Full wwPDB NMR Structure Validation Report (i)

Jun 4, 2023 – 09:32 AM EDT

PDB ID	:	2NBU
BMRB ID	:	25825
Title	:	Solution structure of the Rad23 ubiquitin-like (UBL) domain
Authors	:	Chen, X.; Walters, K.J.
Deposited on	:	2016-03-12

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:

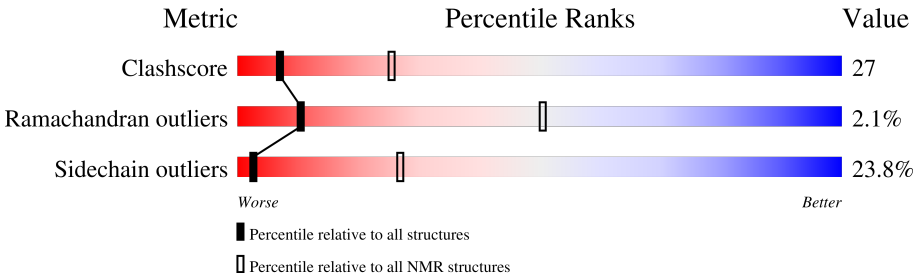
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

The overall completeness of chemical shifts assignment is 95%.

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	99	36% 31% 5% 6% 21%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:73 (72)	0.25	2

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1247 atoms, of which 641 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called UV excision repair protein RAD23.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	78	1247	383	641	97	122	4	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	ASP	-	expression tag	UNP P32628
A	80	PRO	-	expression tag	UNP P32628
A	81	ASN	-	expression tag	UNP P32628
A	82	SER	-	expression tag	UNP P32628
A	83	SER	-	expression tag	UNP P32628
A	84	SER	-	expression tag	UNP P32628
A	85	VAL	-	expression tag	UNP P32628
A	86	ASP	-	expression tag	UNP P32628
A	87	LYS	-	expression tag	UNP P32628
A	88	LEU	-	expression tag	UNP P32628
A	89	ALA	-	expression tag	UNP P32628
A	90	ALA	-	expression tag	UNP P32628
A	91	ALA	-	expression tag	UNP P32628
A	92	LEU	-	expression tag	UNP P32628
A	93	GLU	-	expression tag	UNP P32628
A	94	HIS	-	expression tag	UNP P32628
A	95	HIS	-	expression tag	UNP P32628
A	96	HIS	-	expression tag	UNP P32628
A	97	HIS	-	expression tag	UNP P32628
A	98	HIS	-	expression tag	UNP P32628
A	99	HIS	-	expression tag	UNP P32628

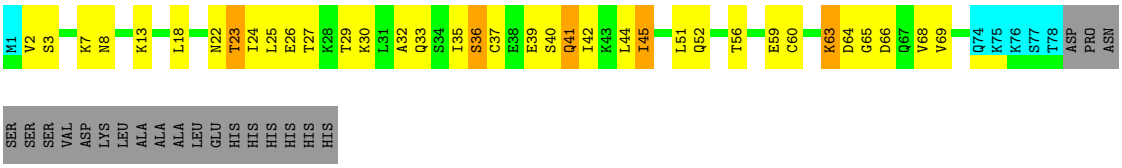
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: UV excision repair protein RAD23

Chain A: 36% 31% 5% 6% 21%



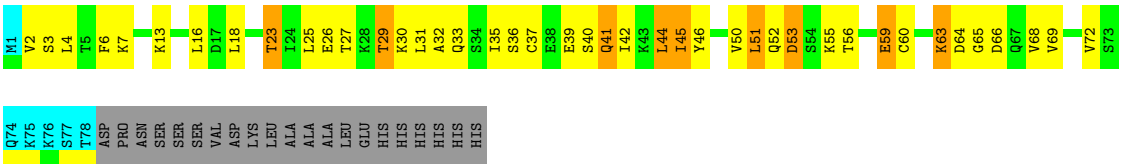
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: UV excision repair protein RAD23

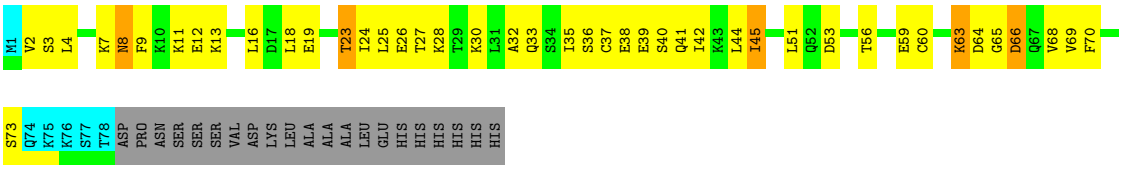
Chain A: 30% 33% 9% 6% 21%



4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: UV excision repair protein RAD23

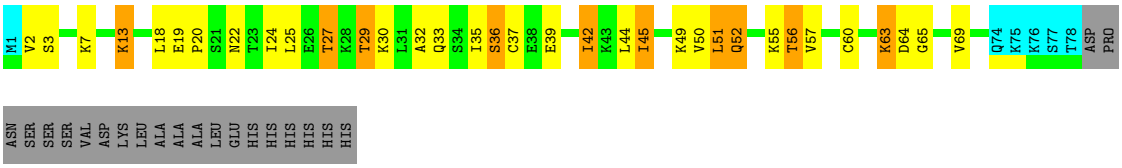
Chain A: 28% 39% 5% 6% 21%



4.2.3 Score per residue for model 3

- Molecule 1: UV excision repair protein RAD23

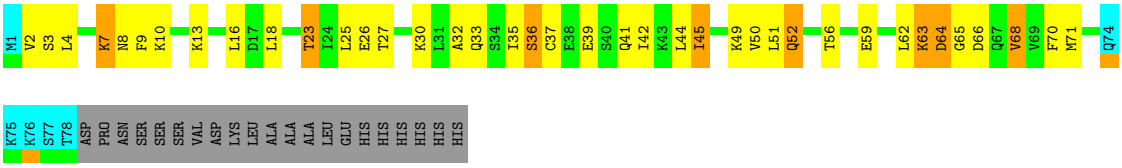
Chain A: 38% 24% 10% 6% 21%



4.2.4 Score per residue for model 4

- Molecule 1: UV excision repair protein RAD23

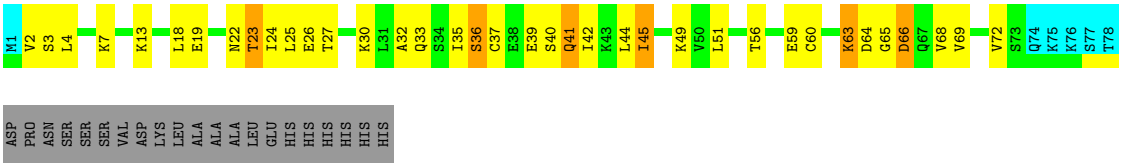
Chain A: 33% 31% 8% 6% 21%



4.2.5 Score per residue for model 5

- Molecule 1: UV excision repair protein RAD23

Chain A: 35% 31% 6% 6% 21%



4.2.6 Score per residue for model 6

- Molecule 1: UV excision repair protein RAD23

Chain A: 39% 25% 8% 6% 21%

M1 V2 S3 L4 T5 F6 K7 L18 T23 T24 L25 E26 T27 K30 L31 A32 Q33 S34 I35 S36 C37 E38 E39 S40 Q41 I42 K43 L44 I45 Y46 L51 Q52 V57 C60 K63 D64 G65 D66 Q67 V68 V69 V72 S73 Q74 K75 K76 S77 T78 ASP PRO ASN SER

SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4.2.7 Score per residue for model 7

- Molecule 1: UV excision repair protein RAD23

Chain A: 37% 29% 6% 6% 21%

M1 V2 S3 K7 N8 K11 E12 K13 L18 T23 T24 L25 E26 T27 K30 L31 A32 Q33 S34 I35 S36 C37 E38 E39 I42 I45 Y46 V50 L51 K55 T56 V57 S58 E59 C60 K63 D64 G65 D66 Q67 V68 V69 S73 Q74 K75 K76 S77 T78 ASP

PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4.2.8 Score per residue for model 8

- Molecule 1: UV excision repair protein RAD23

Chain A: 31% 30% 11% 6% 21%

M1 V2 S3 F6 K7 K13 L18 T23 T24 L25 E26 T27 K28 T29 K30 L31 A32 Q33 S34 I35 S36 C37 E38 E39 S40 Q41 I42 K43 L44 I45 Y46 V50 L51 Q52 T56 E59 C60 K63 D64 G65 V68 V69 F70 M71 V72 S73 Q74 K75 K76 S77 T78

ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4.2.9 Score per residue for model 9

- Molecule 1: UV excision repair protein RAD23

Chain A: 27% 36% 9% 6% 21%

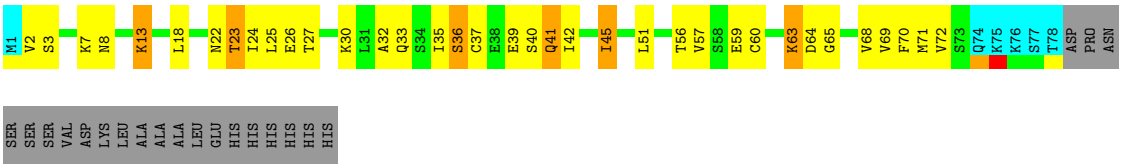
M1 V2 S3 L4 T5 F6 K7 N8 F9 K10 K11 E12 K13 L18 E19 N22 T23 I24 L25 E26 T27 K28 T29 K30 L31 A32 Q33 S34 I35 S36 C37 E38 E39 S40 Q41 I42 K43 L44 I45 L51 Q52 T56 V57 S58 E59 C60 K63 D64 G65 D66 Q67 V68 V69 F70 M71

V72 S73 Q74 K75 K76 S77 T78 ASP PRO ASN SER SER SER VAL ASP LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4.2.10 Score per residue for model 10

- Molecule 1: UV excision repair protein RAD23

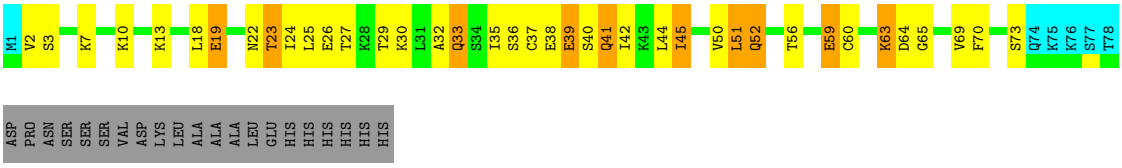
Chain A: 36% 30% 6% 6% 21%



4.2.11 Score per residue for model 11

- Molecule 1: UV excision repair protein RAD23

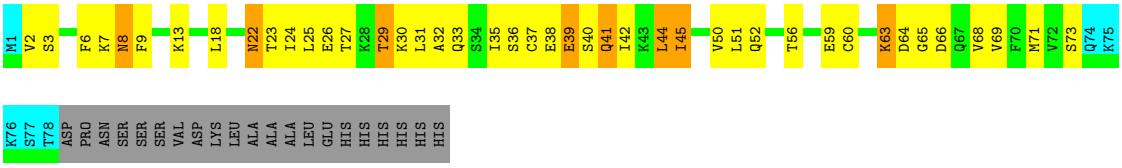
Chain A: 33% 29% 10% 6% 21%



4.2.12 Score per residue for model 12

- Molecule 1: UV excision repair protein RAD23

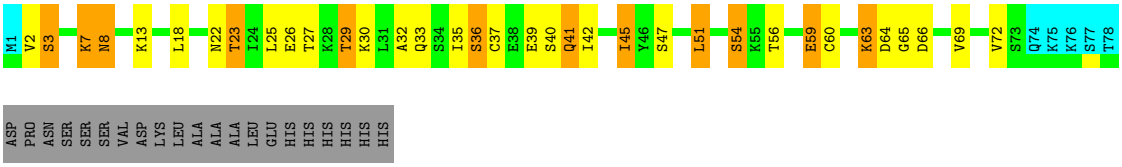
Chain A: 29% 35% 8% 6% 21%



4.2.13 Score per residue for model 13

- Molecule 1: UV excision repair protein RAD23

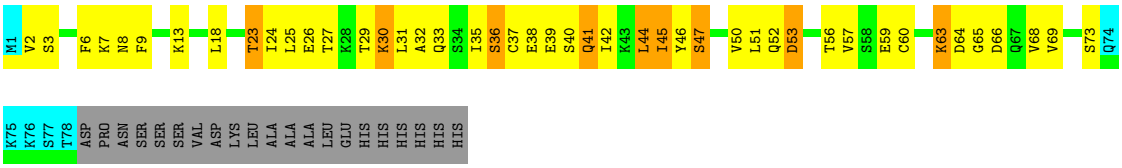
Chain A: 37% 23% 12% 6% 21%



4.2.14 Score per residue for model 14

- Molecule 1: UV excision repair protein RAD23

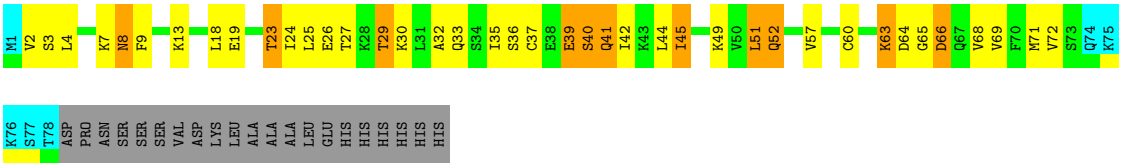
Chain A: 27% 36% 9% 6% 21%



4.2.15 Score per residue for model 15

- Molecule 1: UV excision repair protein RAD23

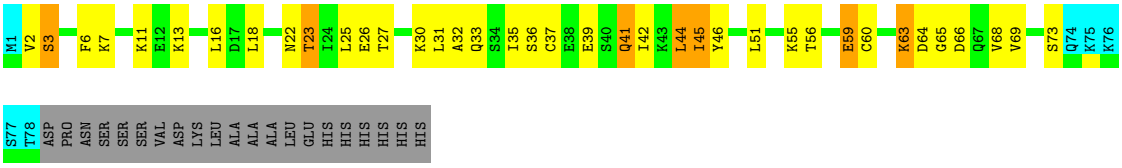
Chain A: 32% 29% 11% 6% 21%



4.2.16 Score per residue for model 16

- Molecule 1: UV excision repair protein RAD23

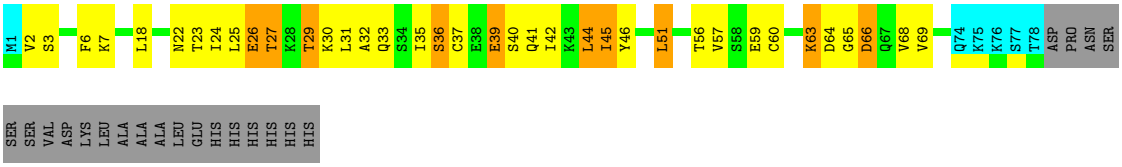
Chain A: 34% 31% 7% 6% 21%



4.2.17 Score per residue for model 17

- Molecule 1: UV excision repair protein RAD23

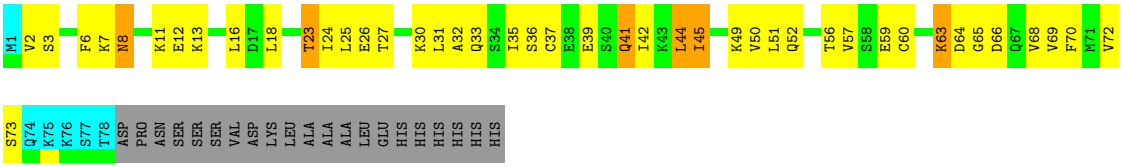
Chain A: 35% 27% 10% 6% 21%



4.2.18 Score per residue for model 18

- Molecule 1: UV excision repair protein RAD23

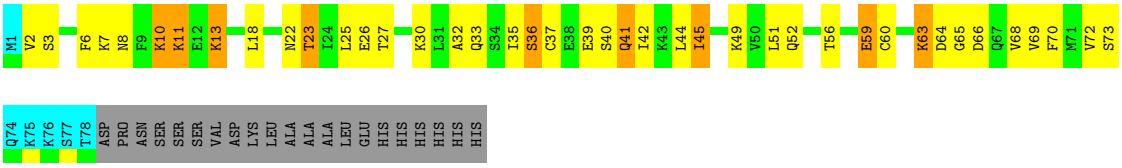
Chain A: 28% 38% 6% 6% 21%



4.2.19 Score per residue for model 19

- Molecule 1: UV excision repair protein RAD23

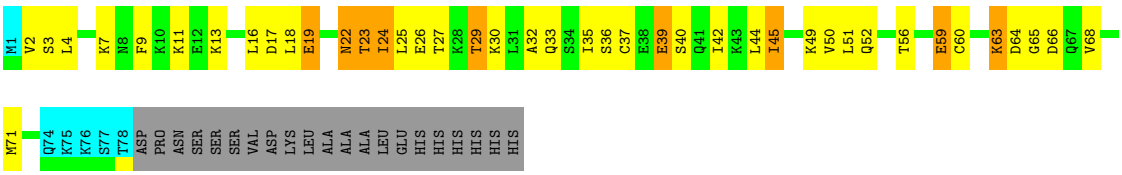
Chain A: 31% 32% 9% 6% 21%



4.2.20 Score per residue for model 20

- Molecule 1: UV excision repair protein RAD23

Chain A: 30% 33% 9% 6% 21%



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
TALOS	structure solution	
TALOS	refinement	
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	
ProcheckNMR	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	95%

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	558	584	584	31±3
All	All	11160	11680	11680	617

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:32:ALA:HB1	1:A:37:CYS:O	0.88	1.68	20	20
1:A:35:ILE:HD11	1:A:37:CYS:SG	0.86	2.11	3	2
1:A:45:ILE:N	1:A:45:ILE:HD13	0.73	1.99	5	20
1:A:25:LEU:C	1:A:25:LEU:HD13	0.71	2.06	14	14
1:A:6:PHE:CE2	1:A:44:LEU:HD11	0.71	2.19	17	9
1:A:45:ILE:N	1:A:45:ILE:CD1	0.71	2.52	5	20
1:A:8:ASN:HD21	1:A:12:GLU:H	0.65	1.32	18	2
1:A:51:LEU:HD21	1:A:60:CYS:SG	0.62	2.35	11	3
1:A:13:LYS:N	1:A:13:LYS:CD	0.61	2.64	3	4
1:A:56:THR:OG1	1:A:57:VAL:N	0.61	2.34	3	1
1:A:8:ASN:ND2	1:A:12:GLU:H	0.60	1.94	18	2
1:A:37:CYS:SG	1:A:41:GLN:NE2	0.60	2.75	2	2
1:A:39:GLU:OE1	1:A:39:GLU:N	0.60	2.34	18	6
1:A:56:THR:O	1:A:59:GLU:N	0.60	2.33	9	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ASN:OD1	1:A:8:ASN:N	0.60	2.35	10	3
1:A:3:SER:O	1:A:65:GLY:N	0.59	2.34	3	19
1:A:32:ALA:O	1:A:37:CYS:N	0.59	2.35	5	20
1:A:9:PHE:CE1	1:A:71:MET:SD	0.59	2.96	4	4
1:A:8:ASN:OD1	1:A:11:LYS:N	0.59	2.36	19	1
1:A:6:PHE:CD2	1:A:31:LEU:HD22	0.58	2.33	1	9
1:A:25:LEU:HD23	1:A:25:LEU:O	0.58	1.98	8	6
1:A:6:PHE:CD1	1:A:16:LEU:HD12	0.57	2.35	18	1
1:A:52:GLN:NE2	1:A:55:LYS:NZ	0.56	2.52	3	1
1:A:50:VAL:HG13	1:A:50:VAL:O	0.56	2.01	3	6
1:A:41:GLN:NE2	1:A:73:SER:O	0.56	2.39	12	4
1:A:25:LEU:HD23	1:A:25:LEU:C	0.56	2.22	19	6
1:A:25:LEU:O	1:A:29:THR:OG1	0.56	2.23	17	11
1:A:7:LYS:O	1:A:70:PHE:CD1	0.55	2.60	19	6
1:A:32:ALA:CB	1:A:37:CYS:O	0.55	2.54	3	2
1:A:13:LYS:CD	1:A:13:LYS:H	0.54	2.14	19	1
1:A:23:THR:O	1:A:26:GLU:N	0.54	2.41	14	17
1:A:22:ASN:ND2	1:A:26:GLU:OE1	0.54	2.41	17	3
1:A:50:VAL:O	1:A:52:GLN:NE2	0.54	2.40	1	5
1:A:37:CYS:SG	1:A:38:GLU:N	0.53	2.81	2	4
1:A:63:LYS:NZ	1:A:66:ASP:OD1	0.53	2.39	14	1
1:A:56:THR:O	1:A:60:CYS:SG	0.53	2.66	3	15
1:A:32:ALA:CB	1:A:39:GLU:OE1	0.52	2.58	4	6
1:A:46:TYR:CE2	1:A:60:CYS:O	0.52	2.62	6	5
1:A:35:ILE:O	1:A:36:SER:CB	0.52	2.58	8	20
1:A:45:ILE:N	1:A:69:VAL:O	0.52	2.43	7	18
1:A:19:GLU:N	1:A:22:ASN:OD1	0.52	2.42	3	1
1:A:55:LYS:NZ	1:A:59:GLU:OE1	0.52	2.39	16	1
1:A:25:LEU:C	1:A:25:LEU:CD1	0.51	2.78	14	14
1:A:9:PHE:CD1	1:A:71:MET:SD	0.51	3.03	4	1
1:A:39:GLU:CD	1:A:40:SER:N	0.51	2.64	15	14
1:A:27:THR:CG2	1:A:44:LEU:CD1	0.51	2.88	3	1
1:A:39:GLU:OE2	1:A:40:SER:N	0.50	2.45	9	2
1:A:22:ASN:ND2	1:A:26:GLU:CD	0.50	2.65	12	1
1:A:64:ASP:OD1	1:A:64:ASP:N	0.50	2.45	17	1
1:A:46:TYR:HB2	1:A:51:LEU:HD11	0.50	1.82	14	7
1:A:50:VAL:O	1:A:50:VAL:HG13	0.50	2.06	1	1
1:A:10:LYS:CD	1:A:10:LYS:O	0.49	2.59	19	1
1:A:10:LYS:O	1:A:10:LYS:CE	0.49	2.60	19	1
1:A:25:LEU:HD13	1:A:25:LEU:O	0.49	2.07	15	14
1:A:16:LEU:HD22	1:A:30:LYS:CD	0.49	2.38	4	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:THR:O	1:A:32:ALA:HB3	0.49	2.07	17	5
1:A:8:ASN:ND2	1:A:8:ASN:H	0.49	2.06	7	5
1:A:28:LYS:NZ	1:A:53:ASP:OD1	0.48	2.44	2	1
1:A:35:ILE:CD1	1:A:37:CYS:SG	0.48	2.96	3	1
1:A:41:GLN:OE1	1:A:72:VAL:CG1	0.48	2.62	1	10
1:A:4:LEU:HD21	1:A:63:LYS:O	0.48	2.08	6	8
1:A:30:LYS:O	1:A:33:GLN:N	0.47	2.47	19	20
1:A:19:GLU:N	1:A:19:GLU:CD	0.47	2.68	20	1
1:A:7:LYS:CD	1:A:7:LYS:C	0.47	2.82	6	3
1:A:44:LEU:CD1	1:A:44:LEU:N	0.47	2.78	9	3
1:A:63:LYS:NZ	1:A:66:ASP:CG	0.47	2.68	7	1
1:A:63:LYS:CD	1:A:64:ASP:N	0.47	2.78	17	20
1:A:59:GLU:C	1:A:59:GLU:OE2	0.47	2.52	20	2
1:A:44:LEU:N	1:A:44:LEU:HD12	0.46	2.26	15	5
1:A:32:ALA:O	1:A:36:SER:N	0.46	2.48	2	14
1:A:53:ASP:OD1	1:A:53:ASP:N	0.45	2.48	1	1
1:A:63:LYS:CD	1:A:64:ASP:O	0.45	2.64	4	15
1:A:10:LYS:O	1:A:11:LYS:HB2	0.45	2.10	19	1
1:A:8:ASN:C	1:A:10:LYS:H	0.45	2.15	4	1
1:A:19:GLU:O	1:A:22:ASN:OD1	0.45	2.35	20	1
1:A:3:SER:O	1:A:65:GLY:CA	0.45	2.64	2	18
1:A:53:ASP:OD1	1:A:53:ASP:C	0.45	2.55	14	1
1:A:6:PHE:CE1	1:A:16:LEU:HD12	0.44	2.47	16	2
1:A:22:ASN:HD21	1:A:26:GLU:CD	0.44	2.14	12	1
1:A:44:LEU:CD2	1:A:44:LEU:N	0.44	2.81	4	1
1:A:30:LYS:O	1:A:32:ALA:N	0.44	2.51	10	6
1:A:24:ILE:HD11	1:A:60:CYS:SG	0.44	2.53	18	7
1:A:52:GLN:N	1:A:52:GLN:CD	0.44	2.70	11	2
1:A:44:LEU:HD12	1:A:70:PHE:HB2	0.44	1.88	11	1
1:A:30:LYS:C	1:A:32:ALA:N	0.44	2.71	3	13
1:A:26:GLU:O	1:A:30:LYS:CD	0.44	2.66	14	1
1:A:56:THR:C	1:A:60:CYS:HG	0.43	2.16	20	2
1:A:9:PHE:CD1	1:A:9:PHE:N	0.43	2.85	2	1
1:A:35:ILE:O	1:A:36:SER:OG	0.43	2.34	6	7
1:A:51:LEU:HD22	1:A:60:CYS:SG	0.43	2.53	3	1
1:A:24:ILE:N	1:A:24:ILE:HD13	0.43	2.29	20	9
1:A:37:CYS:SG	1:A:42:ILE:CD1	0.43	3.07	3	1
1:A:26:GLU:CG	1:A:27:THR:N	0.43	2.82	17	1
1:A:10:LYS:O	1:A:11:LYS:CB	0.43	2.66	19	1
1:A:63:LYS:NZ	1:A:64:ASP:O	0.42	2.41	16	3
1:A:6:PHE:N	1:A:6:PHE:CD1	0.42	2.88	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:VAL:O	1:A:52:GLN:OE1	0.42	2.36	18	1
1:A:47:SER:O	1:A:47:SER:OG	0.42	2.36	14	1
1:A:63:LYS:HZ2	1:A:66:ASP:CG	0.42	2.18	7	1
1:A:16:LEU:O	1:A:17:ASP:OD1	0.42	2.37	20	1
1:A:25:LEU:C	1:A:25:LEU:CD2	0.42	2.89	3	5
1:A:63:LYS:HD3	1:A:64:ASP:N	0.42	2.30	15	3
1:A:44:LEU:N	1:A:44:LEU:CD1	0.42	2.82	20	2
1:A:64:ASP:O	1:A:64:ASP:OD1	0.41	2.37	16	3
1:A:38:GLU:OE2	1:A:40:SER:OG	0.41	2.37	8	1
1:A:19:GLU:CD	1:A:19:GLU:N	0.41	2.73	11	1
1:A:27:THR:CG2	1:A:28:LYS:N	0.41	2.82	8	1
1:A:70:PHE:O	1:A:71:MET:CG	0.41	2.69	8	2
1:A:22:ASN:ND2	1:A:26:GLU:OE2	0.41	2.52	13	1
1:A:52:GLN:CD	1:A:52:GLN:N	0.41	2.73	15	1
1:A:16:LEU:HD22	1:A:30:LYS:HD2	0.41	1.92	16	1
1:A:56:THR:O	1:A:57:VAL:C	0.41	2.59	9	1
1:A:26:GLU:HG2	1:A:27:THR:N	0.41	2.31	17	1
1:A:20:PRO:O	1:A:56:THR:OG1	0.41	2.35	3	1
1:A:23:THR:CB	1:A:55:LYS:O	0.41	2.69	1	1
1:A:45:ILE:O	1:A:69:VAL:O	0.41	2.39	14	1
1:A:27:THR:HG22	1:A:28:LYS:N	0.41	2.31	8	1
1:A:8:ASN:ND2	1:A:8:ASN:N	0.41	2.68	15	1
1:A:8:ASN:OD1	1:A:8:ASN:C	0.41	2.60	19	1
1:A:59:GLU:CD	1:A:59:GLU:C	0.40	2.80	1	1
1:A:9:PHE:O	1:A:9:PHE:CD2	0.40	2.74	9	1
1:A:62:LEU:HD21	1:A:68:VAL:HG22	0.40	1.91	4	1
1:A:54:SER:O	1:A:54:SER:OG	0.40	2.37	13	1
1:A:23:THR:O	1:A:24:ILE:C	0.40	2.59	20	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	72/99 (73%)	63±1 (87±1%)	8±1 (10±1%)	2±1 (2±1%)	10 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1440/1980 (73%)	1259 (87%)	151 (10%)	30 (2%)	10 50

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	51	LEU	17
1	A	66	ASP	9
1	A	24	ILE	2
1	A	36	SER	1
1	A	11	LYS	1

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	68/92 (74%)	52±2 (76±3%)	16±2 (24±3%)	2 27
All	All	1360/1840 (74%)	1037 (76%)	323 (24%)	2 27

All 39 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	2	VAL	20
1	A	18	LEU	20
1	A	27	THR	20
1	A	42	ILE	20
1	A	45	ILE	20
1	A	63	LYS	20
1	A	23	THR	19
1	A	13	LYS	18
1	A	68	VAL	17
1	A	41	GLN	16
1	A	7	LYS	15
1	A	66	ASP	10
1	A	29	THR	9
1	A	36	SER	9

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Mol	Chain	Res	Type	Models (Total)
1	A	44	LEU	8
1	A	52	GLN	8
1	A	59	GLU	7
1	A	49	LYS	7
1	A	39	GLU	7
1	A	57	VAL	7
1	A	8	ASN	6
1	A	11	LYS	6
1	A	19	GLU	6
1	A	22	ASN	6
1	A	53	ASP	2
1	A	33	GLN	2
1	A	73	SER	2
1	A	40	SER	2
1	A	10	LYS	2
1	A	3	SER	2
1	A	47	SER	2
1	A	24	ILE	1
1	A	56	THR	1
1	A	64	ASP	1
1	A	55	LYS	1
1	A	54	SER	1
1	A	9	PHE	1
1	A	30	LYS	1
1	A	26	GLU	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no 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 95% for the well-defined parts and 95% 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	1177
Number of shifts mapped to atoms	1003
Number of unparsed shifts	0
Number of shifts with mapping errors	174
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 174 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	79	ASP	H	8.28	0	1
1	A	79	ASP	HA	4.878	0	1
1	A	79	ASP	HB2	2.774	0	2
1	A	79	ASP	HB3	2.574	0	2
1	A	79	ASP	C	175.013	0	1
1	A	79	ASP	CA	52.087	0	1
1	A	79	ASP	CB	41.205	0	1
1	A	79	ASP	N	124.382	0	1
1	A	80	PRO	HA	4.423	0	1
1	A	80	PRO	HB2	2.3	0	2
1	A	80	PRO	HB3	1.966	0	2
1	A	80	PRO	HG2	2.015	0	2
1	A	80	PRO	HG3	2.015	0	2
1	A	80	PRO	HD2	3.889	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	PRO	HD3	3.835	0	2
1	A	80	PRO	C	177.067	0	1
1	A	80	PRO	CA	63.802	0	1
1	A	80	PRO	CB	32.021	0	1
1	A	80	PRO	CG	26.959	0	1
1	A	80	PRO	CD	50.583	0	1
1	A	81	ASN	H	8.52	0	1
1	A	81	ASN	HA	4.736	0	1
1	A	81	ASN	HB2	2.863	0	2
1	A	81	ASN	HB3	2.789	0	2
1	A	81	ASN	HD21	6.95	0	2
1	A	81	ASN	HD22	7.756	0	2
1	A	81	ASN	C	175.519	0	1
1	A	81	ASN	CA	53.396	0	1
1	A	81	ASN	CB	38.771	0	1
1	A	81	ASN	N	117.478	0	1
1	A	81	ASN	ND2	113.877	0	1
1	A	82	SER	H	8.023	0	1
1	A	82	SER	HA	4.402	0	1
1	A	82	SER	HB2	3.875	0	2
1	A	82	SER	HB3	3.875	0	2
1	A	82	SER	C	174.653	0	1
1	A	82	SER	CA	58.739	0	1
1	A	82	SER	CB	63.802	0	1
1	A	82	SER	N	115.818	0	1
1	A	83	SER	H	8.331	0	1
1	A	83	SER	HA	4.491	0	1
1	A	83	SER	HB2	3.894	0	2
1	A	83	SER	HB3	3.894	0	2
1	A	83	SER	C	174.662	0	1
1	A	83	SER	CA	58.458	0	1
1	A	83	SER	CB	63.802	0	1
1	A	83	SER	N	117.494	0	1
1	A	84	SER	H	8.283	0	1
1	A	84	SER	C	174.886	0	1
1	A	84	SER	CA	58.461	0	1
1	A	84	SER	CB	63.523	0	1
1	A	84	SER	N	117.712	0	1
1	A	85	VAL	H	8.034	0	1
1	A	85	VAL	HA	4.062	0	1
1	A	85	VAL	HB	2.098	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	85	VAL	HG11	0.931	0	2
1	A	85	VAL	HG12	0.931	0	2
1	A	85	VAL	HG13	0.931	0	2
1	A	85	VAL	HG21	0.938	0	2
1	A	85	VAL	HG22	0.938	0	2
1	A	85	VAL	HG23	0.938	0	2
1	A	85	VAL	C	176.142	0	1
1	A	85	VAL	CA	62.889	0	1
1	A	85	VAL	CB	32.518	0	1
1	A	85	VAL	CG1	20.885	0	2
1	A	85	VAL	CG2	20.483	0	2
1	A	85	VAL	N	121.117	0	1
1	A	86	ASP	H	8.269	0	1
1	A	86	ASP	HA	4.565	0	1
1	A	86	ASP	HB2	2.713	0	2
1	A	86	ASP	HB3	2.612	0	2
1	A	86	ASP	C	176.766	0	1
1	A	86	ASP	CA	54.546	0	1
1	A	86	ASP	CB	40.752	0	1
1	A	86	ASP	N	123.029	0	1
1	A	87	LYS	H	8.172	0	1
1	A	87	LYS	HA	4.196	0	1
1	A	87	LYS	HB2	1.858	0	2
1	A	87	LYS	HB3	1.773	0	2
1	A	87	LYS	HG2	1.476	0	2
1	A	87	LYS	HG3	1.417	0	2
1	A	87	LYS	HD2	1.664	0	2
1	A	87	LYS	HD3	1.664	0	2
1	A	87	LYS	HE2	2.986	0	2
1	A	87	LYS	HE3	2.986	0	2
1	A	87	LYS	C	177.35	0	1
1	A	87	LYS	CA	57.052	0	1
1	A	87	LYS	CB	32.583	0	1
1	A	87	LYS	CG	24.709	0	1
1	A	87	LYS	CD	28.927	0	1
1	A	87	LYS	CE	41.865	0	1
1	A	87	LYS	N	121.906	0	1
1	A	88	LEU	H	8.101	0	1
1	A	88	LEU	HA	4.261	0	1
1	A	88	LEU	HB2	1.713	0	2
1	A	88	LEU	HB3	1.592	0	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	88	LEU	HG	1.62	0	1
1	A	88	LEU	HD11	0.909	0	2
1	A	88	LEU	HD12	0.909	0	2
1	A	88	LEU	HD13	0.909	0	2
1	A	88	LEU	HD21	0.851	0	2
1	A	88	LEU	HD22	0.851	0	2
1	A	88	LEU	HD23	0.851	0	2
1	A	88	LEU	C	177.798	0	1
1	A	88	LEU	CA	55.646	0	1
1	A	88	LEU	CB	41.583	0	1
1	A	88	LEU	CG	26.959	0	1
1	A	88	LEU	CD1	24.709	0	2
1	A	88	LEU	CD2	23.302	0	2
1	A	88	LEU	N	121.846	0	1
1	A	89	ALA	H	8.001	0	1
1	A	89	ALA	HA	4.189	0	1
1	A	89	ALA	HB1	1.395	0	1
1	A	89	ALA	HB2	1.395	0	1
1	A	89	ALA	HB3	1.395	0	1
1	A	89	ALA	C	178.382	0	1
1	A	89	ALA	CA	53.389	0	1
1	A	89	ALA	CB	18.521	0	1
1	A	89	ALA	N	123.573	0	1
1	A	90	ALA	H	8.023	0	1
1	A	90	ALA	HA	4.232	0	1
1	A	90	ALA	HB1	1.395	0	1
1	A	90	ALA	HB2	1.395	0	1
1	A	90	ALA	HB3	1.395	0	1
1	A	90	ALA	C	178.119	0	1
1	A	90	ALA	CA	52.833	0	1
1	A	90	ALA	CB	19.084	0	1
1	A	90	ALA	N	121.852	0	1
1	A	91	ALA	H	7.95	0	1
1	A	91	ALA	HA	4.232	0	1
1	A	91	ALA	HB1	1.394	0	1
1	A	91	ALA	HB2	1.394	0	1
1	A	91	ALA	HB3	1.394	0	1
1	A	91	ALA	C	178.1	0	1
1	A	91	ALA	CA	52.552	0	1
1	A	91	ALA	CB	18.802	0	1
1	A	91	ALA	N	121.781	0	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	92	LEU	H	7.928	0	1
1	A	92	LEU	HA	4.24	0	1
1	A	92	LEU	HB2	1.644	0	2
1	A	92	LEU	HB3	1.519	0	2
1	A	92	LEU	HG	1.641	0	1
1	A	92	LEU	HD11	0.889	0	2
1	A	92	LEU	HD12	0.889	0	2
1	A	92	LEU	HD13	0.889	0	2
1	A	92	LEU	HD21	0.835	0	2
1	A	92	LEU	HD22	0.835	0	2
1	A	92	LEU	HD23	0.835	0	2
1	A	92	LEU	C	177.584	0	1
1	A	92	LEU	CA	55.109	0	1
1	A	92	LEU	CB	42.159	0	1
1	A	92	LEU	CG	26.676	0	1
1	A	92	LEU	CD1	24.987	0	2
1	A	92	LEU	CD2	23.298	0	2
1	A	92	LEU	N	120.154	0	1
1	A	93	GLU	H	8.061	0	1
1	A	93	GLU	HA	4.16	0	1
1	A	93	GLU	HB2	1.897	0	2
1	A	93	GLU	HB3	1.897	0	2
1	A	93	GLU	HG2	2.205	0	2
1	A	93	GLU	HG3	2.121	0	2
1	A	93	GLU	C	176.308	0	1
1	A	93	GLU	CA	56.771	0	1
1	A	93	GLU	CB	30.052	0	1
1	A	93	GLU	CG	35.958	0	1
1	A	93	GLU	N	120.382	0	1
1	A	94	HIS	H	8.18	0	1
1	A	94	HIS	HA	4.565	0	1
1	A	94	HIS	HB2	3.057	0	2
1	A	94	HIS	HB3	2.98	0	2
1	A	94	HIS	C	174.955	0	1
1	A	94	HIS	CA	55.927	0	1
1	A	94	HIS	CB	30.333	0	1
1	A	94	HIS	N	119.338	0	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	94	-0.01 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	91	0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	94	-0.05 ± 0.14	None needed (< 0.5 ppm)
^{15}N	90	0.42 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 95%, i.e. 923 atoms were assigned a chemical shift out of a possible 973. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	359/359 (100%)	145/145 (100%)	144/144 (100%)	70/70 (100%)
Sidechain	549/575 (95%)	373/373 (100%)	170/186 (91%)	6/16 (38%)
Aromatic	15/39 (38%)	15/19 (79%)	0/20 (0%)	0/0 (—%)
Overall	923/973 (95%)	533/537 (99%)	314/350 (90%)	76/86 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 95%, i.e. 1003 atoms were assigned a chemical shift out of a possible 1058. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	387/389 (99%)	156/157 (99%)	156/156 (100%)	75/76 (99%)
Sidechain	601/630 (95%)	408/408 (100%)	186/203 (92%)	7/19 (37%)
Aromatic	15/39 (38%)	15/19 (79%)	0/20 (0%)	0/0 (—%)
Overall	1003/1058 (95%)	579/584 (99%)	342/379 (90%)	82/95 (86%)

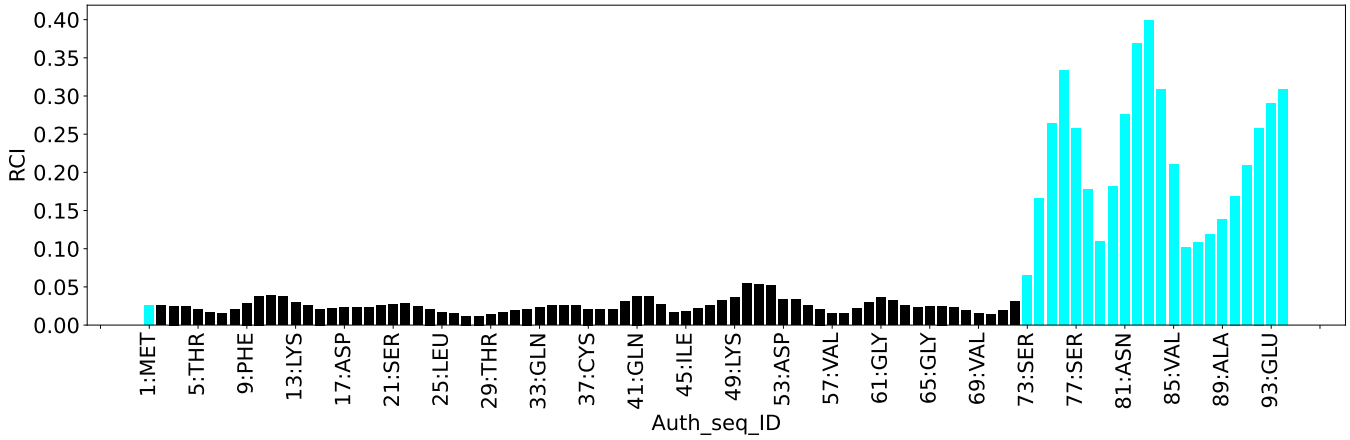
7.1.4 Statistically unusual chemical shifts (i)

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
0.40
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
5:THR
9:PHE
13:LYS
17:ASP
21:SER
25:LEU
29:THR
33:GLN
37:CYS
41:GLN
45:ILE
49:LYS
53:ASP
57:VAL
61:GLY
65:GLY
69:VAL
73:SER
77:SER
81:ASN
85:VAL
89:ALA
93:GLU
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	1362
Intra-residue (|i-j|=0)	556
Sequential (|i-j|=1)	268
Medium range (|i-j|>1 and |i-j|<5)	197
Long range (|i-j|≥5)	293
Inter-chain	0
Hydrogen bond restraints	48
Disulfide bond restraints	0
Total dihedral-angle restraints	137
Number of unmapped restraints	0
Number of restraints per residue	15.1
Number of long range restraints per residue[1]	3.3

[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)	30.9	0.2
0.2-0.5 (Medium)	2.8	0.35
>0.5 (Large)	None	None

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

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

Bins (°)	Average number of violations per model	Max (°)
1.0-10.0 (Small)	8.8	3.3
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

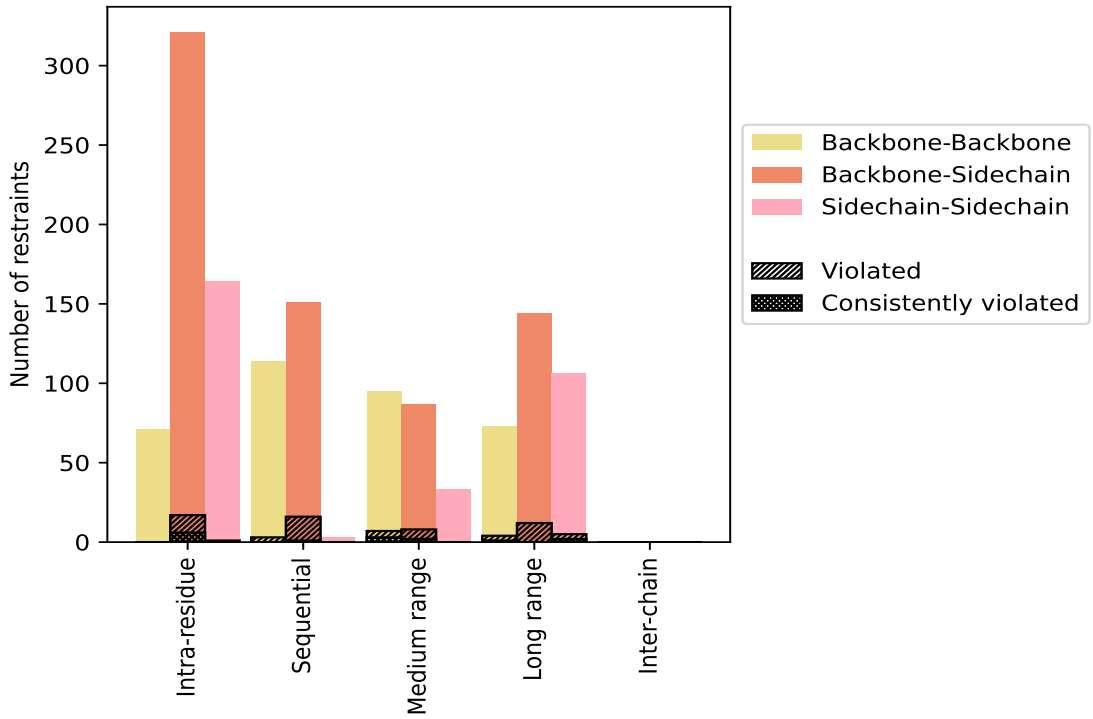
9.1 Summary of distance violations (i)

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)	556	40.8	18	3.2	1.3	6	1.1	0.4
Backbone-Backbone	71	5.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	321	23.6	17	5.3	1.2	6	1.9	0.4
Sidechain-Sidechain	164	12.0	1	0.6	0.1	0	0.0	0.0
Sequential (|i-j|=1)	268	19.7	19	7.1	1.4	1	0.4	0.1
Backbone-Backbone	114	8.4	3	2.6	0.2	0	0.0	0.0
Backbone-Sidechain	151	11.1	16	10.6	1.2	1	0.7	0.1
Sidechain-Sidechain	3	0.2	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	197	14.5	13	6.6	1.0	5	2.5	0.4
Backbone-Backbone	77	5.7	5	6.5	0.4	3	3.9	0.2
Backbone-Sidechain	87	6.4	8	9.2	0.6	2	2.3	0.1
Sidechain-Sidechain	33	2.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	293	21.5	20	6.8	1.5	3	1.0	0.2
Backbone-Backbone	43	3.2	3	7.0	0.2	1	2.3	0.1
Backbone-Sidechain	144	10.6	12	8.3	0.9	0	0.0	0.0
Sidechain-Sidechain	106	7.8	5	4.7	0.4	2	1.9	0.1
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	48	3.5	3	6.2	0.2	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1362	100.0	73	5.4	5.4	15	1.1	1.1
Backbone-Backbone	353	25.9	14	4.0	1.0	4	1.1	0.3
Backbone-Sidechain	703	51.6	53	7.5	3.9	9	1.3	0.7
Sidechain-Sidechain	306	22.5	6	2.0	0.4	2	0.7	0.1

[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	8	9	9	9	0	35	0.14	0.23	0.04	0.13
2	11	8	7	9	0	35	0.14	0.23	0.03	0.14
3	7	4	7	13	0	31	0.14	0.23	0.03	0.13
4	9	7	9	11	0	36	0.14	0.22	0.03	0.14
5	8	8	10	10	0	36	0.14	0.21	0.03	0.13
6	8	7	9	10	0	34	0.15	0.24	0.04	0.14
7	8	4	9	11	0	32	0.14	0.23	0.04	0.13
8	11	8	6	9	0	34	0.14	0.24	0.04	0.12
9	7	10	7	12	0	36	0.14	0.21	0.03	0.14
10	9	6	7	12	0	34	0.15	0.24	0.03	0.14
11	11	11	8	10	0	40	0.14	0.2	0.03	0.13

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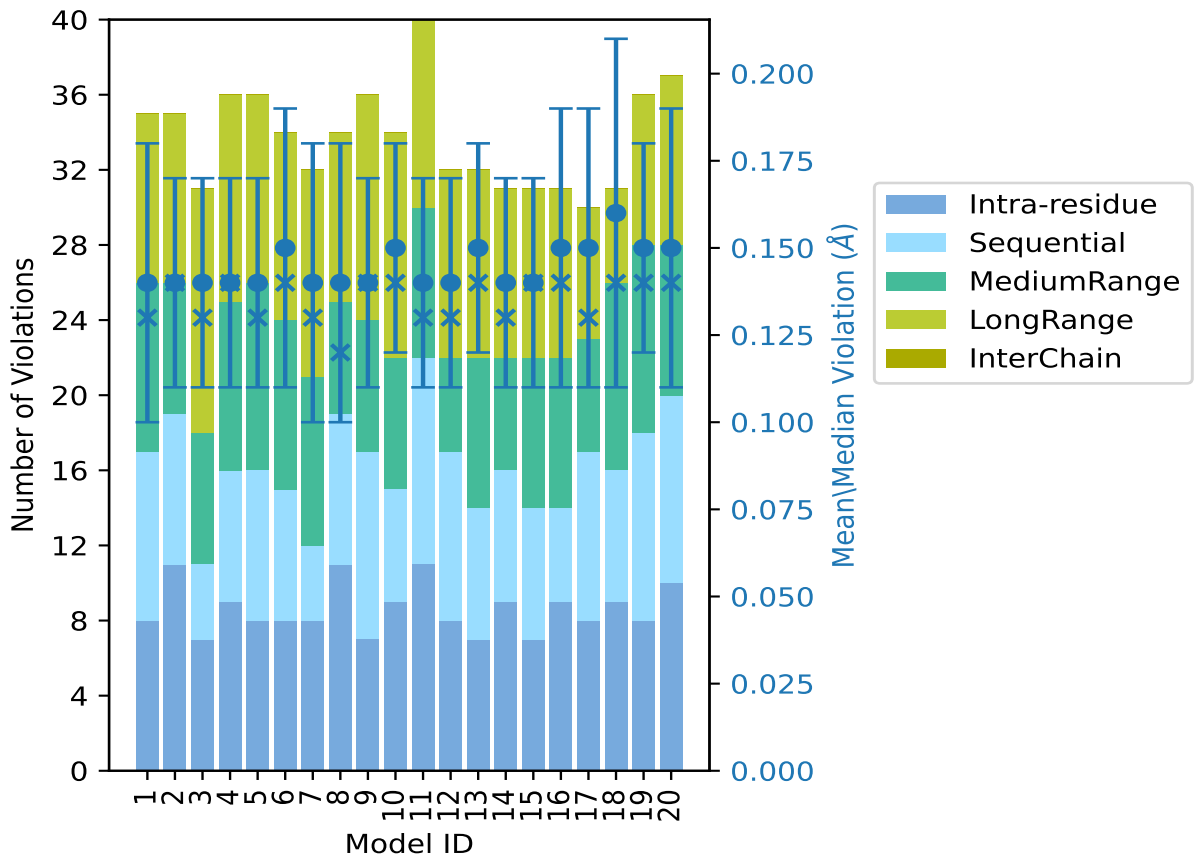
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	8	9	5	10	0	32	0.14	0.23	0.03	0.13
13	7	7	8	10	0	32	0.15	0.23	0.03	0.14
14	9	7	6	9	0	31	0.14	0.23	0.03	0.13
15	7	7	8	9	0	31	0.14	0.21	0.03	0.14
16	9	5	8	9	0	31	0.15	0.23	0.04	0.14
17	8	9	6	7	0	30	0.15	0.24	0.04	0.13
18	9	7	10	5	0	31	0.16	0.35	0.05	0.14
19	8	10	10	8	0	36	0.15	0.23	0.03	0.14
20	10	10	8	9	0	37	0.15	0.26	0.04	0.14

[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

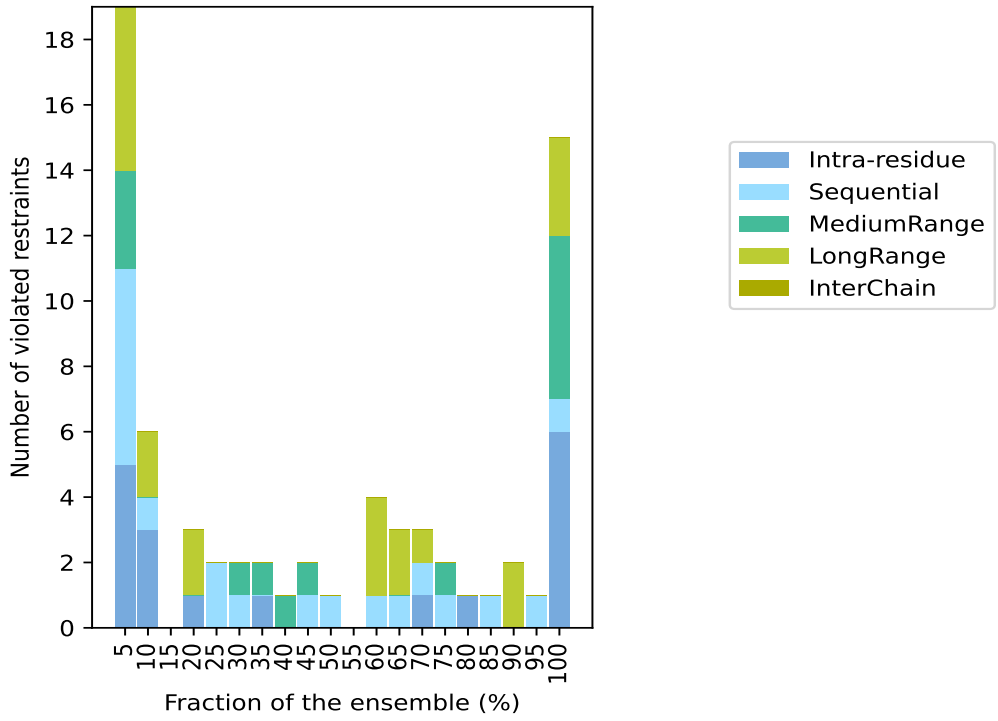
9.3 Distance violation statistics for the ensemble (i)

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, 1244(IR:538, SQ:249, MR:184, LR:273, 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]	%
5	6	3	5	0	19	1	5.0
3	1	0	2	0	6	2	10.0
0	0	0	0	0	0	3	15.0
1	0	0	2	0	3	4	20.0
0	2	0	0	0	2	5	25.0
0	1	1	0	0	2	6	30.0
1	0	1	0	0	2	7	35.0
0	0	1	0	0	1	8	40.0
0	1	1	0	0	2	9	45.0
0	1	0	0	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	1	0	3	0	4	12	60.0
0	1	0	2	0	3	13	65.0
1	1	0	1	0	3	14	70.0
0	1	1	0	0	2	15	75.0
1	0	0	0	0	1	16	80.0
0	1	0	0	0	1	17	85.0
0	0	0	2	0	2	18	90.0
0	1	0	0	0	1	19	95.0
6	1	5	3	0	15	20	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

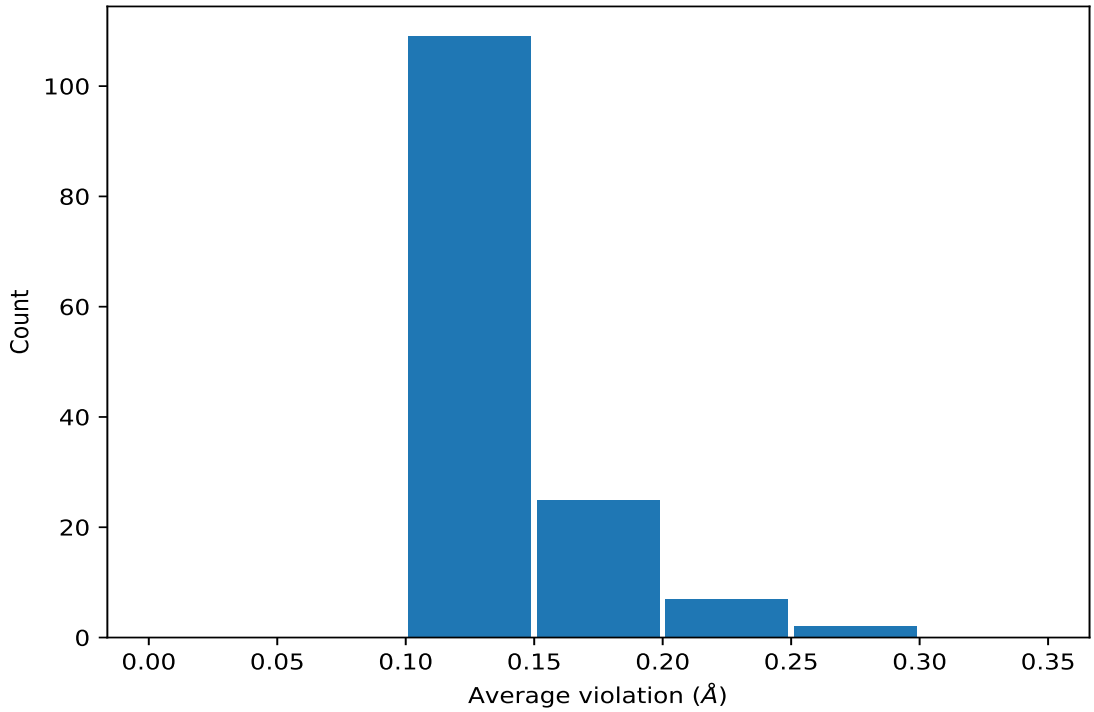
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	20	0.21	0.01	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	20	0.21	0.01	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	20	0.21	0.01	0.21
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	20	0.21	0.03	0.2
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	20	0.21	0.03	0.2
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	20	0.2	0.04	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	20	0.2	0.04	0.21
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	20	0.18	0.04	0.16
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	20	0.18	0.04	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	20	0.17	0.01	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	20	0.17	0.01	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	20	0.17	0.01	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	20	0.17	0.01	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	20	0.17	0.01	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	20	0.17	0.01	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	20	0.17	0.01	0.17

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	20	0.17	0.01	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	20	0.17	0.01	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	20	0.17	0.02	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	20	0.17	0.02	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	20	0.17	0.02	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	20	0.17	0.02	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	20	0.17	0.01	0.17
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	20	0.15	0.01	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	20	0.14	0.01	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	20	0.13	0.02	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	20	0.13	0.01	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	20	0.13	0.01	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	20	0.12	0.01	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	20	0.12	0.01	0.12
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	19	0.19	0.01	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	19	0.19	0.01	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	19	0.19	0.01	0.19
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	18	0.15	0.02	0.15
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	18	0.15	0.02	0.15
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	18	0.13	0.01	0.13
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	17	0.11	0.0	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	17	0.11	0.0	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	16	0.13	0.02	0.13
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	16	0.13	0.02	0.13
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	16	0.13	0.02	0.13
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	15	0.14	0.02	0.15
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	15	0.12	0.02	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	15	0.12	0.02	0.11
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	14	0.14	0.03	0.14
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	14	0.14	0.03	0.14
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	14	0.14	0.03	0.14
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	14	0.13	0.04	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	14	0.13	0.04	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	14	0.13	0.04	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	14	0.11	0.0	0.11
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	13	0.12	0.01	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	13	0.12	0.01	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	13	0.12	0.01	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	13	0.12	0.01	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	13	0.12	0.01	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	13	0.12	0.01	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	13	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	13	0.11	0.0	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	13	0.11	0.0	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	13	0.11	0.0	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	13	0.11	0.0	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	13	0.11	0.0	0.11
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	12	0.13	0.02	0.13
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	12	0.13	0.02	0.13
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	12	0.13	0.02	0.13
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	12	0.13	0.01	0.12
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	12	0.12	0.01	0.12
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	12	0.12	0.01	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	12	0.12	0.01	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	12	0.12	0.01	0.12
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	10	0.12	0.01	0.12
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	10	0.12	0.01	0.12
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	10	0.12	0.01	0.12
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	9	0.14	0.0	0.14
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	9	0.13	0.02	0.12
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	9	0.13	0.02	0.12
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	9	0.13	0.02	0.12
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	8	0.12	0.01	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	8	0.12	0.0	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	8	0.12	0.0	0.12
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	7	0.12	0.01	0.12
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	7	0.12	0.01	0.12
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	7	0.12	0.01	0.12
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	6	0.15	0.0	0.15
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	6	0.11	0.0	0.11
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	6	0.11	0.0	0.11
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	5	0.12	0.01	0.12
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	5	0.12	0.01	0.12
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	5	0.12	0.01	0.12
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	5	0.12	0.0	0.12
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	5	0.12	0.0	0.12
(1,489)	1:A:41:GLN:HB2	1:A:41:GLN:H	4	0.14	0.01	0.14
(1,489)	1:A:41:GLN:HB3	1:A:41:GLN:H	4	0.14	0.01	0.14
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG2	4	0.13	0.01	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG3	4	0.13	0.01	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG2	4	0.13	0.01	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG3	4	0.13	0.01	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG2	4	0.13	0.01	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG3	4	0.13	0.01	0.14
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD11	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD12	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD13	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD21	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD22	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD23	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD11	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD12	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD13	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD21	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD22	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD23	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD11	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD12	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD13	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD21	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD22	4	0.12	0.01	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD23	4	0.12	0.01	0.12
(2,35)	1:A:69:VAL:O	1:A:45:ILE:H	3	0.12	0.01	0.12
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD21	2	0.28	0.07	0.28
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD22	2	0.28	0.07	0.28
(1,337)	1:A:38:GLU:HG2	1:A:38:GLU:H	2	0.16	0.02	0.16
(1,337)	1:A:38:GLU:HG3	1:A:38:GLU:H	2	0.16	0.02	0.16
(1,559)	1:A:15:PRO:HB2	1:A:16:LEU:H	2	0.12	0.0	0.12
(1,559)	1:A:15:PRO:HB3	1:A:16:LEU:H	2	0.12	0.0	0.12
(1,642)	1:A:4:LEU:HD11	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,642)	1:A:4:LEU:HD12	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,642)	1:A:4:LEU:HD13	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,642)	1:A:4:LEU:HD21	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,642)	1:A:4:LEU:HD22	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,642)	1:A:4:LEU:HD23	1:A:64:ASP:H	2	0.11	0.0	0.11
(1,673)	1:A:68:VAL:HB	1:A:68:VAL:H	2	0.11	0.0	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD11	2	0.11	0.0	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD12	2	0.11	0.0	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD13	2	0.11	0.0	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD21	2	0.11	0.0	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD22	2	0.11	0.0	0.11

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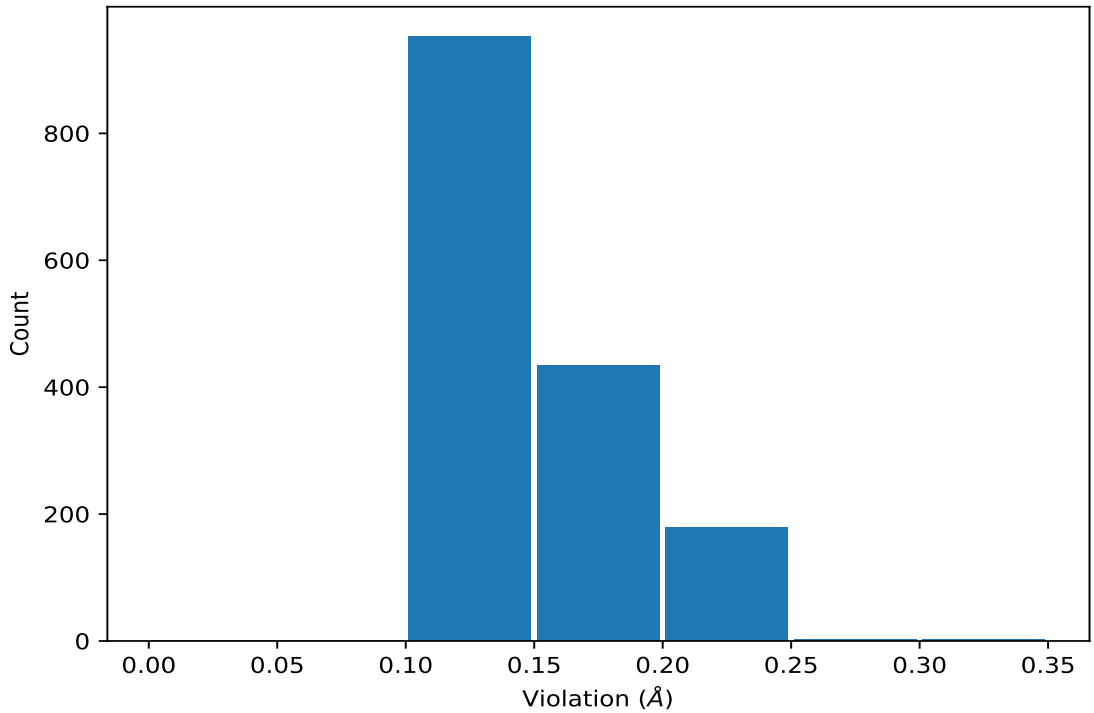
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD23	2	0.11	0.0	0.11

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD21	18	0.35
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD22	18	0.35
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	20	0.26
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	8	0.24
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	8	0.24
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	10	0.24
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	10	0.24
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	17	0.24
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	17	0.24
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	6	0.24
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	6	0.24
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	6	0.24
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	20	0.24
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	20	0.24
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	1	0.23
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	1	0.23
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	2	0.23
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	2	0.23
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	13	0.23
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	13	0.23
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	16	0.23
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	16	0.23
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	17	0.23
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	17	0.23
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	17	0.23
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	12	0.23
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	12	0.23
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	12	0.23
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	14	0.23
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	14	0.23
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	14	0.23
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	12	0.23
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	12	0.23
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	17	0.23
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	17	0.23
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	18	0.23
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	18	0.23
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	19	0.23
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	19	0.23
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	3	0.23
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	3	0.23
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	7	0.23
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	7	0.23
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	16	0.23
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	6	0.22
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	6	0.22
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	1	0.22
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	1	0.22
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	1	0.22
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	3	0.22
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	3	0.22
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	3	0.22
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	7	0.22
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	7	0.22
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	7	0.22
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	18	0.22
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	18	0.22
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	18	0.22
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	1	0.22
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	1	0.22
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	8	0.22
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	8	0.22
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	16	0.22
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	16	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	4	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	4	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	8	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	8	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	10	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	10	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	18	0.22
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	18	0.22
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	15	0.21
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	15	0.21
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	4	0.21
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	4	0.21
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	4	0.21
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	10	0.21
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	10	0.21
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	10	0.21
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	13	0.21
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	13	0.21
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	13	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	5	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	5	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	5	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	6	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	6	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	6	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	8	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	8	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	8	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	10	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	10	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	10	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	13	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	13	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	13	0.21
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	17	0.21
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	17	0.21
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	17	0.21
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	14	0.21
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	14	0.21
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	7	0.21
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	7	0.21
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	7	0.21
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	18	0.21
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	18	0.21
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	18	0.21
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD21	2	0.21
(1,474)	1:A:8:ASN:H	1:A:8:ASN:HD22	2	0.21
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	20	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	1	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	1	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	5	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	5	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	6	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	6	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	9	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	9	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	13	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	13	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	15	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	15	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	19	0.21
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	19	0.21
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	5	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	5	0.2
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	7	0.2
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	7	0.2
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	9	0.2
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	9	0.2
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	11	0.2
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	11	0.2
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	19	0.2
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	19	0.2
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	1	0.2
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	1	0.2
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	1	0.2
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	4	0.2
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	4	0.2
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	4	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	1	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	1	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	1	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	2	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	2	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	2	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	7	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	7	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	7	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	8	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	8	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	8	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	18	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	18	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	18	0.2
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	20	0.2
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	20	0.2
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	20	0.2
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	2	0.2
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	2	0.2
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	2	0.2
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	4	0.2
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	4	0.2
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	4	0.2
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	9	0.2
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	9	0.2
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	16	0.2
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	16	0.2
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	16	0.2
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	20	0.2
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	20	0.2
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	20	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	13	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	13	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	13	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	13	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	13	0.2
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	13	0.2
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	3	0.19
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	3	0.19
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	3	0.19
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	14	0.19
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	14	0.19
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	14	0.19
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	19	0.19
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	19	0.19
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	19	0.19
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	3	0.19
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	3	0.19
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	3	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	9	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	9	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	9	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	12	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	12	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	12	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	14	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	14	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	14	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	15	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	15	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	15	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	16	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	16	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	16	0.19
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	17	0.19
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	17	0.19
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	11	0.19
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	11	0.19
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	11	0.19
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	15	0.19
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	15	0.19
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	15	0.19
(1,636)	1:A:45:ILE:HD11	1:A:49:LYS:H	19	0.19
(1,636)	1:A:45:ILE:HD12	1:A:49:LYS:H	19	0.19
(1,636)	1:A:45:ILE:HD13	1:A:49:LYS:H	19	0.19
(1,507)	1:A:10:LYS:HD2	1:A:10:LYS:H	11	0.19
(1,507)	1:A:10:LYS:HD3	1:A:10:LYS:H	11	0.19
(1,357)	1:A:36:SER:H	1:A:34:SER:H	17	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	16	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	16	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	16	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	16	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	16	0.19
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	16	0.19
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	2	0.19
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	2	0.19
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	11	0.19
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	11	0.19
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	11	0.18
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	11	0.18
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	11	0.18
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	4	0.18
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	4	0.18
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	4	0.18
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	5	0.18
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	5	0.18
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	5	0.18
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	9	0.18
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	9	0.18
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	9	0.18
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	15	0.18
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	15	0.18
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	15	0.18
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	18	0.18
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	18	0.18
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	18	0.18
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	5	0.18
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	5	0.18
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	11	0.18
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	11	0.18
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	11	0.18
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	19	0.18
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	19	0.18
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	19	0.18
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	6	0.18
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	6	0.18
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	10	0.18
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	10	0.18
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	10	0.18
(1,357)	1:A:36:SER:H	1:A:34:SER:H	1	0.18
(1,357)	1:A:36:SER:H	1:A:34:SER:H	6	0.18
(1,357)	1:A:36:SER:H	1:A:34:SER:H	8	0.18
(1,357)	1:A:36:SER:H	1:A:34:SER:H	12	0.18
(1,357)	1:A:36:SER:H	1:A:34:SER:H	15	0.18
(1,337)	1:A:38:GLU:HG2	1:A:38:GLU:H	20	0.18
(1,337)	1:A:38:GLU:HG3	1:A:38:GLU:H	20	0.18
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	20	0.18
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	1	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	4	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	6	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	7	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	7	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	7	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	7	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	7	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	7	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	19	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	20	0.18
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	20	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	1	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	9	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	11	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	13	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	18	0.18
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	19	0.18
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	4	0.17
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	4	0.17
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	14	0.17
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	14	0.17
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	18	0.17
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	18	0.17
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	20	0.17
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	20	0.17
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	20	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	7	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	7	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	7	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	8	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	8	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	8	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	13	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	13	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	13	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	16	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	16	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	16	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	18	0.17
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	18	0.17
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	18	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	2	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	2	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	2	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	6	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	6	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	6	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	7	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	7	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	7	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	8	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	8	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	8	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	10	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	10	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	10	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	12	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	12	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	12	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	14	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	14	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	14	0.17
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	19	0.17
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	19	0.17
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	19	0.17
(1,710)	1:A:56:THR:HG21	1:A:57:VAL:H	6	0.17
(1,710)	1:A:56:THR:HG22	1:A:57:VAL:H	6	0.17
(1,710)	1:A:56:THR:HG23	1:A:57:VAL:H	6	0.17
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	4	0.17
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	9	0.17
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	15	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	4	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	9	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	11	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	13	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	18	0.17
(1,357)	1:A:36:SER:H	1:A:34:SER:H	19	0.17
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	3	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	3	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	3	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	3	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	3	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	3	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	8	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	9	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	10	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	11	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	14	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	15	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	17	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	17	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	17	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	17	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	17	0.17
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	17	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	4	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	8	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	10	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	12	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	14	0.17
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	17	0.17
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	10	0.16
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	10	0.16
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	10	0.16
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	12	0.16
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	12	0.16
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	12	0.16
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	15	0.16
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	15	0.16
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	15	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	1	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	1	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	1	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	11	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	11	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	11	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	13	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	13	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	13	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	16	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	16	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	16	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	17	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	17	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	17	0.16
(1,732)	1:A:24:ILE:HG21	1:A:24:ILE:H	20	0.16
(1,732)	1:A:24:ILE:HG22	1:A:24:ILE:H	20	0.16
(1,732)	1:A:24:ILE:HG23	1:A:24:ILE:H	20	0.16
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	6	0.16
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	6	0.16
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	6	0.16
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	2	0.16
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	3	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	5	0.16
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	7	0.16
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	10	0.16
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	17	0.16
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	10	0.16
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	10	0.16
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	1	0.16
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	19	0.16
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	19	0.16
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	2	0.16
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	10	0.16
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	15	0.16
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	16	0.16
(1,357)	1:A:36:SER:H	1:A:34:SER:H	5	0.16
(1,357)	1:A:36:SER:H	1:A:34:SER:H	10	0.16
(1,357)	1:A:36:SER:H	1:A:34:SER:H	14	0.16
(1,357)	1:A:36:SER:H	1:A:34:SER:H	20	0.16
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	2	0.16
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	2	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	5	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	12	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG11	18	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG12	18	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG13	18	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG21	18	0.16
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG22	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1294)	1:A:62:LEU:HG	1:A:57:VAL:HG23	18	0.16
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	2	0.16
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	5	0.16
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	7	0.16
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	16	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	5	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	5	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	7	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	7	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	9	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	9	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	10	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	10	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	13	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	13	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	20	0.16
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	20	0.16
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	3	0.15
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	3	0.15
(1,864)	1:A:28:LYS:HD2	1:A:28:LYS:HA	12	0.15
(1,864)	1:A:28:LYS:HD3	1:A:28:LYS:HA	12	0.15
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	4	0.15
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	4	0.15
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	4	0.15
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	19	0.15
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	19	0.15
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	19	0.15
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	2	0.15
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	2	0.15
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	2	0.15
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	5	0.15
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	5	0.15
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	5	0.15
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	20	0.15
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	20	0.15
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	20	0.15
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	3	0.15
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	18	0.15
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	19	0.15
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	2	0.15
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	2	0.15
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	4	0.15
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	4	0.15
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	4	0.15
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	9	0.15
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	9	0.15
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	9	0.15
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	6	0.15
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	7	0.15
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	13	0.15
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	19	0.15
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	19	0.15
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	19	0.15
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	1	0.15
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	11	0.15
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	13	0.15
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	11	0.15
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	11	0.15
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	20	0.15
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	20	0.15
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	4	0.15
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	4	0.15
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	4	0.15
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	6	0.15
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	6	0.15
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	6	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	5	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	6	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	8	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	9	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	13	0.15
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	18	0.15
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	12	0.15
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	18	0.15
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	8	0.15
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	5	0.15
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	6	0.15
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	9	0.15
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	19	0.15
(1,357)	1:A:36:SER:H	1:A:34:SER:H	2	0.15
(1,357)	1:A:36:SER:H	1:A:34:SER:H	16	0.15
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	3	0.15
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	15	0.15
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	20	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD11	4	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD12	4	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD13	4	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD21	4	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD22	4	0.15
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD23	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD11	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD12	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD13	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD21	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD22	4	0.15
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD23	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD11	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD12	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD13	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD21	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD22	4	0.15
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD23	4	0.15
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	6	0.15
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	15	0.15
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	2	0.15
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	2	0.15
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	4	0.15
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	4	0.15
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	16	0.14
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG2	4	0.14
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG3	4	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG2	4	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG3	4	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG2	4	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG3	4	0.14
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG2	18	0.14
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG3	18	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG2	18	0.14
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG3	18	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG2	18	0.14
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG3	18	0.14
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	19	0.14
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	19	0.14
(1,766)	1:A:21:SER:HA	1:A:56:THR:HB	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	9	0.14
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	9	0.14
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	9	0.14
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	12	0.14
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	12	0.14
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	12	0.14
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	13	0.14
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	13	0.14
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	13	0.14
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	16	0.14
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	16	0.14
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	16	0.14
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	6	0.14
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	6	0.14
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	6	0.14
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	9	0.14
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	9	0.14
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	9	0.14
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	20	0.14
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	20	0.14
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	20	0.14
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	1	0.14
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	8	0.14
(1,721)	1:A:25:LEU:HG	1:A:26:GLU:H	20	0.14
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	11	0.14
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	11	0.14
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	11	0.14
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	15	0.14
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	15	0.14
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	15	0.14
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	20	0.14
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	20	0.14
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	20	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	6	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	8	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	12	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	14	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	16	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	18	0.14
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	20	0.14
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	10	0.14
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	10	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	13	0.14
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	13	0.14
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	2	0.14
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	2	0.14
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	4	0.14
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	4	0.14
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	7	0.14
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	7	0.14
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	9	0.14
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	9	0.14
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	13	0.14
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	13	0.14
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	5	0.14
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	5	0.14
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	5	0.14
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	14	0.14
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	14	0.14
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	14	0.14
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	7	0.14
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	15	0.14
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	16	0.14
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	4	0.14
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	5	0.14
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	9	0.14
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	11	0.14
(1,489)	1:A:41:GLN:HB2	1:A:41:GLN:H	12	0.14
(1,489)	1:A:41:GLN:HB3	1:A:41:GLN:H	12	0.14
(1,489)	1:A:41:GLN:HB2	1:A:41:GLN:H	17	0.14
(1,489)	1:A:41:GLN:HB3	1:A:41:GLN:H	17	0.14
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	18	0.14
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	18	0.14
(1,441)	1:A:26:GLU:HB2	1:A:27:THR:H	17	0.14
(1,441)	1:A:26:GLU:HB3	1:A:27:THR:H	17	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	2	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	4	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	6	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	16	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	17	0.14
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	20	0.14
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	4	0.14
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	13	0.14
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	9	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	9	0.14
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	20	0.14
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	20	0.14
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	1	0.14
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	5	0.14
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	14	0.14
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	15	0.14
(1,357)	1:A:36:SER:H	1:A:34:SER:H	3	0.14
(1,357)	1:A:36:SER:H	1:A:34:SER:H	7	0.14
(1,337)	1:A:38:GLU:HG2	1:A:38:GLU:H	2	0.14
(1,337)	1:A:38:GLU:HG3	1:A:38:GLU:H	2	0.14
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	10	0.14
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	10	0.14
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	5	0.14
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	9	0.14
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	12	0.14
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	19	0.14
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	20	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	10	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	11	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	17	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	18	0.14
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	19	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	3	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	3	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	12	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	12	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	15	0.14
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	15	0.14
(2,35)	1:A:69:VAL:O	1:A:45:ILE:H	20	0.13
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	18	0.13
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG2	16	0.13
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG3	16	0.13
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG2	16	0.13
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG3	16	0.13
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG2	16	0.13
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG3	16	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	3	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	3	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	7	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	7	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	8	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	8	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	12	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	12	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	16	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	16	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	17	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	17	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	18	0.13
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	18	0.13
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	5	0.13
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	5	0.13
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	5	0.13
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	14	0.13
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	14	0.13
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	14	0.13
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	15	0.13
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	15	0.13
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	15	0.13
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	1	0.13
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	1	0.13
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	1	0.13
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	11	0.13
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	11	0.13
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	11	0.13
(1,740)	1:A:24:ILE:HD11	1:A:28:LYS:H	17	0.13
(1,740)	1:A:24:ILE:HD12	1:A:28:LYS:H	17	0.13
(1,740)	1:A:24:ILE:HD13	1:A:28:LYS:H	17	0.13
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	11	0.13
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	11	0.13
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	11	0.13
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	1	0.13
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	1	0.13
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	1	0.13
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	5	0.13
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	5	0.13
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	5	0.13
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	12	0.13
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	12	0.13
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	12	0.13
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	8	0.13
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	11	0.13
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	11	0.13
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	13	0.13
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	13	0.13
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	13	0.13
(1,638)	1:A:4:LEU:HG	1:A:5:THR:H	19	0.13
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	4	0.13
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	4	0.13
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	3	0.13
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	3	0.13
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	15	0.13
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	15	0.13
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	11	0.13
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	11	0.13
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	11	0.13
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	12	0.13
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	12	0.13
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	12	0.13
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	14	0.13
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	14	0.13
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	14	0.13
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	17	0.13
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	17	0.13
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	17	0.13
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	1	0.13
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	1	0.13
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	1	0.13
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	11	0.13
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	11	0.13
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	11	0.13
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	2	0.13
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	10	0.13
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	18	0.13
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	18	0.13
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	18	0.13
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	18	0.13
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	18	0.13
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	3	0.13
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	4	0.13
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	10	0.13
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	17	0.13
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	20	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	1	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	2	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	6	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	10	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	14	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	19	0.13
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	20	0.13
(1,509)	1:A:10:LYS:HE2	1:A:11:LYS:H	11	0.13
(1,509)	1:A:10:LYS:HE3	1:A:11:LYS:H	11	0.13
(1,489)	1:A:41:GLN:HB2	1:A:41:GLN:H	11	0.13
(1,489)	1:A:41:GLN:HB3	1:A:41:GLN:H	11	0.13
(1,489)	1:A:41:GLN:HB2	1:A:41:GLN:H	14	0.13
(1,489)	1:A:41:GLN:HB3	1:A:41:GLN:H	14	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	1	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	5	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	10	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	11	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	12	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	14	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	15	0.13
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	18	0.13
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	11	0.13
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	2	0.13
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	2	0.13
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	15	0.13
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	15	0.13
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	18	0.13
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	18	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	6	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	8	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	11	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	12	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	16	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	17	0.13
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	20	0.13
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	16	0.13
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	16	0.13
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	6	0.13
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	11	0.13
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	14	0.13
(1,21)	1:A:23:THR:H	1:A:22:ASN:H	17	0.13
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	1	0.13
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	2	0.13
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	5	0.13
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	7	0.13
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	13	0.13
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	5	0.13
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	5	0.13
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	5	0.13
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	13	0.13
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	13	0.13
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	13	0.13
(1,1239)	1:A:23:THR:HB	1:A:56:THR:HB	3	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	6	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	6	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	14	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	14	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	19	0.13
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	19	0.13
(2,39)	1:A:49:LYS:O	1:A:46:TYR:H	5	0.12
(2,35)	1:A:69:VAL:O	1:A:45:ILE:H	3	0.12
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	4	0.12
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	14	0.12
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG2	10	0.12
(1,841)	1:A:32:ALA:HB1	1:A:39:GLU:HG3	10	0.12
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG2	10	0.12
(1,841)	1:A:32:ALA:HB2	1:A:39:GLU:HG3	10	0.12
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG2	10	0.12
(1,841)	1:A:32:ALA:HB3	1:A:39:GLU:HG3	10	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	1	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	1	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	4	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	4	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	5	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	10	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	10	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	11	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	11	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	13	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	13	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	14	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	14	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	20	0.12
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	20	0.12
(1,774)	1:A:23:THR:HA	1:A:56:THR:HG21	3	0.12
(1,774)	1:A:23:THR:HA	1:A:56:THR:HG22	3	0.12
(1,774)	1:A:23:THR:HA	1:A:56:THR:HG23	3	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	2	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	8	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	11	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	13	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	15	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	15	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	15	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	15	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	15	0.12
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	17	0.12
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	17	0.12
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	17	0.12
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	17	0.12
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	17	0.12
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	17	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	2	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	2	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	2	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	7	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	7	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	7	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	10	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	10	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	10	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	11	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	11	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	11	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	18	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	18	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	18	0.12
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	19	0.12
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	19	0.12
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	19	0.12
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	8	0.12
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	8	0.12
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	8	0.12
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	13	0.12
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	13	0.12
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	13	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	1	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	5	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	10	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	14	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	15	0.12
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	16	0.12
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	4	0.12
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	9	0.12
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	14	0.12
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	19	0.12
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	2	0.12
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	2	0.12
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	2	0.12
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	5	0.12
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	5	0.12
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	5	0.12
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	7	0.12
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	7	0.12
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	7	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	3	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	3	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	5	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	5	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	7	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	7	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	9	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	9	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	11	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	11	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	15	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	15	0.12
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	20	0.12
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	20	0.12
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	5	0.12
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	5	0.12
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	5	0.12
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	16	0.12
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	16	0.12
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	16	0.12
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	19	0.12
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	19	0.12
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	19	0.12
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	4	0.12
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	4	0.12
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	4	0.12
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	4	0.12
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	4	0.12
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	4	0.12
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	2	0.12
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	12	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	5	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	8	0.12
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	8	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	9	0.12
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	9	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	12	0.12
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	12	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	14	0.12
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	14	0.12
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	17	0.12
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	17	0.12
(1,559)	1:A:15:PRO:HB2	1:A:16:LEU:H	18	0.12
(1,559)	1:A:15:PRO:HB3	1:A:16:LEU:H	18	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	1	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	1	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	8	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	8	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	11	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	11	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	16	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	16	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	19	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	19	0.12
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	20	0.12
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	20	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	3	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	7	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	8	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	13	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	15	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	16	0.12
(1,538)	1:A:47:SER:HA	1:A:49:LYS:H	17	0.12
(1,523)	1:A:11:LYS:HA	1:A:10:LYS:H	11	0.12
(1,508)	1:A:10:LYS:HE2	1:A:10:LYS:H	19	0.12
(1,508)	1:A:10:LYS:HE3	1:A:10:LYS:H	19	0.12
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	5	0.12
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	5	0.12
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	19	0.12
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	19	0.12
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	20	0.12
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	20	0.12
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	9	0.12
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	13	0.12
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	1	0.12
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	20	0.12
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	1	0.12
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	1	0.12
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	8	0.12
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	8	0.12
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	9	0.12
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	9	0.12
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	6	0.12
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	6	0.12
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	15	0.12
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	15	0.12
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	4	0.12
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	4	0.12
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	7	0.12
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	7	0.12
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	10	0.12
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	10	0.12
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	13	0.12
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	13	0.12
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	2	0.12
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	3	0.12
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	9	0.12
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	13	0.12
(1,388)	1:A:13:LYS:HB2	1:A:14:VAL:H	19	0.12
(1,388)	1:A:13:LYS:HB3	1:A:14:VAL:H	19	0.12
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	4	0.12
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	4	0.12
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	8	0.12
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	8	0.12
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	18	0.12
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	18	0.12
(1,238)	1:A:25:LEU:H	1:A:23:THR:H	1	0.12
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	8	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	2	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	2	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	2	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	6	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	6	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	6	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	8	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	8	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	8	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	9	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	9	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	9	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	15	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	15	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	15	0.12
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	19	0.12
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	19	0.12
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	19	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD11	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD12	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD13	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD21	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD22	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD23	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD11	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD12	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD13	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD21	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD22	1	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD23	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD11	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD12	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD13	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD21	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD22	1	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD23	1	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD11	9	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD12	9	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD13	9	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD21	9	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD22	9	0.12
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD23	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD11	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD12	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD13	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD21	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD22	9	0.12
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD23	9	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD11	9	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD12	9	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD13	9	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD21	9	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD22	9	0.12
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD23	9	0.12
(1,1266)	1:A:45:ILE:HD11	1:A:69:VAL:HB	7	0.12
(1,1266)	1:A:45:ILE:HD12	1:A:69:VAL:HB	7	0.12
(1,1266)	1:A:45:ILE:HD13	1:A:69:VAL:HB	7	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	12	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	12	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	14	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	14	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	17	0.12
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	17	0.12
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	8	0.12
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	8	0.12
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	16	0.12
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	16	0.12
(2,35)	1:A:69:VAL:O	1:A:45:ILE:H	10	0.11
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	1	0.11
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	6	0.11
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	7	0.11
(2,1)	1:A:24:ILE:O	1:A:28:LYS:H	19	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD11	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD12	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD13	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD21	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD22	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD23	10	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD11	11	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD12	11	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD13	11	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD21	11	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD22	11	0.11
(1,882)	1:A:70:PHE:HA	1:A:44:LEU:HD23	11	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	2	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	2	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	6	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	6	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	9	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD2	15	0.11
(1,826)	1:A:63:LYS:HA	1:A:63:LYS:HD3	15	0.11
(1,776)	1:A:56:THR:HA	1:A:23:THR:HG21	3	0.11
(1,776)	1:A:56:THR:HA	1:A:23:THR:HG22	3	0.11
(1,776)	1:A:56:THR:HA	1:A:23:THR:HG23	3	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	3	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	5	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	9	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	10	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	12	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	16	0.11
(1,749)	1:A:18:LEU:HD11	1:A:19:GLU:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,749)	1:A:18:LEU:HD12	1:A:19:GLU:H	20	0.11
(1,749)	1:A:18:LEU:HD13	1:A:19:GLU:H	20	0.11
(1,749)	1:A:18:LEU:HD21	1:A:19:GLU:H	20	0.11
(1,749)	1:A:18:LEU:HD22	1:A:19:GLU:H	20	0.11
(1,749)	1:A:18:LEU:HD23	1:A:19:GLU:H	20	0.11
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	6	0.11
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	6	0.11
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	6	0.11
(1,746)	1:A:24:ILE:HD11	1:A:55:LYS:H	17	0.11
(1,746)	1:A:24:ILE:HD12	1:A:55:LYS:H	17	0.11
(1,746)	1:A:24:ILE:HD13	1:A:55:LYS:H	17	0.11
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	7	0.11
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	7	0.11
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	7	0.11
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	9	0.11
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	9	0.11
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	9	0.11
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	10	0.11
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	10	0.11
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	10	0.11
(1,744)	1:A:24:ILE:HD11	1:A:60:CYS:H	12	0.11
(1,744)	1:A:24:ILE:HD12	1:A:60:CYS:H	12	0.11
(1,744)	1:A:24:ILE:HD13	1:A:60:CYS:H	12	0.11
(1,743)	1:A:24:ILE:HD11	1:A:52:GLN:H	3	0.11
(1,743)	1:A:24:ILE:HD12	1:A:52:GLN:H	3	0.11
(1,743)	1:A:24:ILE:HD13	1:A:52:GLN:H	3	0.11
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	1	0.11
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	1	0.11
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	1	0.11
(1,733)	1:A:24:ILE:HG21	1:A:25:LEU:H	17	0.11
(1,733)	1:A:24:ILE:HG22	1:A:25:LEU:H	17	0.11
(1,733)	1:A:24:ILE:HG23	1:A:25:LEU:H	17	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	6	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	6	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	6	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	7	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	7	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	7	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	8	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	8	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	8	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	10	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	10	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	13	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	13	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	13	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	14	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	14	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	14	0.11
(1,719)	1:A:27:THR:HG21	1:A:27:THR:H	16	0.11
(1,719)	1:A:27:THR:HG22	1:A:27:THR:H	16	0.11
(1,719)	1:A:27:THR:HG23	1:A:27:THR:H	16	0.11
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	3	0.11
(1,69)	1:A:7:LYS:H	1:A:70:PHE:H	4	0.11
(1,673)	1:A:68:VAL:HB	1:A:68:VAL:H	8	0.11
(1,673)	1:A:68:VAL:HB	1:A:68:VAL:H	16	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	2	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	3	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	5	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	6	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	8	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	11	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	12	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	15	0.11
(1,655)	1:A:2:VAL:HB	1:A:3:SER:H	20	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	1	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	1	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	1	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	4	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	4	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	4	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	7	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	7	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	7	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	8	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	8	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	8	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	9	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	9	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	9	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	12	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	12	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	13	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	13	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	13	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	14	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	14	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	14	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	16	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	16	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	16	0.11
(1,651)	1:A:5:THR:HG21	1:A:13:LYS:H	19	0.11
(1,651)	1:A:5:THR:HG22	1:A:13:LYS:H	19	0.11
(1,651)	1:A:5:THR:HG23	1:A:13:LYS:H	19	0.11
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	2	0.11
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	2	0.11
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	2	0.11
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	3	0.11
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	3	0.11
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	3	0.11
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	5	0.11
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	5	0.11
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	5	0.11
(1,648)	1:A:5:THR:HG21	1:A:7:LYS:H	9	0.11
(1,648)	1:A:5:THR:HG22	1:A:7:LYS:H	9	0.11
(1,648)	1:A:5:THR:HG23	1:A:7:LYS:H	9	0.11
(1,643)	1:A:4:LEU:HD11	1:A:5:THR:H	5	0.11
(1,643)	1:A:4:LEU:HD12	1:A:5:THR:H	5	0.11
(1,643)	1:A:4:LEU:HD13	1:A:5:THR:H	5	0.11
(1,643)	1:A:4:LEU:HD21	1:A:5:THR:H	5	0.11
(1,643)	1:A:4:LEU:HD22	1:A:5:THR:H	5	0.11
(1,643)	1:A:4:LEU:HD23	1:A:5:THR:H	5	0.11
(1,642)	1:A:4:LEU:HD11	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD12	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD13	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD21	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD22	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD23	1:A:64:ASP:H	3	0.11
(1,642)	1:A:4:LEU:HD11	1:A:64:ASP:H	9	0.11
(1,642)	1:A:4:LEU:HD12	1:A:64:ASP:H	9	0.11
(1,642)	1:A:4:LEU:HD13	1:A:64:ASP:H	9	0.11
(1,642)	1:A:4:LEU:HD21	1:A:64:ASP:H	9	0.11
(1,642)	1:A:4:LEU:HD22	1:A:64:ASP:H	9	0.11
(1,642)	1:A:4:LEU:HD23	1:A:64:ASP:H	9	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	2	0.11
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	2	0.11
(1,629)	1:A:45:ILE:HG12	1:A:70:PHE:H	6	0.11
(1,629)	1:A:45:ILE:HG13	1:A:70:PHE:H	6	0.11
(1,627)	1:A:45:ILE:HG12	1:A:45:ILE:H	5	0.11
(1,627)	1:A:45:ILE:HG13	1:A:45:ILE:H	5	0.11
(1,600)	1:A:42:ILE:HG21	1:A:40:SER:H	18	0.11
(1,600)	1:A:42:ILE:HG22	1:A:40:SER:H	18	0.11
(1,600)	1:A:42:ILE:HG23	1:A:40:SER:H	18	0.11
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	1	0.11
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	1	0.11
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	1	0.11
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	2	0.11
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	2	0.11
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	2	0.11
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	13	0.11
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	13	0.11
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	13	0.11
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	15	0.11
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	15	0.11
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	15	0.11
(1,599)	1:A:42:ILE:HG21	1:A:41:GLN:H	19	0.11
(1,599)	1:A:42:ILE:HG22	1:A:41:GLN:H	19	0.11
(1,599)	1:A:42:ILE:HG23	1:A:41:GLN:H	19	0.11
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	2	0.11
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	2	0.11
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	2	0.11
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	8	0.11
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	8	0.11
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	8	0.11
(1,589)	1:A:29:THR:HG21	1:A:29:THR:H	20	0.11
(1,589)	1:A:29:THR:HG22	1:A:29:THR:H	20	0.11
(1,589)	1:A:29:THR:HG23	1:A:29:THR:H	20	0.11
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	8	0.11
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	11	0.11
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	11	0.11
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	11	0.11
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	11	0.11
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	11	0.11
(1,585)	1:A:31:LEU:HD11	1:A:31:LEU:H	20	0.11
(1,585)	1:A:31:LEU:HD12	1:A:31:LEU:H	20	0.11
(1,585)	1:A:31:LEU:HD13	1:A:31:LEU:H	20	0.11
(1,585)	1:A:31:LEU:HD21	1:A:31:LEU:H	20	0.11
(1,585)	1:A:31:LEU:HD22	1:A:31:LEU:H	20	0.11
(1,585)	1:A:31:LEU:HD23	1:A:31:LEU:H	20	0.11
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	11	0.11
(1,568)	1:A:35:ILE:HB	1:A:35:ILE:H	14	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	1	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	1	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	2	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	2	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	4	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	4	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	6	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	6	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	7	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	7	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	10	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	10	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	11	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	11	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	15	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	15	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	16	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	16	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	19	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	19	0.11
(1,562)	1:A:20:PRO:HB2	1:A:21:SER:H	20	0.11
(1,562)	1:A:20:PRO:HB3	1:A:21:SER:H	20	0.11
(1,559)	1:A:15:PRO:HB2	1:A:16:LEU:H	19	0.11
(1,559)	1:A:15:PRO:HB3	1:A:16:LEU:H	19	0.11
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	4	0.11
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	4	0.11
(1,551)	1:A:55:LYS:HB2	1:A:59:GLU:H	13	0.11
(1,551)	1:A:55:LYS:HB3	1:A:59:GLU:H	13	0.11
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	3	0.11
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	3	0.11
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	4	0.11
(1,453)	1:A:49:LYS:HG2	1:A:46:TYR:H	15	0.11
(1,453)	1:A:49:LYS:HG3	1:A:46:TYR:H	15	0.11
(1,446)	1:A:26:GLU:HG2	1:A:26:GLU:H	17	0.11
(1,446)	1:A:26:GLU:HG3	1:A:26:GLU:H	17	0.11
(1,44)	1:A:2:VAL:HA	1:A:65:GLY:H	7	0.11
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	7	0.11
(1,437)	1:A:26:GLU:HA	1:A:29:THR:H	18	0.11
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	4	0.11
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	4	0.11
(1,415)	1:A:53:ASP:HB2	1:A:54:SER:H	11	0.11
(1,415)	1:A:53:ASP:HB3	1:A:54:SER:H	11	0.11
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	5	0.11
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	5	0.11
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	7	0.11
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	7	0.11
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	10	0.11
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	10	0.11
(1,41)	1:A:58:SER:HB2	1:A:60:CYS:H	18	0.11
(1,41)	1:A:58:SER:HB3	1:A:60:CYS:H	18	0.11
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	1	0.11
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	1	0.11
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	6	0.11
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	6	0.11
(1,405)	1:A:17:ASP:HB2	1:A:18:LEU:H	12	0.11
(1,405)	1:A:17:ASP:HB3	1:A:18:LEU:H	12	0.11
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	4	0.11
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	7	0.11
(1,401)	1:A:17:ASP:HA	1:A:3:SER:H	10	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	1	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	1	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	6	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	6	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	9	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	9	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	12	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	12	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	13	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	13	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	14	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	14	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	17	0.11
(1,336)	1:A:38:GLU:HG2	1:A:39:GLU:H	19	0.11
(1,336)	1:A:38:GLU:HG3	1:A:39:GLU:H	19	0.11
(1,278)	1:A:75:LYS:HB2	1:A:75:LYS:H	3	0.11
(1,278)	1:A:75:LYS:HB3	1:A:75:LYS:H	3	0.11
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	4	0.11
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	6	0.11
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	12	0.11
(1,209)	1:A:24:ILE:HA	1:A:27:THR:H	16	0.11
(1,174)	1:A:70:PHE:H	1:A:69:VAL:H	9	0.11
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	1	0.11
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	1	0.11
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	1	0.11
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	11	0.11
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	11	0.11
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	11	0.11
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	12	0.11
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	12	0.11
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	12	0.11
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	14	0.11
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	14	0.11
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	14	0.11
(1,135)	1:A:32:ALA:HB1	1:A:40:SER:H	20	0.11
(1,135)	1:A:32:ALA:HB2	1:A:40:SER:H	20	0.11
(1,135)	1:A:32:ALA:HB3	1:A:40:SER:H	20	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD11	12	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD12	12	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD13	12	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD21	12	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD22	12	0.11
(1,1304)	1:A:27:THR:HG21	1:A:16:LEU:HD23	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD11	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD12	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD13	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD21	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD22	12	0.11
(1,1304)	1:A:27:THR:HG22	1:A:16:LEU:HD23	12	0.11
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD11	12	0.11
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD12	12	0.11
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD13	12	0.11
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD21	12	0.11
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD22	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1304)	1:A:27:THR:HG23	1:A:16:LEU:HD23	12	0.11
(1,130)	1:A:32:ALA:HB1	1:A:36:SER:H	17	0.11
(1,130)	1:A:32:ALA:HB2	1:A:36:SER:H	17	0.11
(1,130)	1:A:32:ALA:HB3	1:A:36:SER:H	17	0.11
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG2	11	0.11
(1,1139)	1:A:41:GLN:HA	1:A:41:GLN:HG3	11	0.11
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG12	17	0.11
(1,1010)	1:A:50:VAL:HA	1:A:45:ILE:HG13	17	0.11
(1,1005)	1:A:75:LYS:HB2	1:A:75:LYS:HE2	8	0.11
(1,1005)	1:A:75:LYS:HB2	1:A:75:LYS:HE3	8	0.11
(1,1005)	1:A:75:LYS:HB3	1:A:75:LYS:HE2	8	0.11
(1,1005)	1:A:75:LYS:HB3	1:A:75:LYS:HE3	8	0.11

10 Dihedral-angle violation analysis (i)

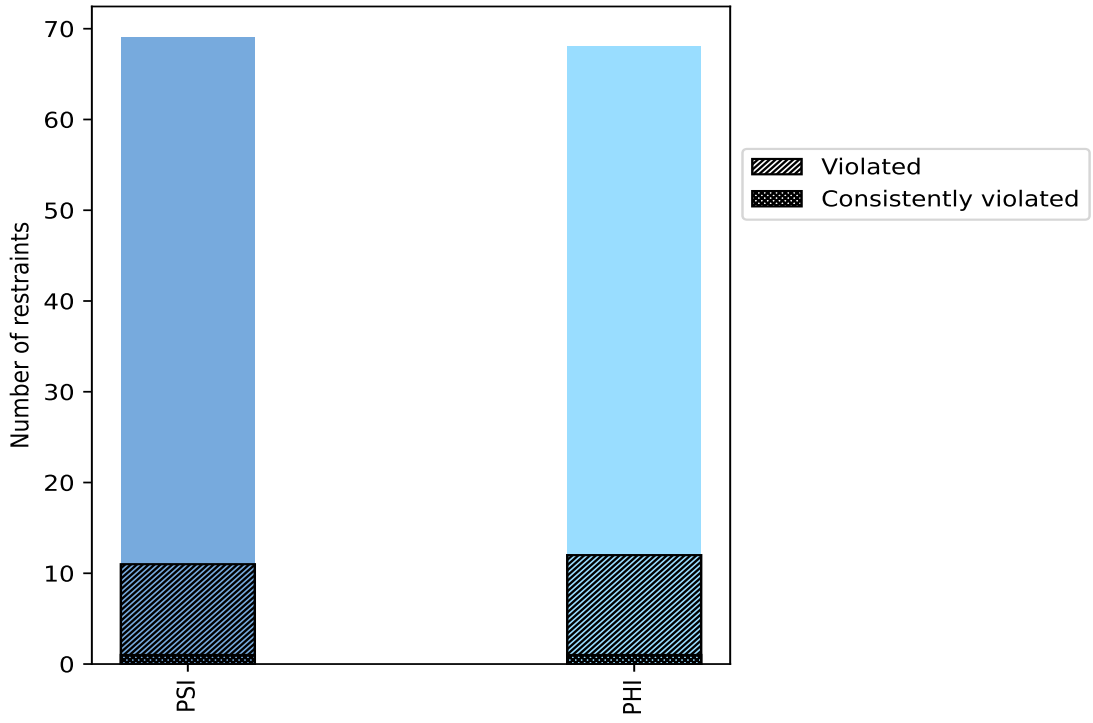
10.1 Summary of dihedral-angle violations (i)

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	69	50.4	11	15.9	8.0	1	1.4	0.7
PHI	68	49.6	12	17.6	8.8	1	1.5	0.7
Total	137	100.0	23	16.8	16.8	2	1.5	1.5

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

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



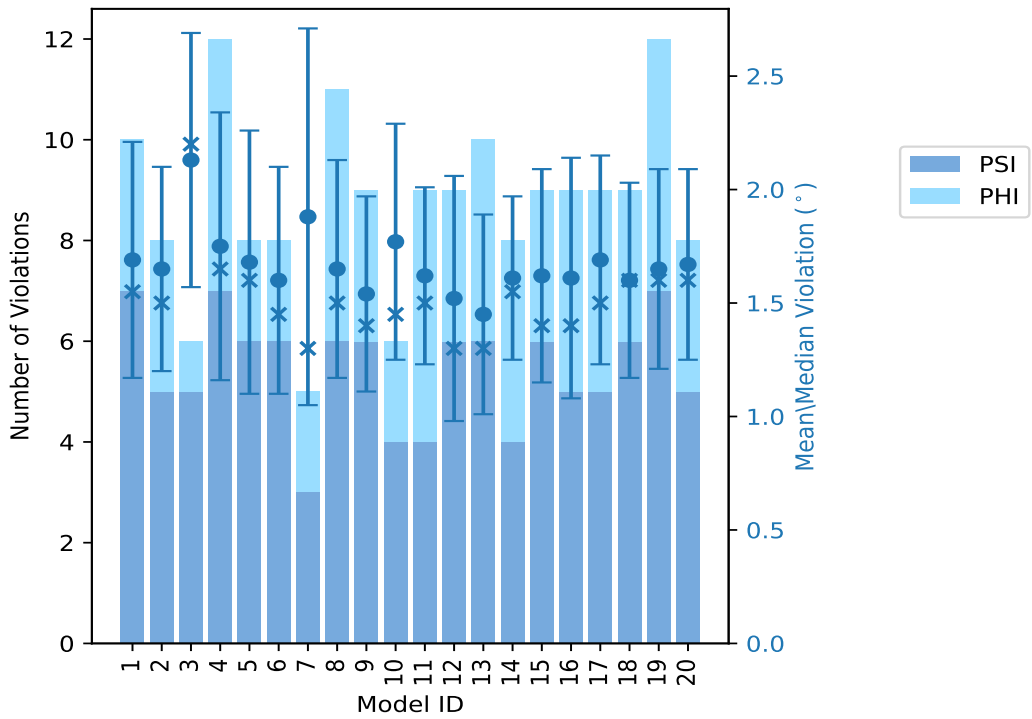
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model (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	7	3	10	1.69	2.8	0.52	1.55
2	5	3	8	1.65	2.4	0.45	1.5
3	5	1	6	2.13	3.0	0.56	2.2
4	7	5	12	1.75	3.3	0.59	1.65
5	6	2	8	1.68	2.6	0.58	1.6
6	6	2	8	1.6	2.4	0.5	1.45
7	3	2	5	1.88	3.2	0.83	1.3
8	6	5	11	1.65	2.7	0.48	1.5
9	6	3	9	1.54	2.4	0.43	1.4
10	4	2	6	1.77	2.6	0.52	1.45
11	4	5	9	1.62	2.5	0.39	1.5
12	6	3	9	1.52	2.6	0.54	1.3
13	6	4	10	1.45	2.4	0.44	1.3
14	4	4	8	1.61	2.4	0.36	1.55
15	6	3	9	1.62	2.5	0.47	1.4
16	5	4	9	1.61	2.6	0.53	1.4
17	5	4	9	1.69	2.7	0.46	1.5
18	6	3	9	1.6	2.4	0.43	1.6
19	7	5	12	1.65	2.7	0.44	1.6
20	5	3	8	1.67	2.5	0.42	1.6

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]	%
2	4	6	1	5.0
0	1	1	2	10.0
1	3	4	3	15.0
1	0	1	4	20.0
0	0	0	5	25.0
1	0	1	6	30.0
0	0	0	7	35.0
1	1	2	8	40.0
0	0	0	9	45.0
0	1	1	10	50.0
0	0	0	11	55.0

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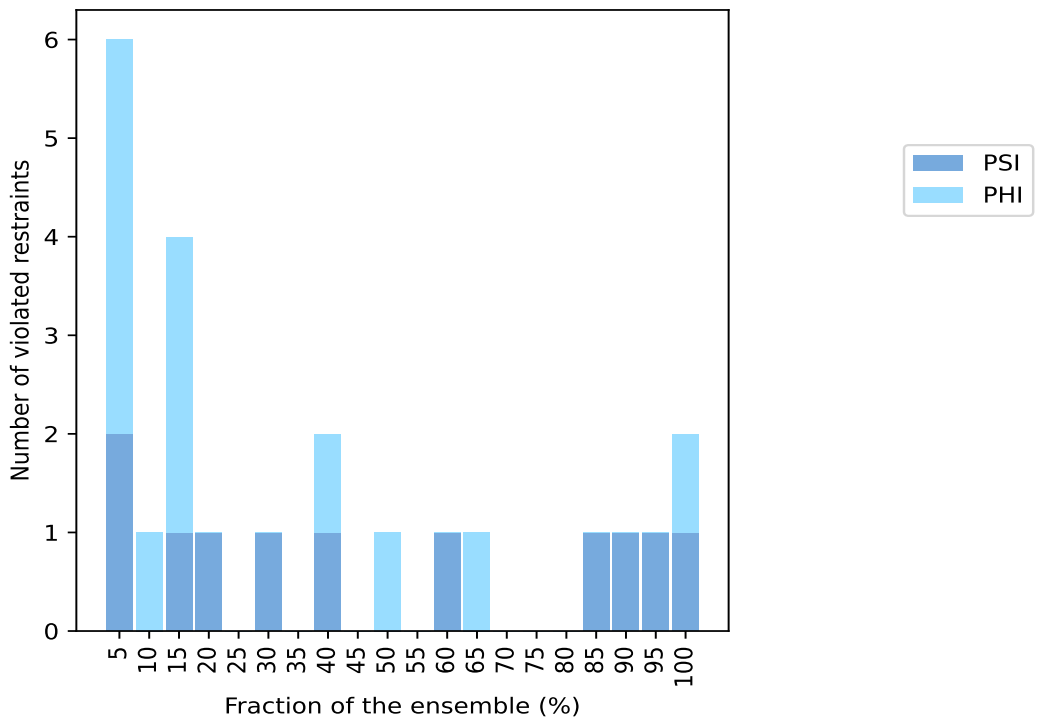
Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count[1]	%
1	0	1	12	60.0
0	1	1	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
1	0	1	18	90.0
1	0	1	19	95.0
1	1	2	20	100.0

[1] Number of models with violations

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

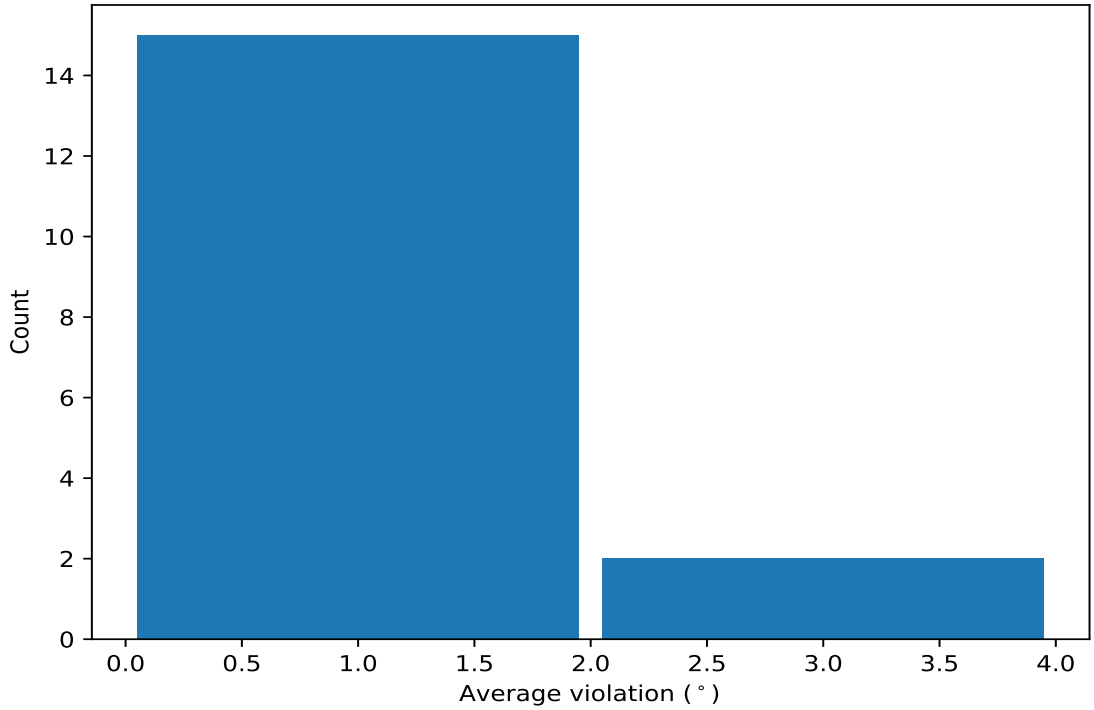


10.4 Most violated dihedral-angle restraints in the ensemble (i)

10.4.1 Histogram : Distribution of mean dihedral-angle violations (i)

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

in the ensemble



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

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

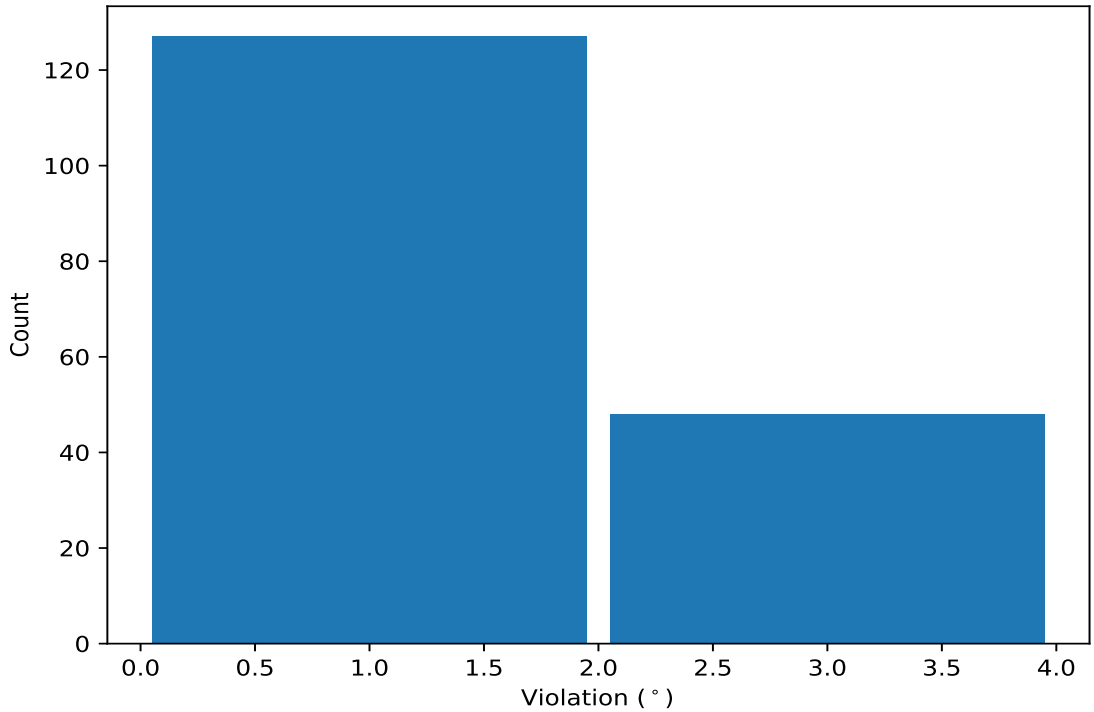
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	20	2.42	0.22	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	20	2.41	0.3	2.4
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	19	1.64	0.2	1.6
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	18	1.32	0.14	1.3
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	17	1.59	0.29	1.6
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	13	1.39	0.15	1.4
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	12	1.16	0.08	1.1
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	10	1.19	0.09	1.15
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	8	1.55	0.32	1.45
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	8	1.52	0.33	1.45
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	6	1.37	0.14	1.4
(1,95)	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	1:A:52:GLN:N	4	1.6	0.28	1.6
(1,104)	1:A:55:LYS:C	1:A:56:THR:N	1:A:56:THR:CA	1:A:56:THR:C	3	1.43	0.47	1.1
(1,58)	1:A:31:LEU:C	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	3	1.37	0.09	1.3
(1,22)	1:A:12:GLU:C	1:A:13:LYS:N	1:A:13:LYS:CA	1:A:13:LYS:C	3	1.23	0.09	1.3
(1,91)	1:A:49:LYS:N	1:A:49:LYS:CA	1:A:49:LYS:C	1:A:50:VAL:N	3	1.17	0.05	1.2
(1,112)	1:A:59:GLU:C	1:A:60:CYS:N	1:A:60:CYS:CA	1:A:60:CYS:C	2	1.5	0.1	1.5

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

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:A:56:THR:N	1:A:56:THR:CA	1:A:56:THR:C	1:A:57:VAL:N	4	3.3
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	7	3.2
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	3	3.0
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	1	2.8
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	8	2.7
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	19	2.7
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	17	2.7
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	10	2.6
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	12	2.6
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	16	2.6
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	5	2.6
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	7	2.5
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	15	2.5
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	20	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	11	2.5
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	16	2.5
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	2	2.4
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	6	2.4
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	9	2.4
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	13	2.4
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	18	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	1	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	6	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	8	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	10	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	12	2.4
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	14	2.4
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	3	2.3
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	5	2.3
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	17	2.3
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	2	2.3
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	3	2.2
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	3	2.2
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	13	2.2
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	15	2.2
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	18	2.2
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	19	2.2
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	4	2.2
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	11	2.1
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	9	2.1
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	20	2.1
(1,104)	1:A:55:LYS:C	1:A:56:THR:N	1:A:56:THR:CA	1:A:56:THR:C	4	2.1
(1,95)	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	1:A:52:GLN:N	3	2.0
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	5	2.0
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	5	2.0
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	4	2.0
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	1	2.0
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	8	2.0
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	15	1.9
(1,84)	1:A:44:LEU:C	1:A:45:ILE:N	1:A:45:ILE:CA	1:A:45:ILE:C	14	1.9
(1,61)	1:A:33:GLN:N	1:A:33:GLN:CA	1:A:33:GLN:C	1:A:34:SER:N	4	1.9
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	19	1.9
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	19	1.8
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	20	1.8
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	2	1.8
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	15	1.8
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	18	1.7
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	4	1.7
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	6	1.7
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	9	1.7
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	18	1.7
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	8	1.7
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	19	1.7
(1,95)	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	1:A:52:GLN:N	1	1.6
(1,95)	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	1:A:52:GLN:N	14	1.6

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	4	1.6
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	9	1.6
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	16	1.6
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	17	1.6
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	14	1.6
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	16	1.6
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	17	1.6
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	19	1.6
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	20	1.6
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	18	1.6
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	2	1.6
(1,18)	1:A:10:LYS:C	1:A:11:LYS:N	1:A:11:LYS:CA	1:A:11:LYS:C	19	1.6
(1,112)	1:A:59:GLU:C	1:A:60:CYS:N	1:A:60:CYS:CA	1:A:60:CYS:C	1	1.6
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	20	1.6
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	1	1.5
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	6	1.5
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	8	1.5
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	8	1.5
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	11	1.5
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	10	1.5
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	11	1.5
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	17	1.5
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	14	1.5
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	17	1.5
(1,58)	1:A:31:LEU:C	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	11	1.5
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	11	1.5
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	11	1.5
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	19	1.5
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	1	1.4
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	10	1.4
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	12	1.4
(1,87)	1:A:46:TYR:N	1:A:46:TYR:CA	1:A:46:TYR:C	1:A:47:SER:N	13	1.4
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	2	1.4
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	4	1.4
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	20	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	4	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	10	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	11	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	13	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	16	1.4
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	17	1.4
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	6	1.4
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	9	1.4
(1,112)	1:A:59:GLU:C	1:A:60:CYS:N	1:A:60:CYS:CA	1:A:60:CYS:C	8	1.4
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	13	1.4
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	12	1.4
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	15	1.4
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	2	1.3
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	10	1.3
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	1	1.3
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	7	1.3

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	12	1.3
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	14	1.3
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	15	1.3
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	12	1.3
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	18	1.3
(1,58)	1:A:31:LEU:C	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	14	1.3
(1,58)	1:A:31:LEU:C	1:A:32:ALA:N	1:A:32:ALA:CA	1:A:32:ALA:C	18	1.3
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	2	1.3
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	15	1.3
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	7	1.3
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	8	1.3
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	14	1.3
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	17	1.3
(1,22)	1:A:12:GLU:C	1:A:13:LYS:N	1:A:13:LYS:CA	1:A:13:LYS:C	17	1.3
(1,22)	1:A:12:GLU:C	1:A:13:LYS:N	1:A:13:LYS:CA	1:A:13:LYS:C	19	1.3
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	8	1.3
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	16	1.3
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	9	1.3
(1,95)	1:A:51:LEU:N	1:A:51:LEU:CA	1:A:51:LEU:C	1:A:52:GLN:N	8	1.2
(1,91)	1:A:49:LYS:N	1:A:49:LYS:CA	1:A:49:LYS:C	1:A:50:VAL:N	4	1.2
(1,91)	1:A:49:LYS:N	1:A:49:LYS:CA	1:A:49:LYS:C	1:A:50:VAL:N	5	1.2
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	9	1.2
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	13	1.2
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	16	1.2
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	19	1.2
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	20	1.2
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	6	1.2
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	8	1.2
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	13	1.2
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	16	1.2
(1,33)	1:A:18:LEU:N	1:A:18:LEU:CA	1:A:18:LEU:C	1:A:19:GLU:N	20	1.2
(1,110)	1:A:58:SER:C	1:A:59:GLU:N	1:A:59:GLU:CA	1:A:59:GLU:C	1	1.2
(1,10)	1:A:6:PHE:C	1:A:7:LYS:N	1:A:7:LYS:CA	1:A:7:LYS:C	19	1.2
(1,91)	1:A:49:LYS:N	1:A:49:LYS:CA	1:A:49:LYS:C	1:A:50:VAL:N	3	1.1
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	12	1.1
(1,89)	1:A:48:GLY:N	1:A:48:GLY:CA	1:A:48:GLY:C	1:A:49:LYS:N	13	1.1
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	5	1.1
(1,73)	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	1:A:40:SER:N	6	1.1
(1,72)	1:A:38:GLU:C	1:A:39:GLU:N	1:A:39:GLU:CA	1:A:39:GLU:C	6	1.1
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	12	1.1
(1,69)	1:A:37:CYS:N	1:A:37:CYS:CA	1:A:37:CYS:C	1:A:38:GLU:N	13	1.1
(1,56)	1:A:30:LYS:C	1:A:31:LEU:N	1:A:31:LEU:CA	1:A:31:LEU:C	15	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	1	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	4	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	5	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	7	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	16	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	18	1.1
(1,39)	1:A:21:SER:N	1:A:21:SER:CA	1:A:21:SER:C	1:A:22:ASN:N	19	1.1
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	2	1.1
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	4	1.1

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	5	1.1
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	12	1.1
(1,34)	1:A:18:LEU:C	1:A:19:GLU:N	1:A:19:GLU:CA	1:A:19:GLU:C	15	1.1
(1,22)	1:A:12:GLU:C	1:A:13:LYS:N	1:A:13:LYS:CA	1:A:13:LYS:C	9	1.1
(1,128)	1:A:68:VAL:C	1:A:69:VAL:N	1:A:69:VAL:CA	1:A:69:VAL:C	9	1.1
(1,104)	1:A:55:LYS:C	1:A:56:THR:N	1:A:56:THR:CA	1:A:56:THR:C	11	1.1
(1,104)	1:A:55:LYS:C	1:A:56:THR:N	1:A:56:THR:CA	1:A:56:THR:C	13	1.1
(1,101)	1:A:54:SER:N	1:A:54:SER:CA	1:A:54:SER:C	1:A:55:LYS:N	18	1.1