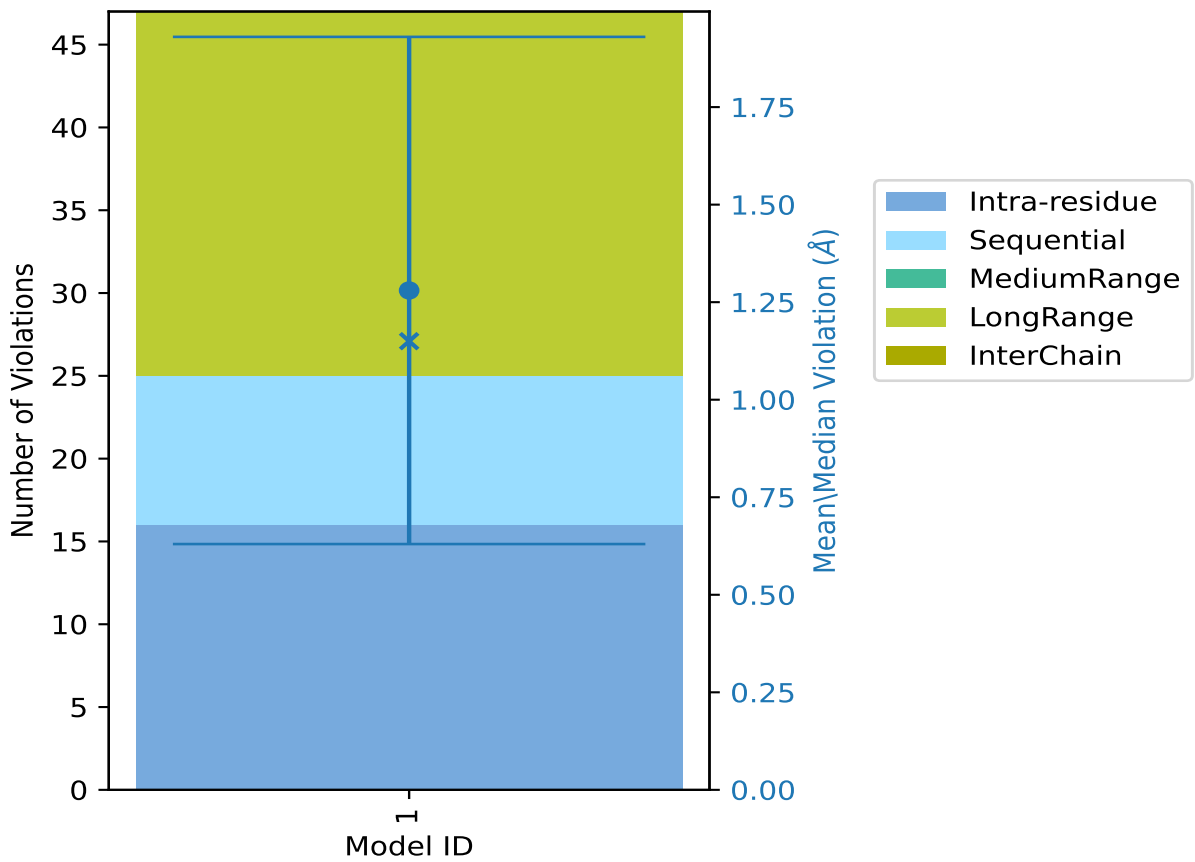
9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	16	9	0	22	0	47	1.28	2.34	0.65	1.15

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

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



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

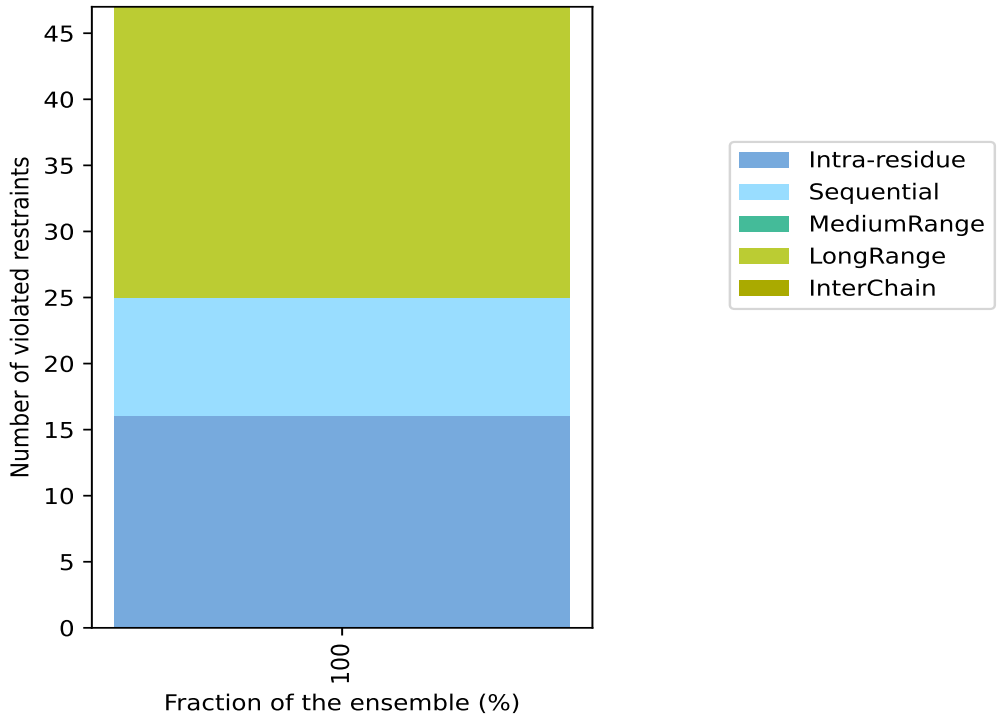
9.3 Distance violation statistics for the ensemble (i)

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, 328(IR:8, SQ:5, MR:67, LR:248, 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]	%
16	9	0	22	0	47	1	100.0

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

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



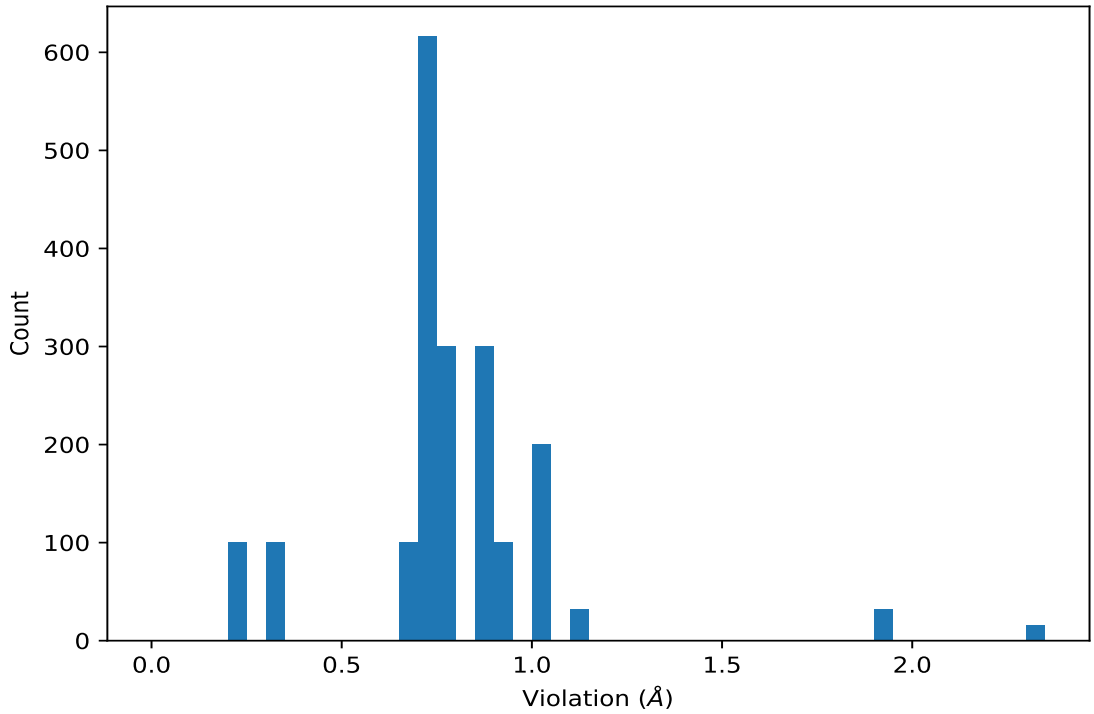
9.4 Most violated distance restraints in the ensemble (i)

No violations found

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)
(1,375)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,375)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,374)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,374)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,373)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,373)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,372)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,372)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,371)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,371)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,370)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,370)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,369)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,369)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,368)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34
(1,368)	1:J:79:GLN:NE2	1:J:79:GLN:CD	1	2.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,359)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,359)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,359)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,357)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,357)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,357)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,357)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,355)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,355)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,355)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,355)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,353)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,353)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,353)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,353)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,351)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,351)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,351)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,351)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,349)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,349)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,349)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,349)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,347)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,347)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,347)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,347)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,345)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,345)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,345)	1:J:46:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,345)	1:J:83:GLU:OE2	1:J:80:LYS:NZ	1	1.92
(1,358)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,358)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,358)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,358)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,356)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,356)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,356)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,356)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,354)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,354)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,354)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,354)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,352)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,352)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,352)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,352)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,350)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,350)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,350)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,350)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,348)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,348)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,348)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,348)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,346)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,346)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,346)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,346)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,344)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,344)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,344)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,344)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	1.15
(1,280)	1:A:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:A:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:A:76:ALA:N	1:J:77:VAL:CG2	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:B:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:B:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:B:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:C:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:C:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:A:77:VAL:CG2	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:D:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:D:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:D:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:E:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:E:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:B:77:VAL:CG2	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:F:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:F:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:F:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:G:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:G:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:C:77:VAL:CG2	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:H:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:H:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:H:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:D:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:I:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:I:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:A:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:A:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:B:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:B:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:C:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:C:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:D:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:D:77:VAL:CG2	1	1.03

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,280)	1:J:76:ALA:N	1:E:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:E:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:F:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:F:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:G:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:G:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:H:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:H:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:I:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:I:77:VAL:CG2	1	1.03
(1,280)	1:J:76:ALA:N	1:J:77:VAL:CG1	1	1.03
(1,280)	1:J:76:ALA:N	1:J:77:VAL:CG2	1	1.03
(1,265)	1:A:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:A:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:B:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:C:79:GLN:NE2	1:J:89:ALA:CB	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:D:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:D:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:E:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:F:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:G:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:B:89:ALA:CB	1	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,265)	1:H:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:H:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:I:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:A:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:B:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:C:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:D:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:E:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:F:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:G:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:H:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:I:89:ALA:CB	1	0.9
(1,265)	1:J:79:GLN:NE2	1:J:89:ALA:CB	1	0.9
(1,55)	1:A:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:A:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:D:86:GLY:CA	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:B:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:B:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:C:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:D:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:E:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:F:86:GLY:CA	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:F:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:F:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:G:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:H:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:H:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:I:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:A:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:B:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:C:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:D:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:E:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:F:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:G:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:H:86:GLY:CA	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,55)	1:J:87:SER:CA	1:I:86:GLY:CA	1	0.86
(1,55)	1:J:87:SER:CA	1:J:86:GLY:CA	1	0.86
(1,181)	1:A:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:A:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:B:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:C:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:D:46:GLU:CD	1:J:80:LYS:NZ	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:E:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:E:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:F:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:G:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:H:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:B:80:LYS:NZ	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:I:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:I:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:J:46:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:A:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:B:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:D:80:LYS:NZ	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:C:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:C:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:D:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:E:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:F:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:F:80:LYS:NZ	1	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,181)	1:G:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:G:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:H:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:I:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:A:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:B:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:C:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:D:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:E:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:F:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:G:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:H:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:I:80:LYS:NZ	1	0.86
(1,181)	1:J:83:GLU:CD	1:J:80:LYS:NZ	1	0.86
(1,48)	1:A:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:H:92:THR:CA	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:A:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:A:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:B:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:C:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:D:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:E:93:GLY:CA	1:J:92:THR:CA	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:F:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:F:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:G:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:H:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:B:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:I:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:A:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:B:92:THR:CA	1	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,48)	1:J:93:GLY:CA	1:C:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:D:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:E:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:F:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:G:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:H:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:I:92:THR:CA	1	0.78
(1,48)	1:J:93:GLY:CA	1:J:92:THR:CA	1	0.78
(1,54)	1:A:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:A:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:B:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:C:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:D:68:GLY:CA	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:D:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:D:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:E:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:F:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:G:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:F:68:GLY:CA	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,54)	1:H:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:H:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:I:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:A:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:B:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:C:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:D:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:E:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:F:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:G:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:H:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:I:68:GLY:CA	1	0.76
(1,54)	1:J:69:ALA:CA	1:J:68:GLY:CA	1	0.76
(1,50)	1:A:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:A:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:H:47:GLY:CA	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:B:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:B:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:C:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:D:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:E:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:F:48:VAL:CA	1:J:47:GLY:CA	1	0.75

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,50)	1:G:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:G:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:H:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:I:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:A:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:B:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:C:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:D:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:E:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:F:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:G:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:H:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:I:47:GLY:CA	1	0.75
(1,50)	1:J:48:VAL:CA	1:J:47:GLY:CA	1	0.75
(1,53)	1:A:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:B:71:VAL:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:A:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:A:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:B:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:C:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:D:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:D:71:VAL:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:E:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:E:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:F:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:G:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:H:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:F:71:VAL:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,53)	1:I:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:I:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:A:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:B:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:C:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:D:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:E:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:F:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:G:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:H:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:I:71:VAL:CA	1	0.74
(1,53)	1:J:72:THR:CA	1:J:71:VAL:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:A:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:B:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:H:72:THR:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:C:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:C:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:D:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:E:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:F:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:G:73:GLY:CA	1:J:72:THR:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,52)	1:H:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:H:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:I:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:A:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:B:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:C:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:D:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:E:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:F:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:G:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:H:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:I:72:THR:CA	1	0.74
(1,52)	1:J:73:GLY:CA	1:J:72:THR:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:A:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:B:93:GLY:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:B:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:B:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:C:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:D:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:E:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:D:93:GLY:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:F:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:F:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:G:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:H:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:F:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:I:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:A:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:B:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:C:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:D:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:E:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:F:93:GLY:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,51)	1:J:94:PHE:CA	1:G:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:H:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:I:93:GLY:CA	1	0.74
(1,51)	1:J:94:PHE:CA	1:J:93:GLY:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:A:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:B:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:C:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:H:94:PHE:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:D:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:D:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:E:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:F:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:G:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:H:93:GLY:CA	1:J:94:PHE:CA	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,49)	1:I:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:I:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:A:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:B:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:C:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:D:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:E:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:F:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:G:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:H:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:I:94:PHE:CA	1	0.74
(1,49)	1:J:93:GLY:CA	1:J:94:PHE:CA	1	0.74
(1,367)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,367)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,366)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,366)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,365)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,365)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,364)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,364)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,363)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,363)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,362)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,362)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,361)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,361)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,360)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,360)	1:J:79:GLN:NE2	1:J:79:GLN:OE1	1	0.74
(1,270)	1:A:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:C:71:VAL:CG2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:A:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:A:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:A:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:B:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:B:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:D:71:VAL:CG2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:C:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:C:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:C:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:D:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:D:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:E:71:VAL:CG2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:E:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:E:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:E:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:F:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:F:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:F:71:VAL:CG2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:G:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:G:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:G:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:H:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:H:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:G:71:VAL:CG2	1	0.74

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,270)	1:I:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:I:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:I:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:A:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:A:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:B:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:B:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:C:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:C:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:D:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:D:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:E:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:E:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:F:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:F:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:G:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:G:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:H:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:H:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:I:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:I:71:VAL:CG2	1	0.74
(1,270)	1:J:93:GLY:N	1:J:71:VAL:CG1	1	0.74
(1,270)	1:J:93:GLY:N	1:J:71:VAL:CG2	1	0.74
(1,262)	1:A:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:A:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:F:78:ALA:CB	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:B:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:B:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:C:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:D:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:E:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:H:78:ALA:CB	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,262)	1:F:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:F:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:G:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:H:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:I:48:VAL:N	1:J:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:A:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:B:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:C:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:D:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:E:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:F:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:G:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:H:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:I:78:ALA:CB	1	0.68
(1,262)	1:J:48:VAL:N	1:J:78:ALA:CB	1	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:A:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:A:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:B:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:C:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:D:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:B:89:ALA:C	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:E:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:E:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:F:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:G:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:H:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:D:89:ALA:C	1	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,264)	1:I:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:I:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:A:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:B:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:C:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:D:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:E:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:F:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:G:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:H:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:I:89:ALA:C	1	0.31
(1,264)	1:J:79:GLN:NE2	1:J:89:ALA:C	1	0.31
(1,261)	1:A:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:A:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:B:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:F:78:ALA:CB	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:C:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:C:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:D:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:E:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:F:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:H:78:ALA:CB	1	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,261)	1:G:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:G:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:H:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:I:49:VAL:N	1:J:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:A:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:B:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:C:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:D:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:E:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:F:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:G:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:H:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:I:78:ALA:CB	1	0.24
(1,261)	1:J:49:VAL:N	1:J:78:ALA:CB	1	0.24

10 Dihedral-angle violation analysis (i)

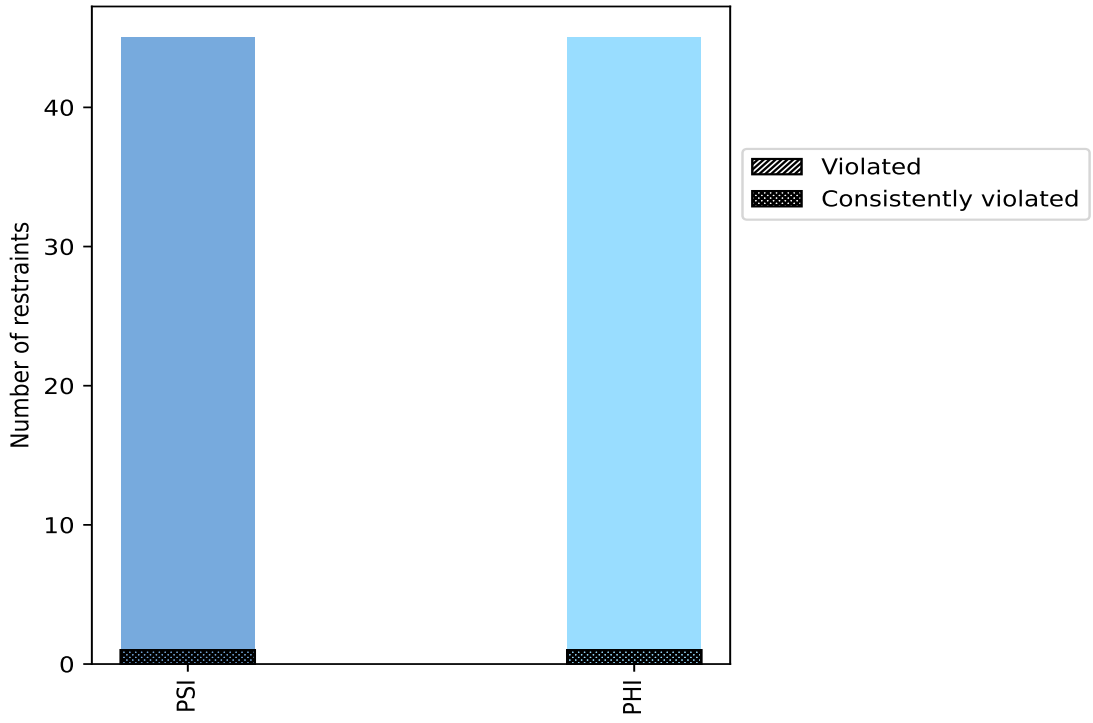
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	45	50.0	1	2.2	1.1	1	2.2	1.1
PHI	45	50.0	1	2.2	1.1	1	2.2	1.1
Total	90	100.0	2	2.2	2.2	2	2.2	2.2

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

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



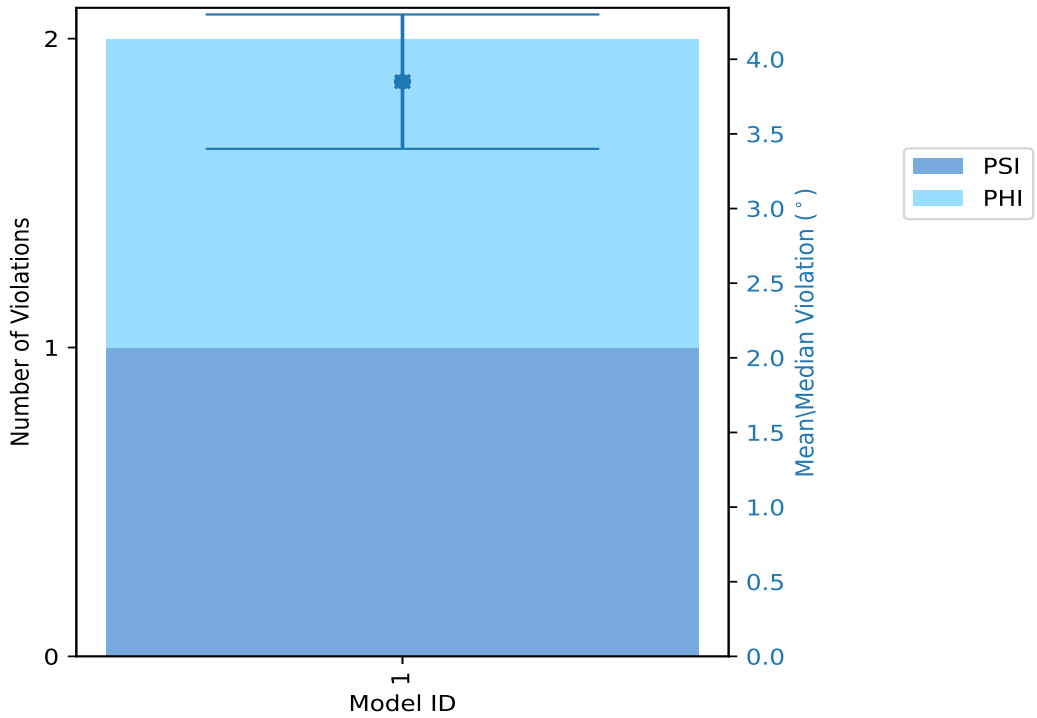
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	1	1	2	3.85	4.3	0.45	3.85

10.2.1 Bar graph : Dihedral violation statistics for each model (i)



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

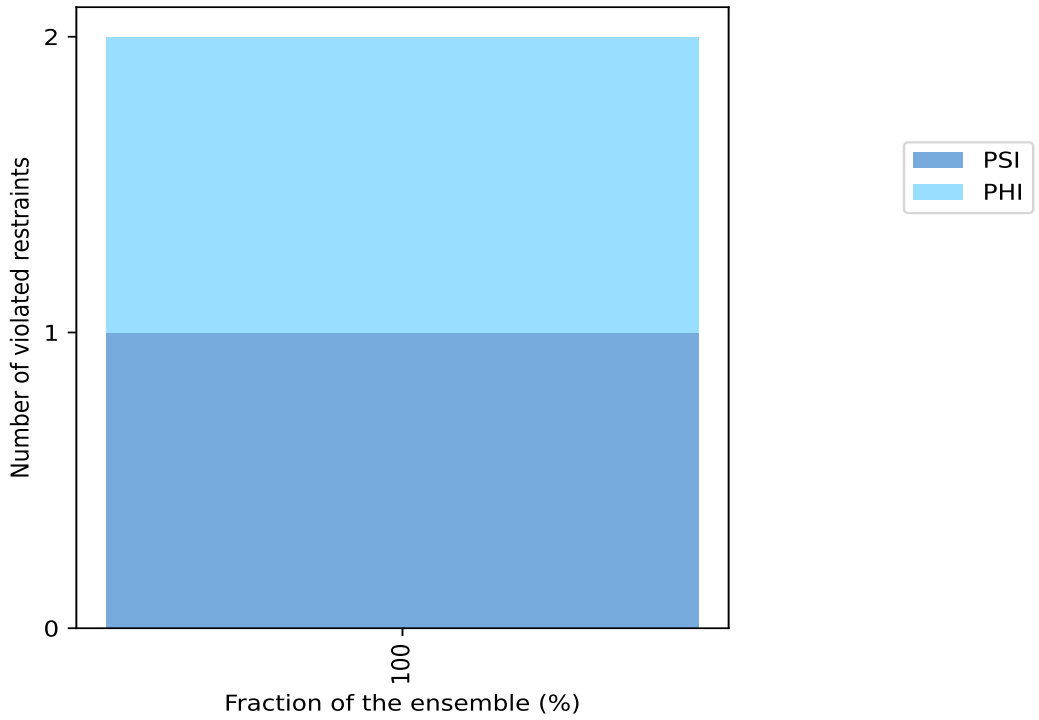
10.3 Dihedral-angle violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in very few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of ensemble.

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	1	2	1	100.0

[1] Number of models with violations

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



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

No violations found

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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

10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,3)	1:J:32:LYS:C	1:J:33:THR:N	1:J:33:THR:CA	1:J:33:THR:C	1	4.3
(1,2)	1:J:32:LYS:N	1:J:32:LYS:CA	1:J:32:LYS:C	1:J:33:THR:N	1	3.4