



Full wwPDB NMR Structure Validation Report ⓘ

Dec 25, 2024 – 02:57 AM EST

PDB ID : 2WCY
BMRB ID : 15996
Title : NMR solution structure of factor I-like modules of complement C7.
Authors : Phelan, M.M.; Thai, C.T.; Soares, D.C.; Ogata, R.T.; Barlow, P.N.; Bramham, J.
Deposited on : 2009-03-17

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.40

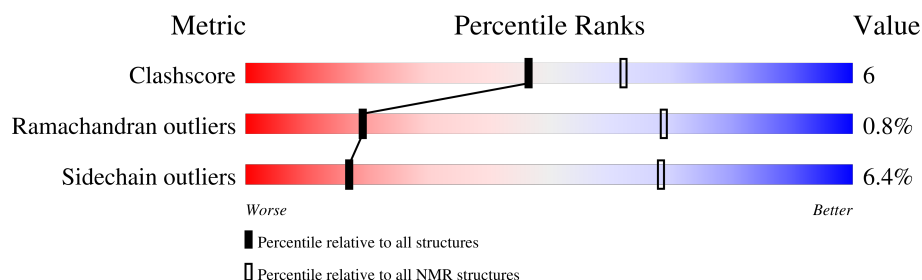
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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

Mol	Chain	Length	Quality of chain
1	A	155	

2 Ensemble composition and analysis

This entry contains 48 models. Model 44 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:701-A:766, A:778-A:780, A:790-A:840 (120)	1.00	44

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 8 clusters and 2 single-model clusters were found.

Cluster number	Models
1	4, 6, 8, 16, 17, 18, 20, 22, 23, 24, 33, 34, 37, 39, 44, 46
2	1, 3, 5, 7, 9, 10, 11, 13, 15, 19, 21, 28, 41
3	12, 38, 42, 43
4	14, 36, 40, 45
5	2, 32, 48
6	27, 29
7	35, 47
8	25, 26
Single-model clusters	30; 31

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2296 atoms, of which 1129 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT COMPONENT C7.

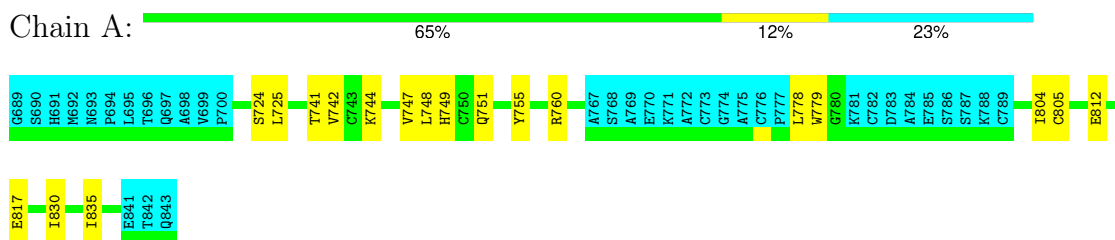
Mol	Chain	Residues	Atoms						Trace
1	A	155	Total	C	H	N	O	S	0
			2296	701	1129	214	230	22	

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: COMPLEMENT COMPONENT C7

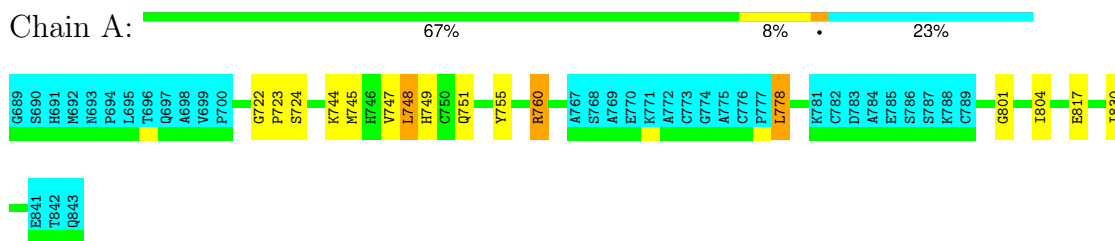


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

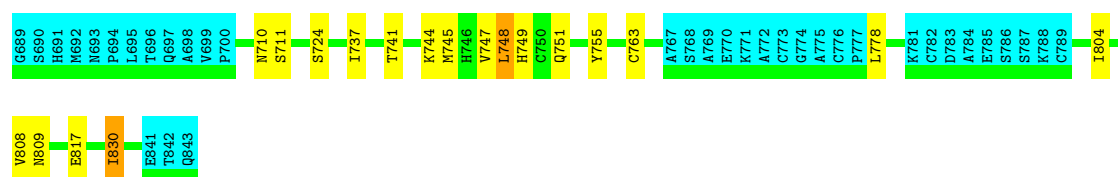
- Molecule 1: COMPLEMENT COMPONENT C7



4.2.2 Score per residue for model 2

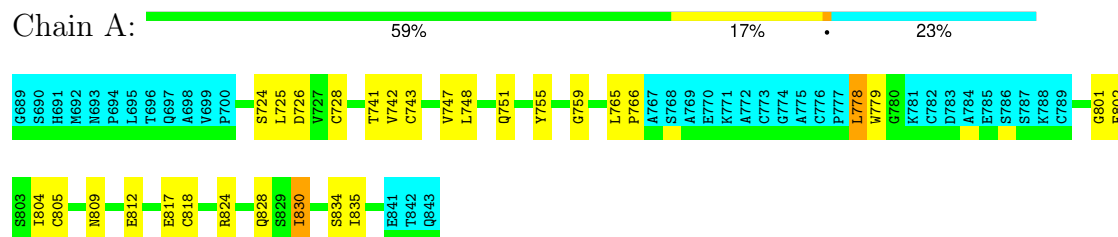
- Molecule 1: COMPLEMENT COMPONENT C7





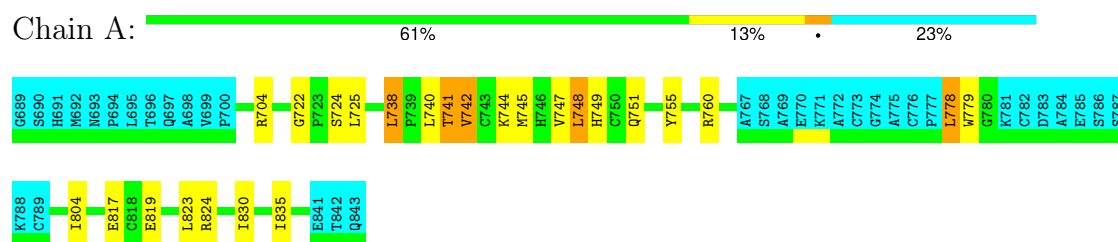
4.2.3 Score per residue for model 3

- Molecule 1: COMPLEMENT COMPONENT C7



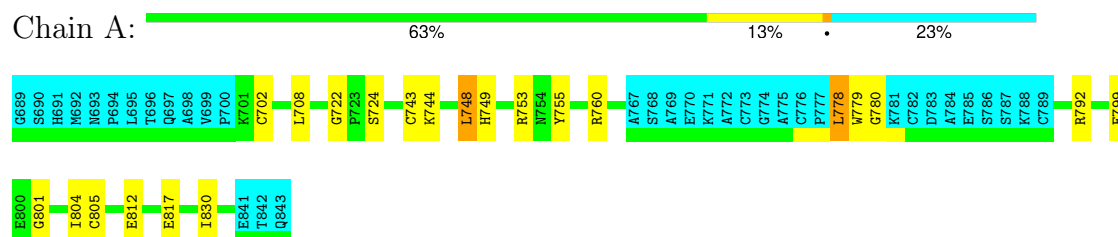
4.2.4 Score per residue for model 4

- Molecule 1: COMPLEMENT COMPONENT C7



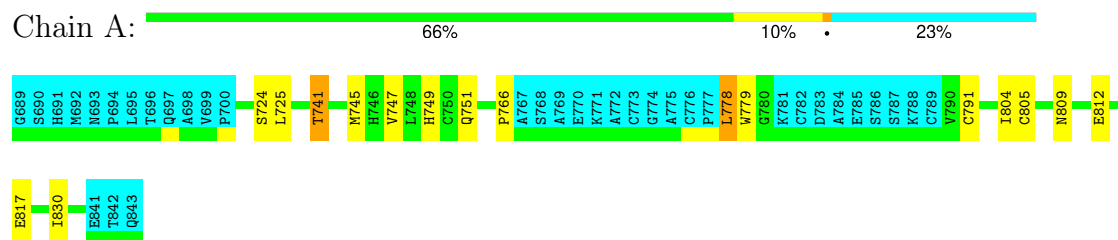
4.2.5 Score per residue for model 5

- Molecule 1: COMPLEMENT COMPONENT C7



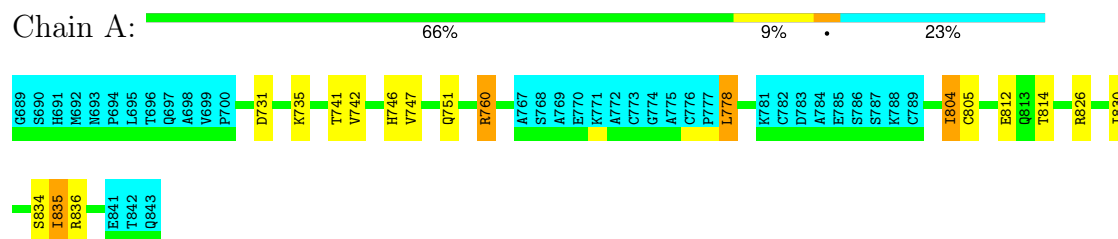
4.2.6 Score per residue for model 6

- Molecule 1: COMPLEMENT COMPONENT C7



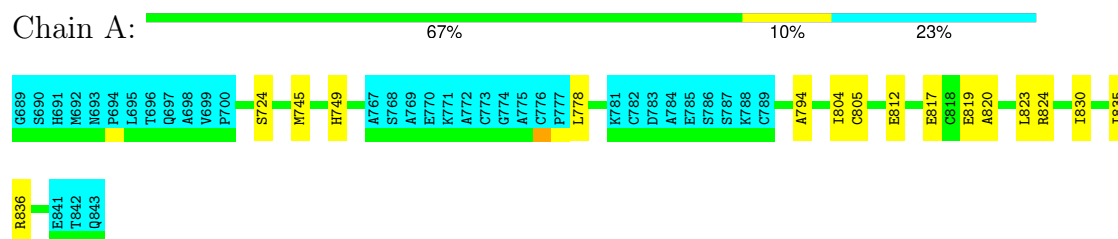
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT COMPONENT C7



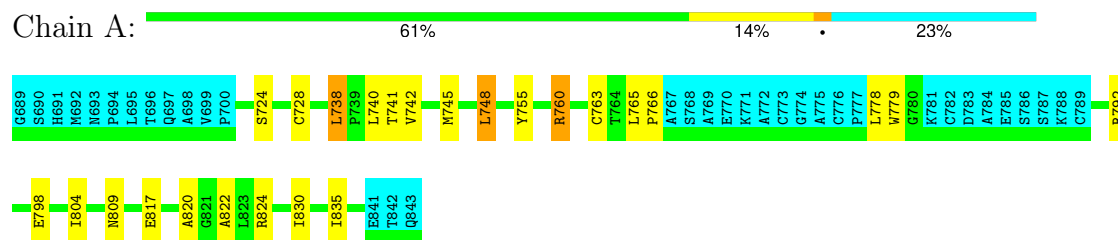
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT COMPONENT C7



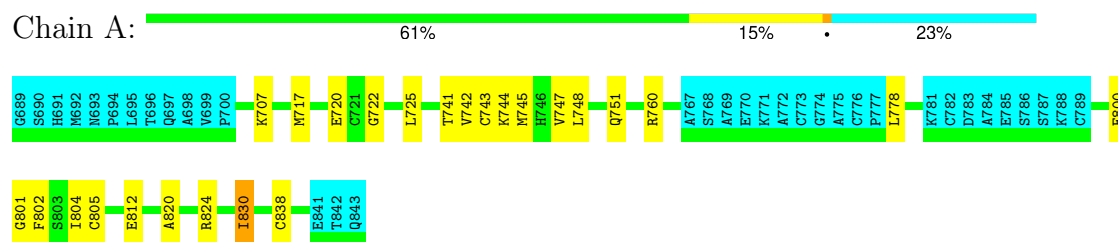
4.2.9 Score per residue for model 9

- Molecule 1: COMPLEMENT COMPONENT C7



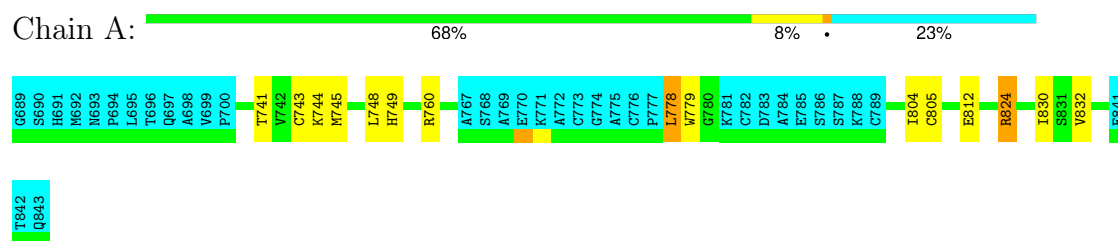
4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT COMPONENT C7



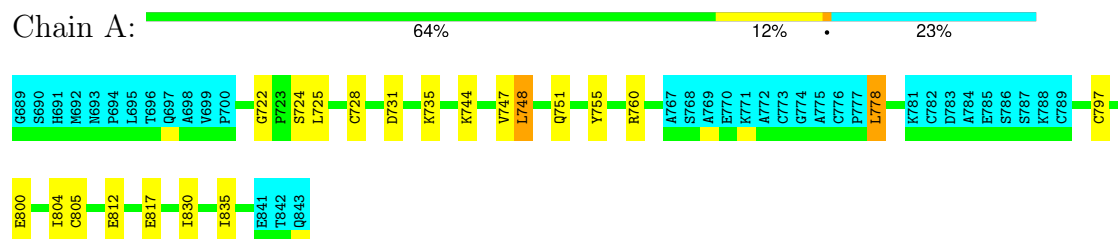
4.2.11 Score per residue for model 11

- Molecule 1: COMPLEMENT COMPONENT C7



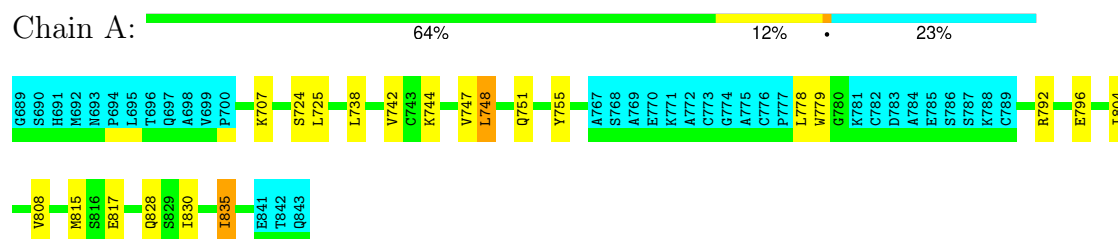
4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT COMPONENT C7



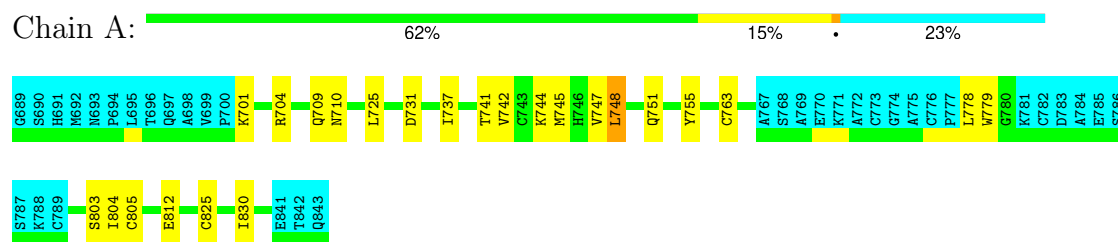
4.2.13 Score per residue for model 13

- Molecule 1: COMPLEMENT COMPONENT C7



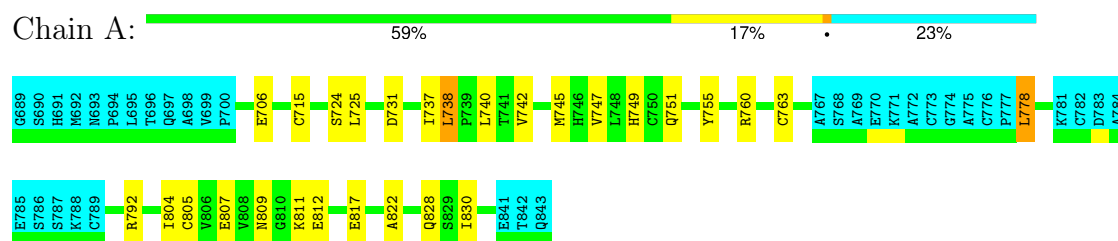
4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT COMPONENT C7



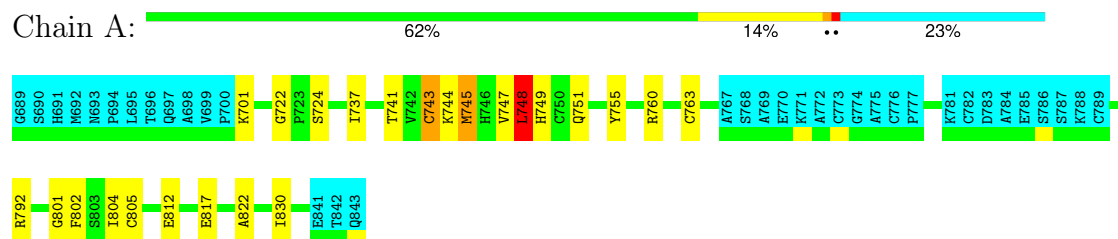
4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT COMPONENT C7



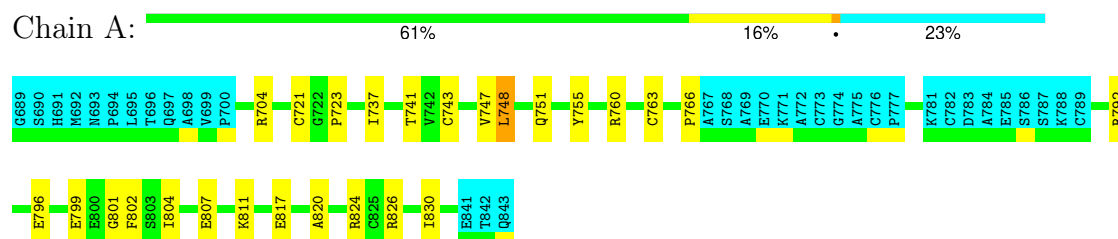
4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT COMPONENT C7



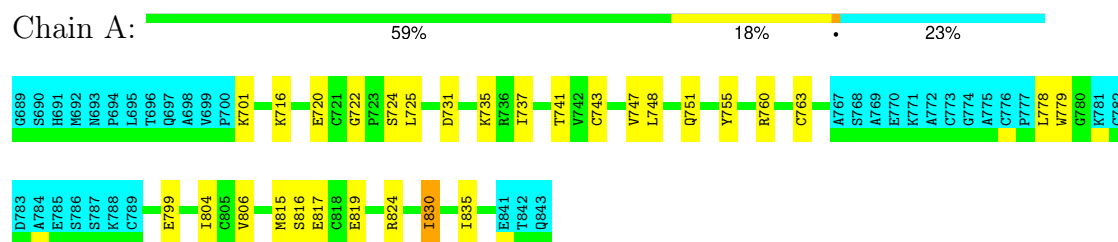
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT COMPONENT C7



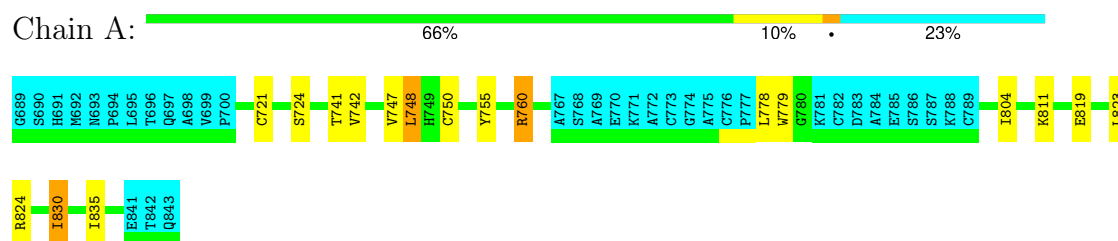
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT COMPONENT C7



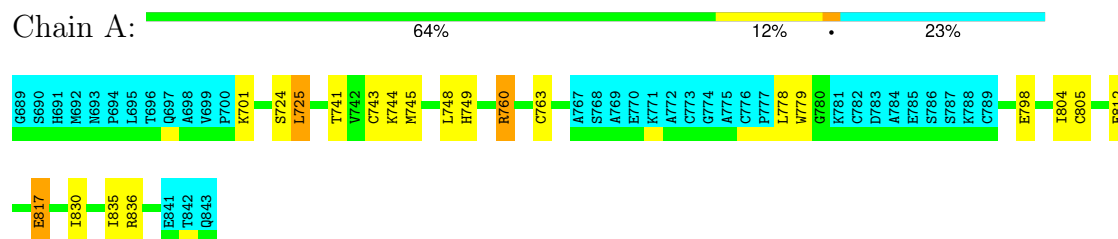
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT COMPONENT C7



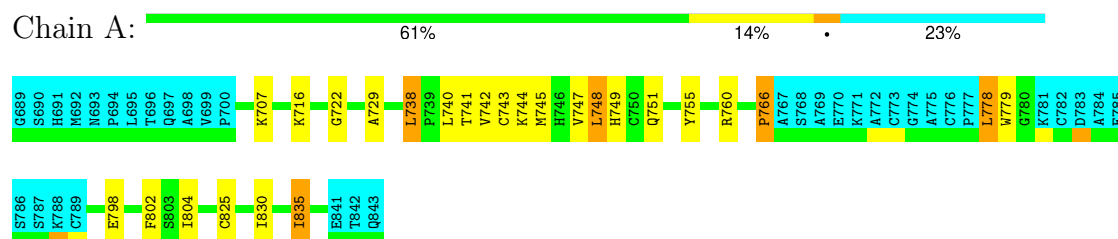
4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT COMPONENT C7



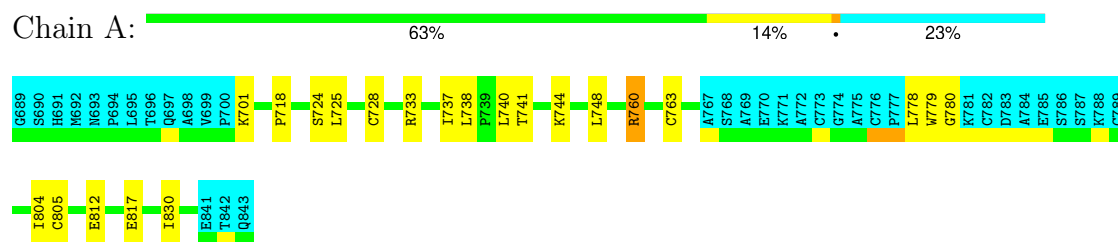
4.2.21 Score per residue for model 21

- Molecule 1: COMPLEMENT COMPONENT C7



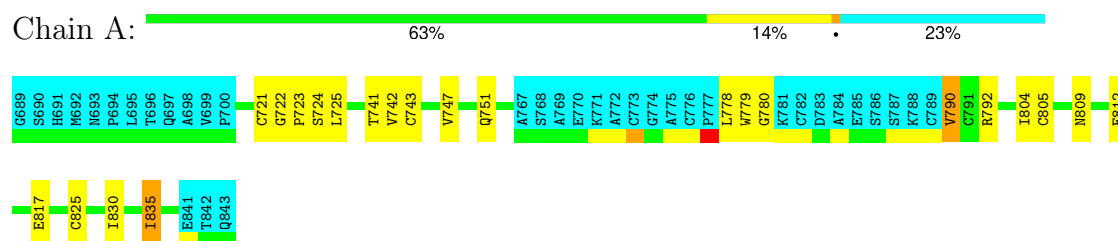
4.2.22 Score per residue for model 22

- Molecule 1: COMPLEMENT COMPONENT C7



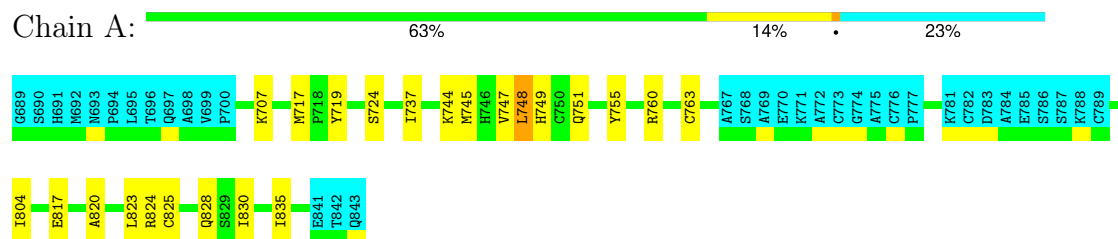
4.2.23 Score per residue for model 23

- Molecule 1: COMPLEMENT COMPONENT C7



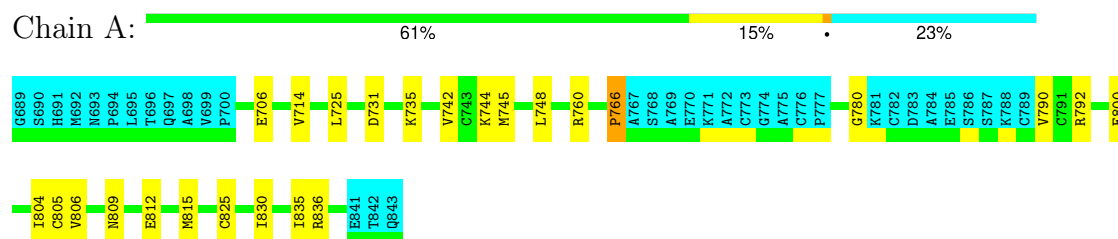
4.2.24 Score per residue for model 24

- Molecule 1: COMPLEMENT COMPONENT C7



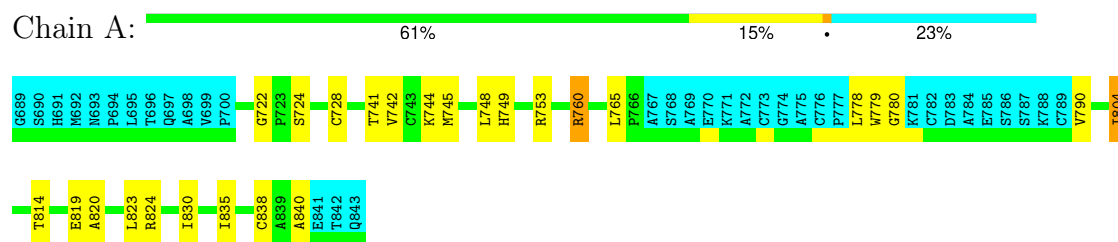
4.2.25 Score per residue for model 25

- Molecule 1: COMPLEMENT COMPONENT C7



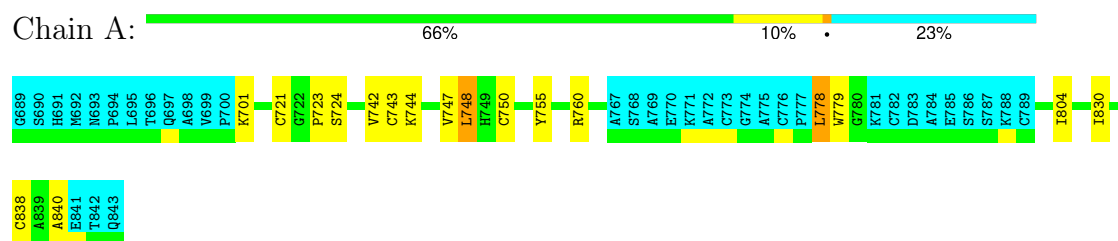
4.2.26 Score per residue for model 26

- Molecule 1: COMPLEMENT COMPONENT C7



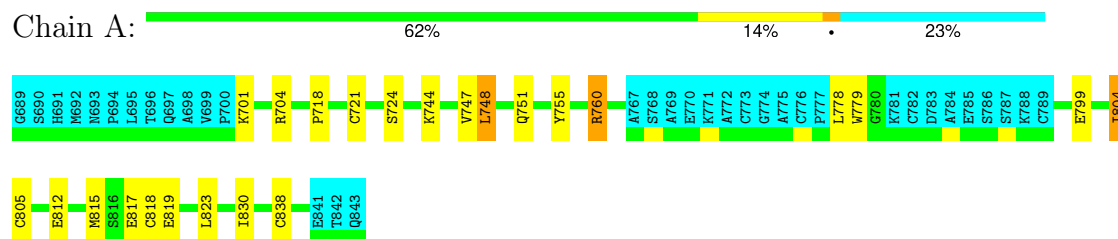
4.2.27 Score per residue for model 27

- Molecule 1: COMPLEMENT COMPONENT C7



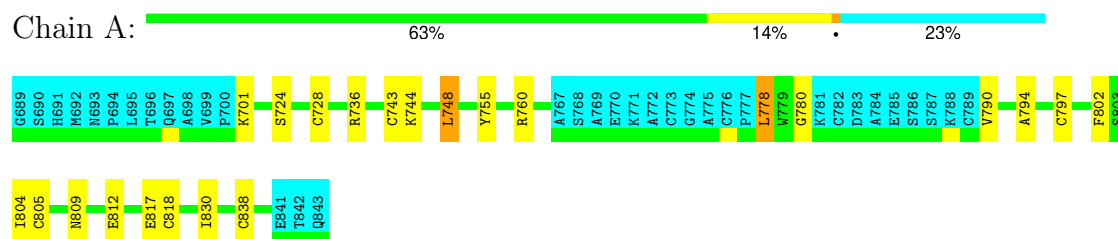
4.2.28 Score per residue for model 28

- Molecule 1: COMPLEMENT COMPONENT C7



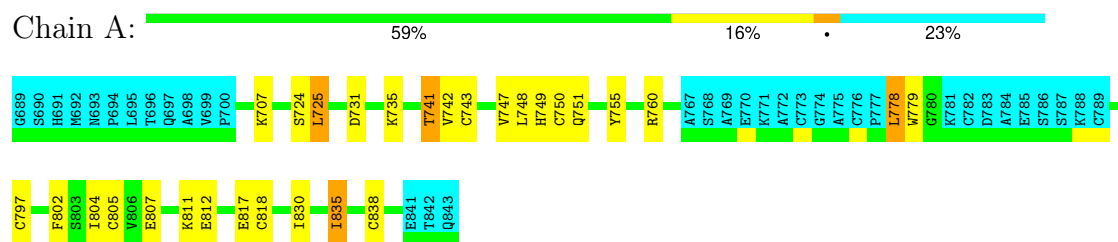
4.2.29 Score per residue for model 29

- Molecule 1: COMPLEMENT COMPONENT C7



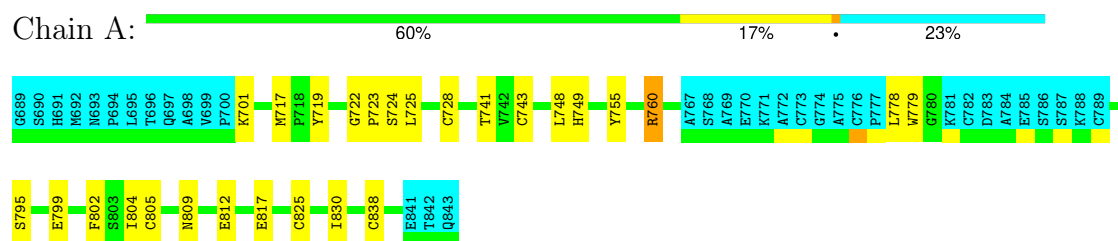
4.2.30 Score per residue for model 30

• Molecule 1: COMPLEMENT COMPONENT C7



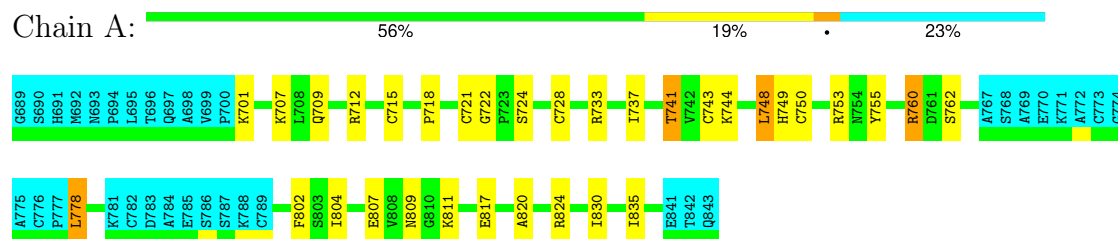
4.2.31 Score per residue for model 31

• Molecule 1: COMPLEMENT COMPONENT C7



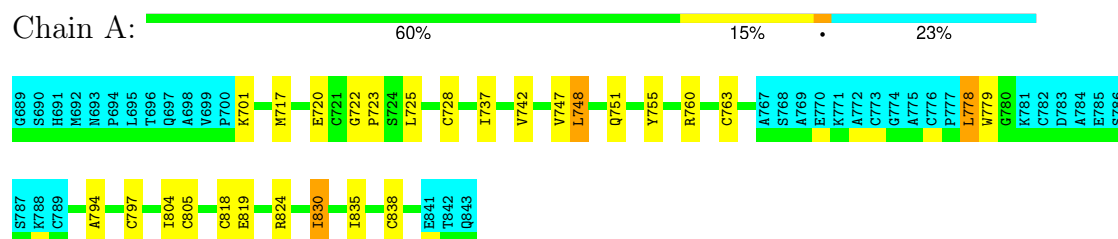
4.2.32 Score per residue for model 32

• Molecule 1: COMPLEMENT COMPONENT C7



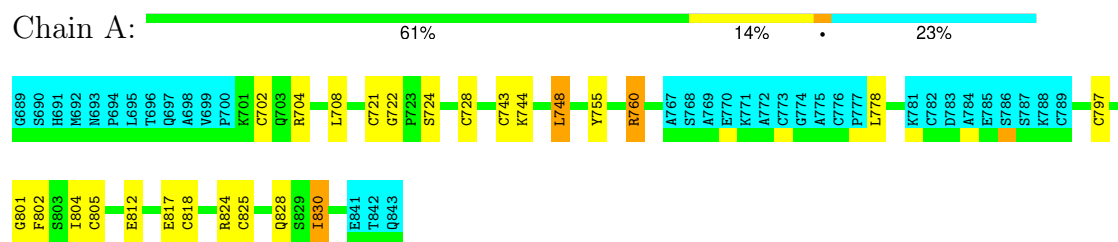
4.2.33 Score per residue for model 33

• Molecule 1: COMPLEMENT COMPONENT C7



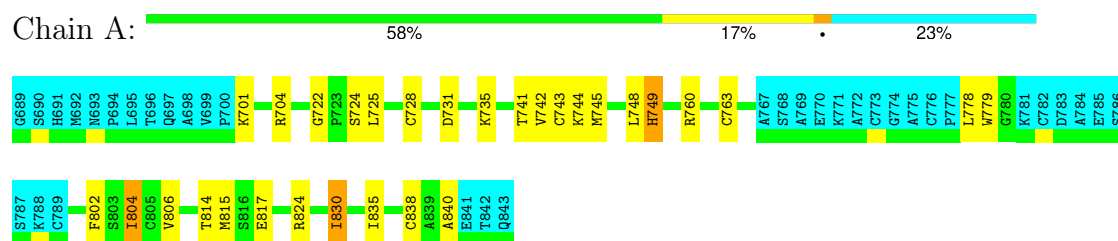
4.2.34 Score per residue for model 34

- Molecule 1: COMPLEMENT COMPONENT C7



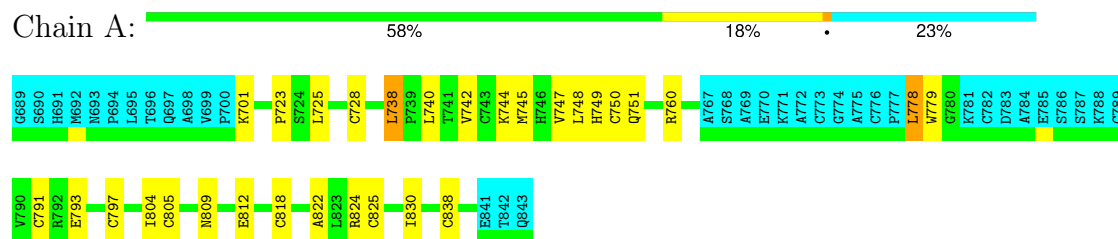
4.2.35 Score per residue for model 35

- Molecule 1: COMPLEMENT COMPONENT C7



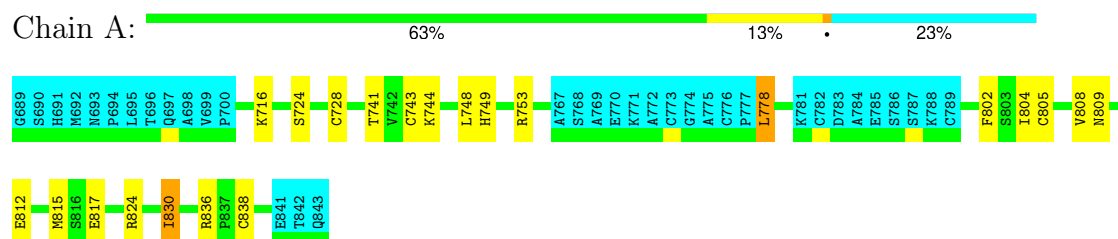
4.2.36 Score per residue for model 36

- Molecule 1: COMPLEMENT COMPONENT C7



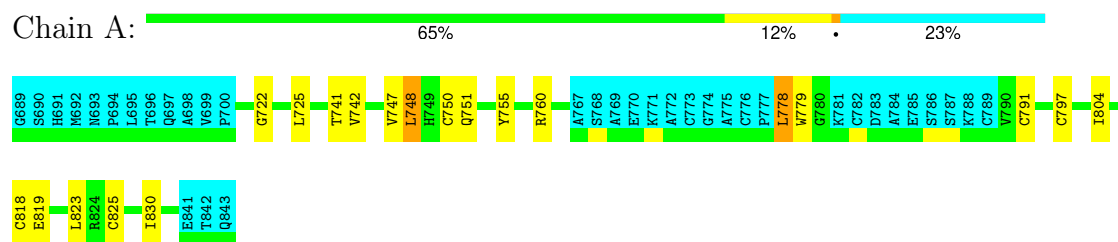
4.2.37 Score per residue for model 37

- Molecule 1: COMPLEMENT COMPONENT C7



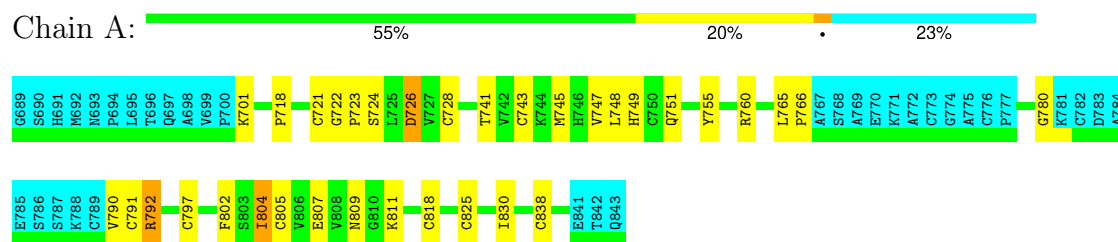
4.2.38 Score per residue for model 38

- Molecule 1: COMPLEMENT COMPONENT C7



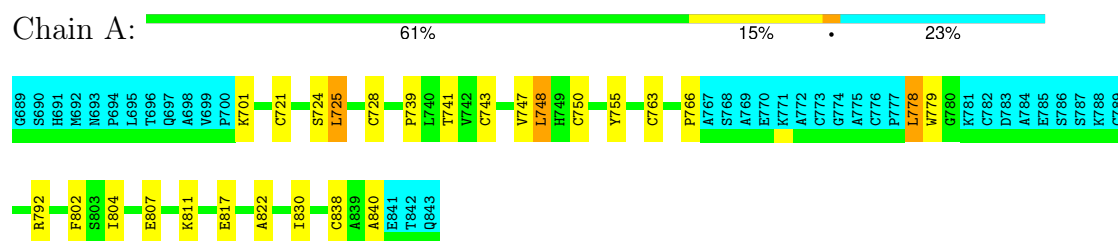
4.2.42 Score per residue for model 42

- Molecule 1: COMPLEMENT COMPONENT C7



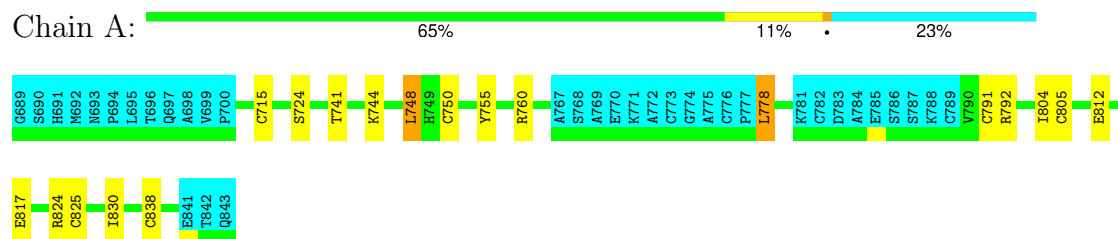
4.2.43 Score per residue for model 43

- Molecule 1: COMPLEMENT COMPONENT C7



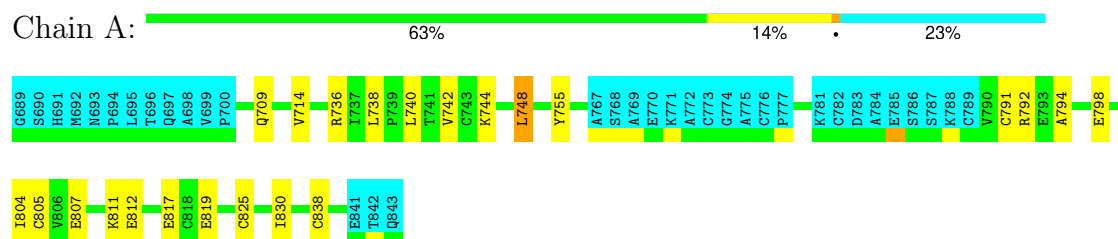
4.2.44 Score per residue for model 44 (medoid)

- Molecule 1: COMPLEMENT COMPONENT C7



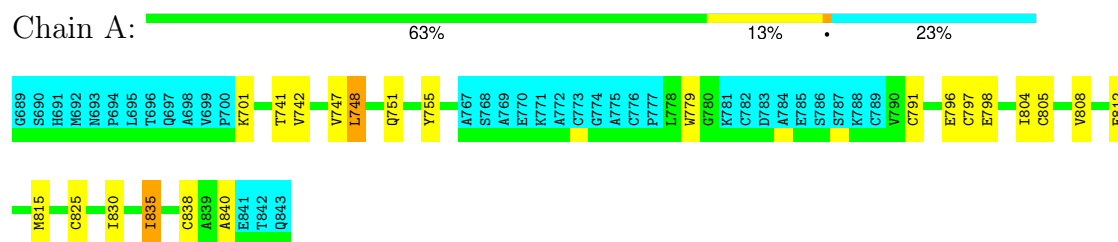
4.2.45 Score per residue for model 45

- Molecule 1: COMPLEMENT COMPONENT C7



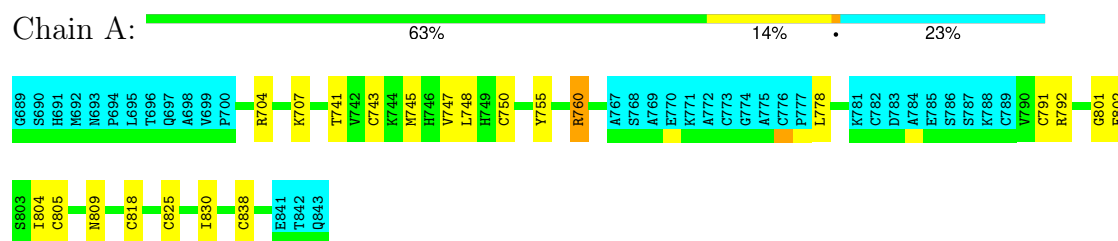
4.2.46 Score per residue for model 46

- Molecule 1: COMPLEMENT COMPONENT C7



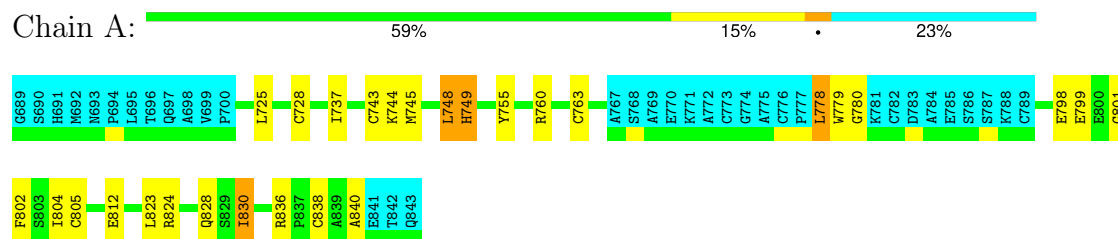
4.2.47 Score per residue for model 47

- Molecule 1: COMPLEMENT COMPONENT C7



4.2.48 Score per residue for model 48

- Molecule 1: COMPLEMENT COMPONENT C7



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, RESTRAINED MOLECULAR DYNAMICS*.

Of the 200 calculated structures, 48 were deposited, based on the following criterion: *CONVERGED DATASETS OF 100 STRUCTURES EACH (1-25 AND 26-48)*.

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

Software name	Classification	Version
CNS	refinement	1.2
TopSpin	structure solution	1.3
CcpNmr Analysis	structure solution	1.0.15
CYANA	structure solution	2.1
CNS	structure solution	1.2

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	1676
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.86±0.02	0±0/938 (0.0± 0.0%)	0.69±0.03	0±0/1263 (0.0± 0.0%)
All	All	0.86	0/45024 (0.0%)	0.69	1/60624 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.4±0.6
All	All	0	17

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	748	LEU	CA-CB-CG	5.05	126.91	115.30	16	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	760	ARG	Sidechain	5
1	A	824	ARG	Sidechain	4
1	A	792	ARG	Sidechain	4
1	A	836	ARG	Sidechain	2
1	A	826	ARG	Sidechain	1
1	A	704	ARG	Sidechain	1

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	924	900	912	11±3
All	All	44352	43200	43426	519

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:728:CYS:SG	1:A:760:ARG:HA	0.75	2.21	26	10
1:A:794:ALA:HB1	1:A:819:GLU:HG2	0.75	1.58	33	1
1:A:725:LEU:HD13	1:A:779:TRP:CH2	0.69	2.22	3	5
1:A:738:LEU:HD13	1:A:740:LEU:HG	0.68	1.63	15	3
1:A:797:CYS:SG	1:A:818:CYS:HB2	0.68	2.28	42	5
1:A:797:CYS:SG	1:A:800:GLU:HA	0.68	2.29	12	1
1:A:724:SER:OG	1:A:742:VAL:HB	0.67	1.89	27	2
1:A:748:LEU:HD11	1:A:755:TYR:CD1	0.65	2.25	16	6
1:A:808:VAL:HG21	1:A:815:MET:HE1	0.65	1.69	37	3
1:A:748:LEU:HD11	1:A:755:TYR:CD2	0.65	2.25	14	4
1:A:721:CYS:SG	1:A:743:CYS:HB2	0.63	2.33	43	1
1:A:778:LEU:H	1:A:778:LEU:HD23	0.62	1.54	36	12
1:A:805:CYS:SG	1:A:812:GLU:HB3	0.62	2.35	40	28
1:A:724:SER:HA	1:A:817:GLU:CD	0.61	2.16	4	17
1:A:748:LEU:HD21	1:A:755:TYR:CD1	0.60	2.32	30	11
1:A:743:CYS:HA	1:A:802:PHE:CZ	0.59	2.32	42	10
1:A:824:ARG:HG2	1:A:830:ILE:HD11	0.59	1.74	34	6
1:A:838:CYS:SG	1:A:840:ALA:HB3	0.59	2.37	48	6
1:A:728:CYS:SG	1:A:739:PRO:HA	0.59	2.37	43	1
1:A:748:LEU:HD21	1:A:755:TYR:CD2	0.59	2.32	12	11
1:A:743:CYS:HA	1:A:802:PHE:CE1	0.59	2.32	17	3
1:A:724:SER:HA	1:A:817:GLU:OE1	0.58	1.98	18	7
1:A:724:SER:HA	1:A:817:GLU:OE2	0.58	1.99	9	6
1:A:805:CYS:SG	1:A:838:CYS:HB2	0.57	2.39	42	11
1:A:724:SER:OG	1:A:741:THR:HB	0.57	2.00	42	2
1:A:742:VAL:HG23	1:A:835:ILE:HB	0.57	1.77	35	10
1:A:824:ARG:HD2	1:A:830:ILE:HD11	0.56	1.75	37	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:744:LYS:O	1:A:748:LEU:HB3	0.56	2.00	2	19
1:A:728:CYS:SG	1:A:737:ILE:HG22	0.56	2.40	48	2
1:A:724:SER:HB2	1:A:741:THR:HG22	0.56	1.78	31	6
1:A:743:CYS:HA	1:A:802:PHE:CE2	0.56	2.34	31	4
1:A:728:CYS:SG	1:A:763:CYS:HB3	0.56	2.41	41	4
1:A:791:CYS:SG	1:A:825:CYS:HB3	0.56	2.41	44	6
1:A:791:CYS:HB3	1:A:825:CYS:SG	0.55	2.42	38	2
1:A:838:CYS:SG	1:A:840:ALA:HB2	0.54	2.42	46	1
1:A:728:CYS:SG	1:A:765:LEU:HD13	0.54	2.42	42	5
1:A:738:LEU:CD1	1:A:740:LEU:HG	0.54	2.32	15	5
1:A:725:LEU:HD13	1:A:817:GLU:HG3	0.54	1.80	4	1
1:A:778:LEU:HB2	1:A:779:TRP:CE3	0.53	2.38	18	6
1:A:745:MET:O	1:A:749:HIS:HB2	0.53	2.03	21	16
1:A:820:ALA:O	1:A:824:ARG:HG3	0.53	2.04	9	8
1:A:778:LEU:HG	1:A:779:TRP:CE3	0.53	2.38	40	11
1:A:737:ILE:HG22	1:A:763:CYS:HB3	0.53	1.80	14	8
1:A:724:SER:OG	1:A:743:CYS:HB3	0.53	2.04	41	1
1:A:780:GLY:HA2	1:A:790:VAL:O	0.53	2.04	23	3
1:A:747:VAL:O	1:A:751:GLN:HG3	0.52	2.04	4	9
1:A:824:ARG:HB3	1:A:830:ILE:HD11	0.52	1.81	3	1
1:A:819:GLU:O	1:A:823:LEU:HG	0.51	2.05	41	7
1:A:731:ASP:O	1:A:735:LYS:HA	0.51	2.06	35	6
1:A:738:LEU:HD23	1:A:740:LEU:HG	0.51	1.82	21	2
1:A:747:VAL:HA	1:A:750:CYS:SG	0.51	2.45	43	7
1:A:742:VAL:HG13	1:A:817:GLU:OE2	0.51	2.05	9	1
1:A:792:ARG:HD2	1:A:796:GLU:OE2	0.51	2.06	39	1
1:A:779:TRP:HA	1:A:797:CYS:SG	0.51	2.44	46	2
1:A:805:CYS:HB2	1:A:836:ARG:O	0.50	2.07	25	1
1:A:794:ALA:HA	1:A:797:CYS:SG	0.50	2.46	29	1
1:A:717:MET:O	1:A:720:GLU:HG3	0.50	2.06	33	1
1:A:718:PRO:HA	1:A:721:CYS:SG	0.50	2.45	28	3
1:A:807:GLU:HA	1:A:811:LYS:O	0.50	2.06	42	7
1:A:747:VAL:O	1:A:751:GLN:HG2	0.50	2.07	46	16
1:A:749:HIS:HA	1:A:753:ARG:O	0.49	2.08	40	4
1:A:823:LEU:HD23	1:A:828:GLN:HG2	0.49	1.84	24	2
1:A:741:THR:OG1	1:A:744:LYS:HD3	0.49	2.06	41	1
1:A:728:CYS:HB2	1:A:759:GLY:O	0.49	2.07	3	1
1:A:744:LYS:O	1:A:748:LEU:HG	0.49	2.06	35	10
1:A:725:LEU:CD2	1:A:817:GLU:HG3	0.49	2.37	23	1
1:A:792:ARG:HA	1:A:792:ARG:NE	0.49	2.23	44	2
1:A:717:MET:HB2	1:A:720:GLU:CG	0.49	2.38	33	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:743:CYS:SG	1:A:744:LYS:N	0.49	2.86	20	1
1:A:702:CYS:SG	1:A:708:LEU:HB2	0.49	2.48	34	2
1:A:778:LEU:H	1:A:778:LEU:HD13	0.48	1.67	3	11
1:A:792:ARG:O	1:A:822:ALA:HB1	0.48	2.08	9	4
1:A:709:GLN:CD	1:A:710:ASN:HB2	0.48	2.29	14	1
1:A:731:ASP:HA	1:A:755:TYR:CE1	0.48	2.44	14	1
1:A:725:LEU:HD22	1:A:779:TRP:CH2	0.48	2.43	20	1
1:A:806:VAL:HG11	1:A:815:MET:SD	0.47	2.48	25	3
1:A:721:CYS:HB2	1:A:743:CYS:SG	0.47	2.49	27	2
1:A:742:VAL:HG13	1:A:817:GLU:OE1	0.47	2.10	35	1
1:A:715:CYS:HB3	1:A:750:CYS:SG	0.47	2.49	40	2
1:A:709:GLN:OE1	1:A:714:VAL:HG22	0.47	2.10	45	1
1:A:725:LEU:HD23	1:A:779:TRP:CH2	0.47	2.45	48	2
1:A:792:ARG:HE	1:A:796:GLU:HG3	0.47	1.70	13	1
1:A:824:ARG:HA	1:A:830:ILE:HD11	0.47	1.86	18	1
1:A:778:LEU:HD12	1:A:778:LEU:H	0.47	1.69	22	1
1:A:748:LEU:HD11	1:A:755:TYR:CG	0.47	2.45	42	3
1:A:717:MET:HB3	1:A:719:TYR:CE1	0.46	2.45	31	1
1:A:725:LEU:O	1:A:742:VAL:HG23	0.46	2.11	10	7
1:A:731:ASP:HA	1:A:755:TYR:CE2	0.46	2.46	15	1
1:A:716:LYS:NZ	1:A:720:GLU:HB3	0.46	2.25	18	1
1:A:725:LEU:HD23	1:A:817:GLU:HG3	0.46	1.88	20	1
1:A:701:LYS:N	1:A:701:LYS:HD2	0.46	2.25	27	1
1:A:704:ARG:HA	1:A:704:ARG:CZ	0.46	2.39	47	1
1:A:794:ALA:HB1	1:A:819:GLU:HG3	0.46	1.85	45	3
1:A:721:CYS:SG	1:A:744:LYS:HA	0.46	2.50	34	1
1:A:709:GLN:HE22	1:A:714:VAL:HG11	0.46	1.71	45	1
1:A:726:ASP:O	1:A:765:LEU:HD21	0.45	2.11	3	1
1:A:723:PRO:CB	1:A:778:LEU:HG	0.45	2.42	41	1
1:A:834:SER:OG	1:A:836:ARG:HG2	0.45	2.11	7	1
1:A:760:ARG:HA	1:A:763:CYS:SG	0.45	2.51	20	2
1:A:748:LEU:HD11	1:A:755:TYR:CZ	0.45	2.46	30	1
1:A:709:GLN:O	1:A:712:ARG:HG2	0.45	2.12	32	1
1:A:748:LEU:HD12	1:A:749:HIS:N	0.45	2.26	37	1
1:A:742:VAL:HG13	1:A:835:ILE:HB	0.45	1.89	21	2
1:A:706:GLU:HA	1:A:714:VAL:O	0.45	2.11	25	1
1:A:724:SER:HG	1:A:743:CYS:HB3	0.45	1.70	41	1
1:A:742:VAL:HG22	1:A:835:ILE:HB	0.45	1.88	30	1
1:A:717:MET:O	1:A:720:GLU:HB3	0.44	2.11	10	1
1:A:824:ARG:CG	1:A:830:ILE:HD11	0.44	2.43	34	1
1:A:715:CYS:SG	1:A:750:CYS:HB3	0.44	2.53	32	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:725:LEU:HD12	1:A:779:TRP:CZ3	0.44	2.48	38	1
1:A:724:SER:CB	1:A:741:THR:HG22	0.44	2.42	44	1
1:A:742:VAL:CG2	1:A:835:ILE:HB	0.44	2.42	7	1
1:A:745:MET:HG3	1:A:835:ILE:HD13	0.43	1.90	20	1
1:A:726:ASP:OD2	1:A:765:LEU:HG	0.43	2.12	42	1
1:A:745:MET:HG2	1:A:835:ILE:CD1	0.43	2.43	26	2
1:A:741:THR:HB	1:A:743:CYS:SG	0.43	2.54	20	1
1:A:704:ARG:HD2	1:A:801:GLY:O	0.43	2.14	34	1
1:A:742:VAL:HB	1:A:817:GLU:OE2	0.43	2.13	45	1
1:A:745:MET:CG	1:A:835:ILE:HD13	0.43	2.43	20	1
1:A:804:ILE:O	1:A:814:THR:HA	0.43	2.13	35	3
1:A:721:CYS:O	1:A:723:PRO:HD2	0.43	2.14	17	1
1:A:704:ARG:HD3	1:A:801:GLY:O	0.43	2.14	17	1
1:A:778:LEU:HG	1:A:779:TRP:CZ3	0.43	2.48	33	2
1:A:725:LEU:HD12	1:A:779:TRP:CH2	0.43	2.49	31	1
1:A:728:CYS:HB2	1:A:763:CYS:SG	0.43	2.54	35	2
1:A:801:GLY:HA3	1:A:817:GLU:OE1	0.43	2.14	39	1
1:A:725:LEU:HD22	1:A:817:GLU:HG3	0.43	1.91	23	1
1:A:716:LYS:O	1:A:747:VAL:HG13	0.42	2.14	21	1
1:A:792:ARG:HB3	1:A:796:GLU:HB2	0.42	1.91	41	1
1:A:805:CYS:SG	1:A:838:CYS:HB3	0.42	2.55	31	3
1:A:778:LEU:HB2	1:A:818:CYS:SG	0.42	2.55	47	1
1:A:808:VAL:HG22	1:A:830:ILE:HG22	0.42	1.90	2	1
1:A:801:GLY:HA3	1:A:817:GLU:HB3	0.42	1.92	17	1
1:A:745:MET:HA	1:A:748:LEU:HB3	0.42	1.91	9	1
1:A:792:ARG:HD2	1:A:796:GLU:CD	0.42	2.35	17	1
1:A:804:ILE:HD13	1:A:804:ILE:H	0.42	1.73	28	2
1:A:793:GLU:HA	1:A:822:ALA:CB	0.42	2.44	36	1
1:A:706:GLU:HG2	1:A:715:CYS:SG	0.42	2.54	15	1
1:A:704:ARG:HA	1:A:704:ARG:NE	0.42	2.30	47	1
1:A:725:LEU:HD23	1:A:817:GLU:HG2	0.42	1.92	18	1
1:A:778:LEU:HD12	1:A:818:CYS:SG	0.42	2.54	28	2
1:A:728:CYS:SG	1:A:737:ILE:CG2	0.41	3.07	33	2
1:A:717:MET:C	1:A:747:VAL:HG11	0.41	2.36	39	1
1:A:725:LEU:O	1:A:742:VAL:HG12	0.41	2.14	40	1
1:A:725:LEU:HD22	1:A:817:GLU:CG	0.41	2.45	30	1
1:A:778:LEU:HD21	1:A:779:TRP:CZ3	0.41	2.50	35	1
1:A:746:HIS:NE2	1:A:835:ILE:HG12	0.41	2.31	7	1
1:A:717:MET:HB3	1:A:719:TYR:CE2	0.41	2.51	24	1
1:A:778:LEU:H	1:A:778:LEU:CD1	0.41	2.29	9	1
1:A:778:LEU:HA	1:A:799:GLU:HB3	0.41	1.93	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:815:MET:HB3	1:A:819:GLU:HG3	0.41	1.91	28	1
1:A:728:CYS:CB	1:A:763:CYS:SG	0.41	3.08	43	1
1:A:725:LEU:HB2	1:A:817:GLU:HG3	0.41	1.93	6	1
1:A:729:ALA:O	1:A:738:LEU:HD22	0.41	2.15	21	1
1:A:718:PRO:O	1:A:744:LYS:HG2	0.41	2.16	22	1
1:A:797:CYS:HB3	1:A:818:CYS:SG	0.41	2.56	33	1
1:A:824:ARG:NH2	1:A:832:VAL:HG21	0.41	2.31	11	1
1:A:723:PRO:HB2	1:A:778:LEU:CD2	0.41	2.46	27	1
1:A:737:ILE:HG21	1:A:762:SER:CB	0.41	2.45	32	1
1:A:724:SER:HB3	1:A:741:THR:CG2	0.40	2.46	4	1
1:A:724:SER:OG	1:A:743:CYS:HB2	0.40	2.16	30	1
1:A:778:LEU:H	1:A:778:LEU:HD12	0.40	1.76	31	1
1:A:805:CYS:HB3	1:A:834:SER:OG	0.40	2.16	3	1
1:A:816:SER:O	1:A:819:GLU:HB3	0.40	2.16	18	1
1:A:760:ARG:HD2	1:A:760:ARG:C	0.40	2.36	30	1
1:A:724:SER:HB2	1:A:741:THR:HB	0.40	1.94	6	1
1:A:748:LEU:HD21	1:A:755:TYR:CE2	0.40	2.52	33	1
1:A:797:CYS:CB	1:A:818:CYS:HB2	0.40	2.46	38	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	120/155 (77%)	112±2 (93±2%)	7±2 (6±2%)	1±1 (1±1%)	19	69
All	All	5760/7440 (77%)	5373 (93%)	340 (6%)	47 (1%)	19	69

All 10 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	722	GLY	17
1	A	766	PRO	9
1	A	801	GLY	8
1	A	723	PRO	6

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Mol	Chain	Res	Type	Models (Total)
1	A	800	GLU	2
1	A	710	ASN	1
1	A	711	SER	1
1	A	799	GLU	1
1	A	798	GLU	1
1	A	701	LYS	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	106/133 (80%)	99±1 (94±1%)	7±1 (6±1%)	17	68
All	All	5088/6384 (80%)	4763 (94%)	325 (6%)	17	68

All 40 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	804	ILE	48
1	A	830	ILE	48
1	A	760	ARG	31
1	A	778	LEU	29
1	A	748	LEU	27
1	A	741	THR	24
1	A	701	LYS	15
1	A	809	ASN	14
1	A	835	ILE	14
1	A	707	LYS	7
1	A	738	LEU	6
1	A	743	CYS	5
1	A	799	GLU	5
1	A	798	GLU	5
1	A	725	LEU	5
1	A	828	GLN	4
1	A	745	MET	4
1	A	749	HIS	4
1	A	704	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	742	VAL	2
1	A	836	ARG	2
1	A	721	CYS	2
1	A	766	PRO	2
1	A	733	ARG	2
1	A	736	ARG	2
1	A	818	CYS	1
1	A	791	CYS	1
1	A	838	CYS	1
1	A	803	SER	1
1	A	826	ARG	1
1	A	811	LYS	1
1	A	817	GLU	1
1	A	790	VAL	1
1	A	795	SER	1
1	A	716	LYS	1
1	A	728	CYS	1
1	A	753	ARG	1
1	A	802	PHE	1
1	A	726	ASP	1
1	A	796	GLU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 89% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1676
Number of shifts mapped to atoms	1676
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	-0.09 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	136	0.32 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	136	-0.94 ± 0.37	Should be applied
^{15}N	137	0.16 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 89%, i.e. 1404 atoms were assigned a chemical shift out of a possible 1578. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	590/598 (99%)	241/243 (99%)	235/240 (98%)	114/115 (99%)
Sidechain	762/912 (84%)	518/588 (88%)	226/279 (81%)	18/45 (40%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	52/68 (76%)	26/33 (79%)	24/29 (83%)	2/6 (33%)
Overall	1404/1578 (89%)	785/864 (91%)	485/548 (89%)	134/166 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1676 atoms were assigned a chemical shift out of a possible 1971. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	713/769 (93%)	293/312 (94%)	283/310 (91%)	137/147 (93%)
Sidechain	909/1126 (81%)	619/727 (85%)	270/348 (78%)	20/51 (39%)
Aromatic	54/76 (71%)	27/37 (73%)	25/31 (81%)	2/8 (25%)
Overall	1676/1971 (85%)	939/1076 (87%)	578/689 (84%)	159/206 (77%)

7.1.4 Statistically unusual chemical shifts [i](#)

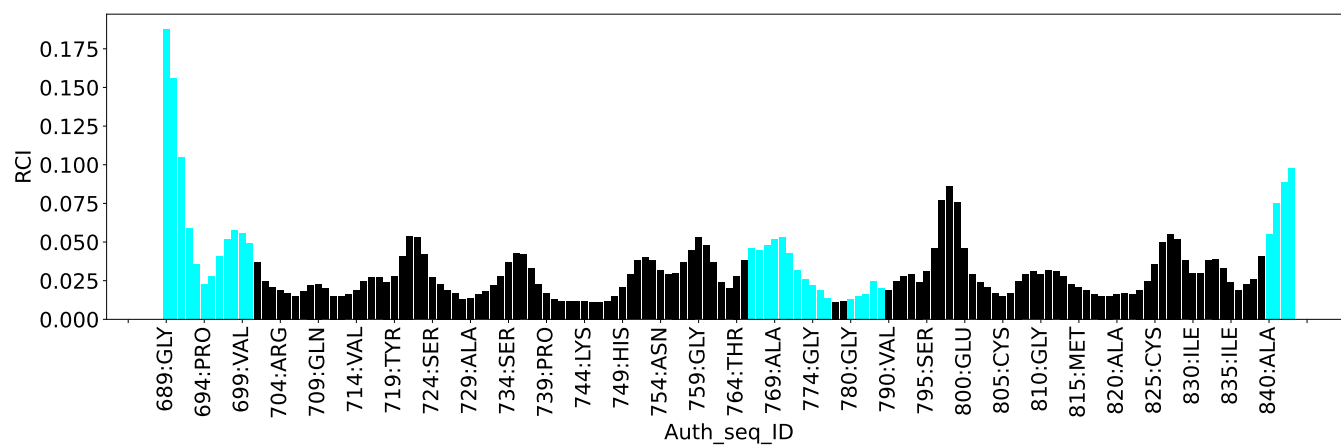
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	703	GLN	HB2	-0.16	0.80 – 3.29	-8.9
1	A	792	ARG	HG2	-0.34	0.26 – 2.87	-7.3
1	A	703	GLN	HB3	0.27	0.71 – 3.33	-6.7
1	A	744	LYS	CE	36.15	37.57 – 46.21	-6.6

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	2739
Intra-residue ($ i-j =0$)	618
Sequential ($ i-j =1$)	770
Medium range ($ i-j >1$ and $ i-j <5$)	401
Long range ($ i-j \geq 5$)	911
Inter-chain	0
Hydrogen bond restraints	28
Disulfide bond restraints	11
Total dihedral-angle restraints	154
Number of unmapped restraints	0
Number of restraints per residue	18.7
Number of long range restraints per residue ¹	6.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	13.9	0.2
0.2-0.5 (Medium)	1.8	0.39
>0.5 (Large)	5.5	5.93

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)	5.6	6.71
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis ⓘ

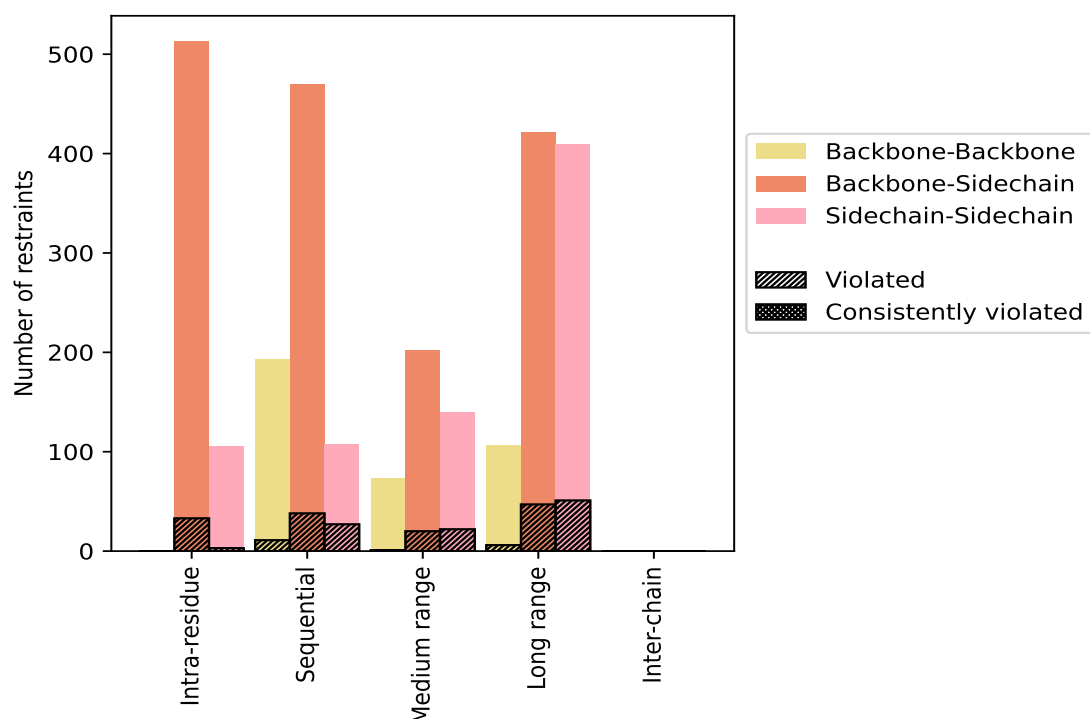
9.1 Summary of distance violations ⓘ

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	618	22.6	36	5.8	1.3	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	513	18.7	33	6.4	1.2	0	0.0	0.0
Sidechain-Sidechain	105	3.8	3	2.9	0.1	0	0.0	0.0
Sequential ($i-j =1$)	770	28.1	76	9.9	2.8	0	0.0	0.0
Backbone-Backbone	193	7.0	11	5.7	0.4	0	0.0	0.0
Backbone-Sidechain	470	17.2	38	8.1	1.4	0	0.0	0.0
Sidechain-Sidechain	107	3.9	27	25.2	1.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	401	14.6	41	10.2	1.5	0	0.0	0.0
Backbone-Backbone	73	2.7	1	1.4	0.0	0	0.0	0.0
Backbone-Sidechain	190	6.9	20	10.5	0.7	0	0.0	0.0
Sidechain-Sidechain	138	5.0	20	14.5	0.7	0	0.0	0.0
Long range ($i-j \geq 5$)	911	33.3	94	10.3	3.4	0	0.0	0.0
Backbone-Backbone	106	3.9	6	5.7	0.2	0	0.0	0.0
Backbone-Sidechain	405	14.8	46	11.4	1.7	0	0.0	0.0
Sidechain-Sidechain	400	14.6	42	10.5	1.5	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	28	1.0	1	3.6	0.0	0	0.0	0.0
Disulfide bond	11	0.4	11	100.0	0.4	0	0.0	0.0
Total	2739	100.0	259	9.5	9.5	0	0.0	0.0
Backbone-Backbone	372	13.6	18	4.8	0.7	0	0.0	0.0
Backbone-Sidechain	1606	58.6	138	8.6	5.0	0	0.0	0.0
Sidechain-Sidechain	761	27.8	103	13.5	3.8	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	4	2	2	0	13	0.16	0.31	0.06	0.13
2	3	4	2	10	0	19	0.15	0.27	0.04	0.13
3	3	5	2	5	0	15	0.14	0.22	0.03	0.13
4	2	5	0	9	0	16	0.17	0.31	0.05	0.16
5	5	6	5	7	0	23	0.14	0.3	0.05	0.13
6	2	4	1	5	0	12	0.14	0.27	0.05	0.12
7	3	5	1	3	0	12	0.14	0.18	0.02	0.14
8	5	3	1	2	0	11	0.13	0.21	0.03	0.12
9	4	6	5	11	0	26	0.13	0.2	0.03	0.12
10	3	6	1	5	0	15	0.13	0.22	0.03	0.13

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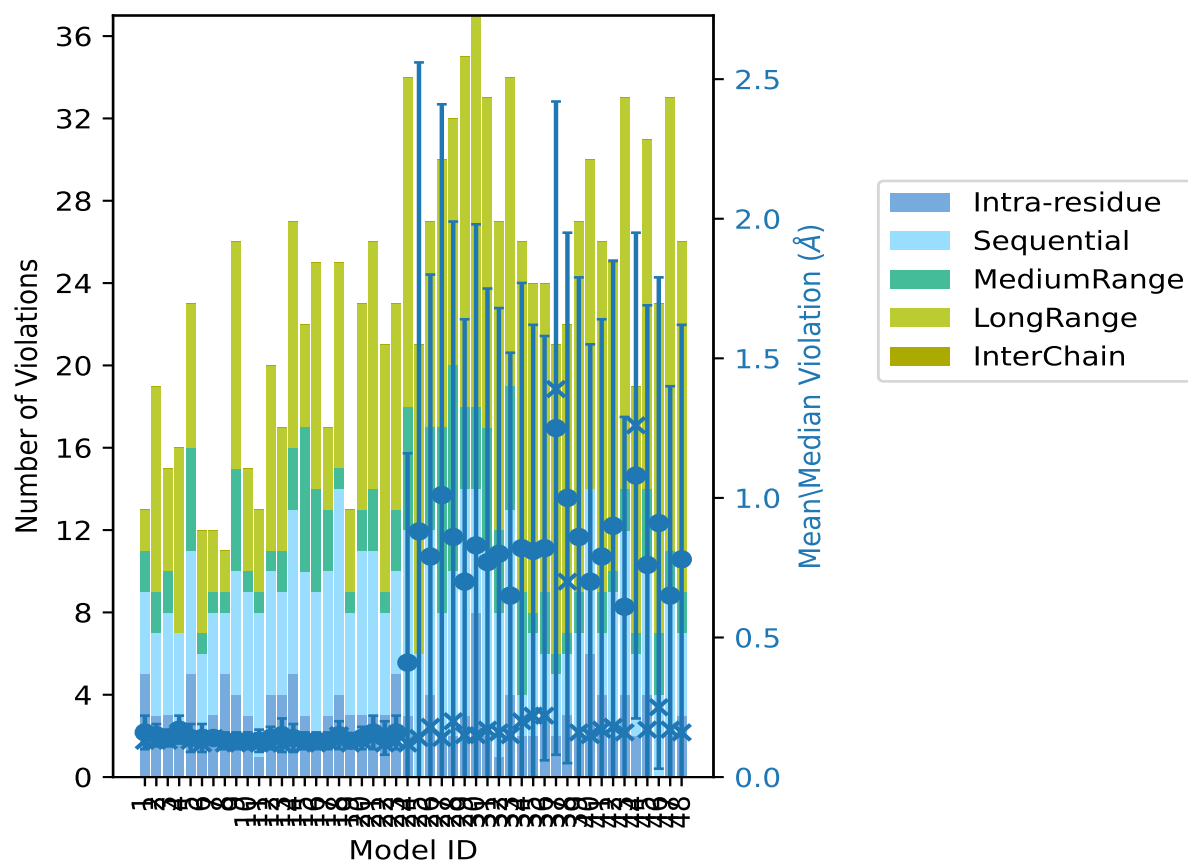
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	7	1	4	0	13	0.13	0.24	0.04	0.12
12	4	6	1	9	0	20	0.14	0.27	0.04	0.12
13	4	5	2	6	0	17	0.15	0.29	0.06	0.12
14	5	8	3	11	0	27	0.14	0.32	0.05	0.13
15	3	7	7	5	0	22	0.13	0.21	0.03	0.12
16	2	7	5	11	0	25	0.13	0.23	0.03	0.12
17	3	7	3	4	0	17	0.13	0.19	0.03	0.13
18	4	10	1	10	0	25	0.15	0.3	0.05	0.15
19	3	5	1	4	0	13	0.13	0.18	0.02	0.12
20	3	8	2	10	0	23	0.14	0.25	0.04	0.13
21	3	8	3	12	0	26	0.16	0.28	0.06	0.14
22	3	5	1	12	0	21	0.14	0.33	0.06	0.12
23	5	5	3	10	0	23	0.16	0.3	0.06	0.13
24	3	9	6	16	0	34	0.41	2.56	0.75	0.12
25	0	6	0	15	0	21	0.88	5.93	1.68	0.14
26	4	8	5	10	0	27	0.79	4.53	1.01	0.18
27	2	6	9	13	0	30	1.01	4.49	1.4	0.14
28	2	8	10	12	0	32	0.86	4.58	1.13	0.2
29	3	11	4	17	0	35	0.7	3.83	0.94	0.15
30	8	6	4	19	0	37	0.83	4.03	1.15	0.15
31	2	9	6	16	0	33	0.77	4.38	0.98	0.17
32	1	7	4	15	0	27	0.8	3.15	0.88	0.16
33	4	9	6	15	0	34	0.65	4.14	0.87	0.15
34	2	2	5	17	0	26	0.82	3.76	0.95	0.2
35	2	5	1	16	0	24	0.81	3.33	0.81	0.22
36	3	3	3	15	0	24	0.82	2.36	0.76	0.22
37	2	3	1	15	0	21	1.25	3.52	1.17	1.39
38	3	3	1	15	0	22	1.0	3.43	0.95	0.7
39	2	5	2	18	0	27	0.86	2.81	0.93	0.16
40	6	8	0	16	0	30	0.7	3.63	0.85	0.15
41	4	3	2	17	0	26	0.79	2.63	0.85	0.17
42	2	7	1	15	0	25	0.9	3.02	0.95	0.18
43	4	8	2	19	0	33	0.61	2.19	0.68	0.16
44	2	4	1	12	0	19	1.08	2.41	0.87	1.26
45	4	6	4	17	0	31	0.76	3.9	0.93	0.17
46	0	4	3	16	0	23	0.91	2.81	0.88	0.25
47	2	7	2	22	0	33	0.65	2.68	0.75	0.17
48	3	4	2	17	0	26	0.78	2.9	0.84	0.16

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2453(IR:582, SQ:694, MR:360, LR:817, 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	%
17	29	12	46	0	104	1	2.1
3	15	12	14	0	44	2	4.2
3	9	7	7	0	26	3	6.2
2	7	3	9	0	21	4	8.3
1	2	3	3	0	9	5	10.4
3	1	2	0	0	6	6	12.5

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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
1	2	2	1	0	6	7	14.6
0	3	0	2	0	5	8	16.7
0	2	0	1	0	3	9	18.8
1	0	0	4	0	5	10	20.8
0	1	0	0	0	1	11	22.9
1	1	0	2	0	4	12	25.0
1	1	0	1	0	3	13	27.1
2	1	0	0	0	3	14	29.2
1	0	0	0	0	1	15	31.2
0	1	0	2	0	3	16	33.3
0	0	0	1	0	1	17	35.4
0	0	0	0	0	0	18	37.5
0	0	0	1	0	1	19	39.6
0	0	0	0	0	0	20	41.7
0	0	0	0	0	0	21	43.8
0	0	0	0	0	0	22	45.8
0	0	0	0	0	0	23	47.9
0	0	0	0	0	0	24	50.0
0	0	0	0	0	0	25	52.1
0	0	0	0	0	0	26	54.2
0	0	0	0	0	0	27	56.2
0	0	0	0	0	0	28	58.3
0	0	0	0	0	0	29	60.4
0	0	0	0	0	0	30	62.5
0	0	0	0	0	0	31	64.6
0	0	0	0	0	0	32	66.7
0	0	0	0	0	0	33	68.8
0	0	0	0	0	0	34	70.8
0	1	0	0	0	1	35	72.9
0	0	0	0	0	0	36	75.0
0	0	0	0	0	0	37	77.1
0	0	0	0	0	0	38	79.2
0	0	0	0	0	0	39	81.2
0	0	0	0	0	0	40	83.3
0	0	0	0	0	0	41	85.4
0	0	0	0	0	0	42	87.5
0	0	0	0	0	0	43	89.6
0	0	0	0	0	0	44	91.7
0	0	0	0	0	0	45	93.8
0	0	0	0	0	0	46	95.8
0	0	0	0	0	0	47	97.9

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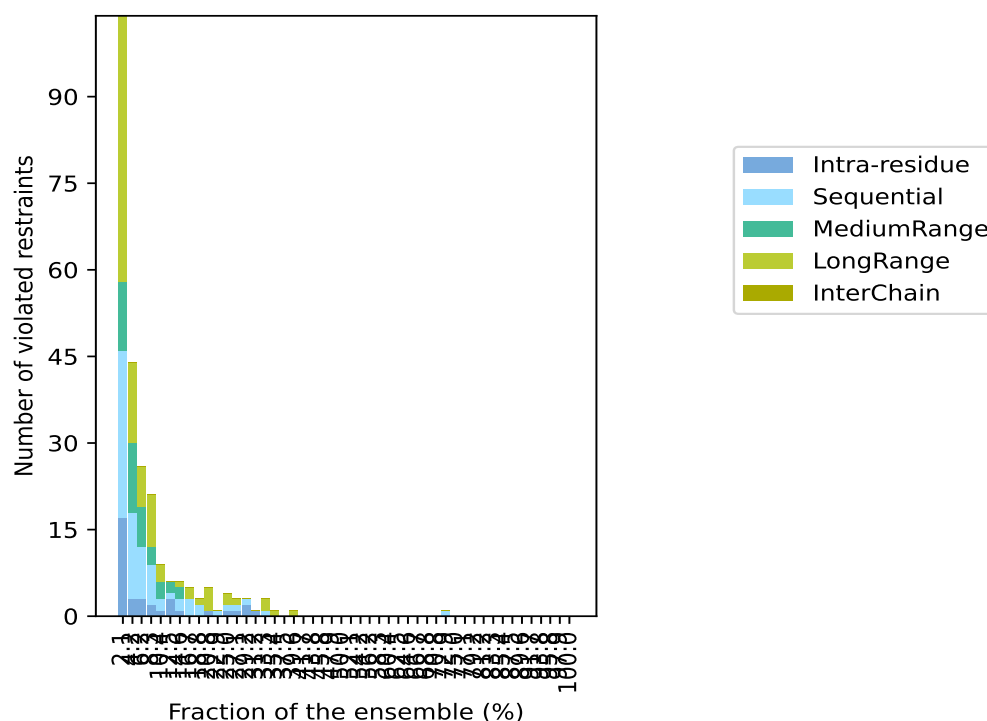
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	0	0	48	100.0

¹Intra-residue restraints, ²Sequential restraints, ³Medium range restraints, ⁴Long range restraints,

⁵Inter-chain restraints, ⁶ Number of models with violations

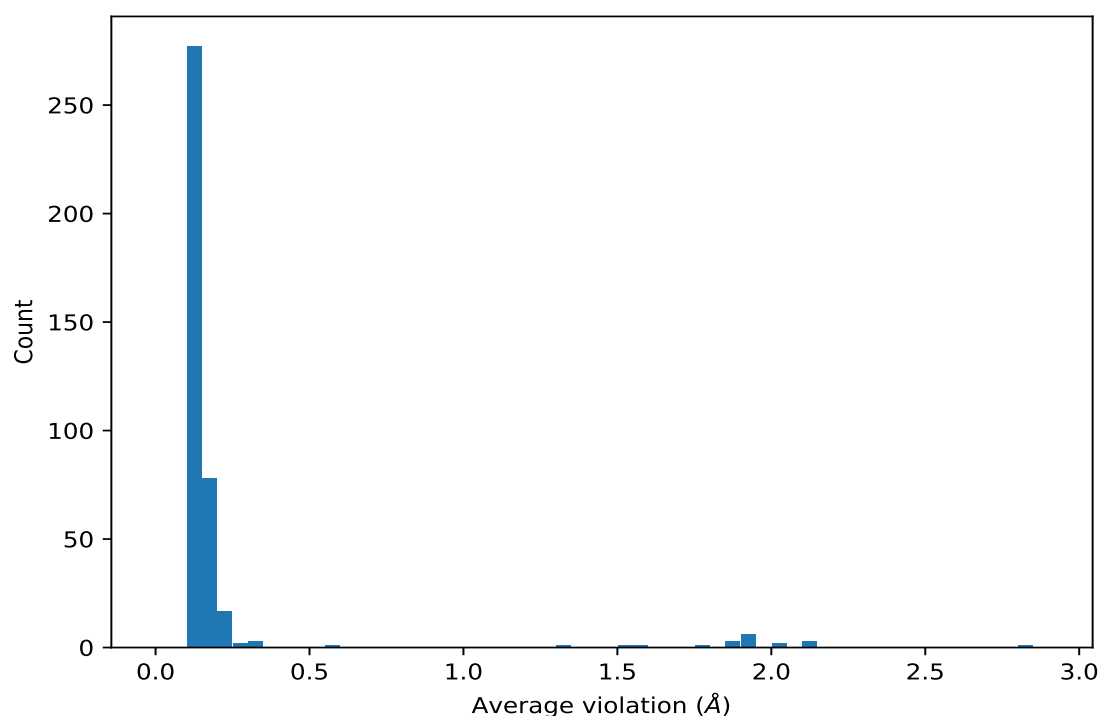
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	35	0.15	0.03	0.15
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	35	0.15	0.03	0.15
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	35	0.15	0.03	0.15
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	25	2.11	1.0	1.75
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	25	2.11	1.0	1.75
(1,2703)	1:782:A:CYS:SG	1:776:A:CYS:SG	25	2.11	1.0	1.75
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	25	1.9	0.79	1.63
(1,2701)	1:773:A:CYS:SG	1:789:A:CYS:SG	25	1.9	0.79	1.63
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	25	1.9	0.79	1.63
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	25	1.9	0.79	1.63
(1,2704)	1:789:A:CYS:SG	1:773:A:CYS:SG	25	1.9	0.79	1.63
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	25	1.9	0.79	1.63
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	25	1.88	0.79	1.59
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	25	1.88	0.79	1.59
(1,2702)	1:776:A:CYS:SG	1:782:A:CYS:SG	25	1.88	0.79	1.59
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	23	2.84	1.11	2.46

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	23	2.02	0.59	2.01
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	23	2.0	0.67	1.73
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	23	1.77	0.78	1.38
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	23	1.56	0.29	1.53
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	23	1.53	0.29	1.42
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	23	1.33	0.41	1.25
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	19	0.14	0.02	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	19	0.14	0.02	0.13
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	17	0.24	0.02	0.24
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	16	0.14	0.02	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	16	0.14	0.02	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	16	0.14	0.02	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	16	0.14	0.03	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	16	0.14	0.03	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	16	0.14	0.03	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	16	0.14	0.03	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	16	0.14	0.03	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	16	0.14	0.03	0.13
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	16	0.14	0.02	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	15	0.13	0.01	0.13
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	14	0.18	0.07	0.14
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	14	0.12	0.01	0.13
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	14	0.11	0.01	0.11
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	13	0.14	0.04	0.12
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	13	0.12	0.01	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	13	0.11	0.01	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	13	0.11	0.01	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	13	0.11	0.01	0.11
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	12	0.18	0.03	0.18
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	12	0.18	0.03	0.18
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	12	0.18	0.03	0.18
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	12	0.18	0.03	0.18
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	12	0.18	0.03	0.18
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	12	0.18	0.03	0.18
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	12	0.14	0.04	0.14
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	12	0.12	0.02	0.12
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	12	0.12	0.01	0.12
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	11	0.13	0.02	0.13
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	10	0.21	0.03	0.2
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	10	0.19	0.05	0.18
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	10	0.19	0.05	0.18
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	10	0.18	0.05	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	10	0.13	0.02	0.13
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	10	0.13	0.02	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	10	0.13	0.02	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	10	0.13	0.02	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	10	0.13	0.02	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	10	0.13	0.02	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	10	0.12	0.02	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	10	0.12	0.02	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	10	0.12	0.02	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	10	0.12	0.02	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	10	0.12	0.02	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	10	0.12	0.02	0.13
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	9	0.15	0.02	0.16
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	9	0.15	0.02	0.16
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	9	0.15	0.02	0.16
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	9	0.14	0.03	0.14
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	9	0.14	0.03	0.14
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	9	0.14	0.03	0.14
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	9	0.13	0.03	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	9	0.13	0.03	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	9	0.13	0.03	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	9	0.13	0.03	0.11
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	8	0.24	0.05	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	8	0.24	0.05	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	8	0.24	0.05	0.24
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	8	0.17	0.03	0.16
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	8	0.13	0.03	0.12
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	8	0.13	0.03	0.12
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	8	0.13	0.03	0.12
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	8	0.12	0.01	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	8	0.12	0.02	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	8	0.12	0.02	0.12
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	7	0.2	0.06	0.2
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	7	0.18	0.03	0.18
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	7	0.18	0.03	0.18
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	7	0.18	0.03	0.18
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	7	0.18	0.03	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	7	0.18	0.03	0.18
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	7	0.18	0.03	0.18
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	7	0.15	0.04	0.16
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	7	0.12	0.02	0.11
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	7	0.12	0.02	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	7	0.11	0.01	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	7	0.11	0.01	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	7	0.11	0.01	0.11
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	6	0.26	0.01	0.27
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	6	0.16	0.02	0.16
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	6	0.16	0.05	0.16
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	6	0.16	0.05	0.16
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	6	0.14	0.03	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	6	0.14	0.03	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	6	0.14	0.03	0.14
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	6	0.12	0.01	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	6	0.11	0.01	0.11
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	6	0.11	0.01	0.11
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	5	0.16	0.05	0.16
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	5	0.14	0.02	0.14
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	5	0.12	0.01	0.13
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	5	0.12	0.01	0.12
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	5	0.12	0.01	0.12
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	5	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	5	0.11	0.01	0.11
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	5	0.11	0.01	0.11
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	5	0.11	0.01	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	5	0.11	0.01	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	5	0.11	0.01	0.11
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	5	0.11	0.01	0.11
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	5	0.11	0.01	0.11
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	5	0.11	0.01	0.11
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	5	0.11	0.01	0.11
(1,811)	1:709:A:GLN:HG3	1:710:A:ASN:HD21	4	0.57	0.79	0.12
(1,2240)	1:742:A:VAL:HG11	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,2240)	1:742:A:VAL:HG12	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,2240)	1:742:A:VAL:HG13	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,2240)	1:742:A:VAL:HG21	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,2240)	1:742:A:VAL:HG22	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,2240)	1:742:A:VAL:HG23	1:746:A:HIS:HA	4	0.23	0.08	0.22
(1,1741)	1:738:A:LEU:HA	1:738:A:LEU:HG	4	0.2	0.06	0.24
(1,1201)	1:725:A:LEU:HG	1:779:A:TRP:HZ2	4	0.15	0.03	0.15
(1,2339)	1:760:A:ARG:HG2	1:762:A:SER:H	4	0.15	0.06	0.11
(1,2339)	1:760:A:ARG:HG3	1:762:A:SER:H	4	0.15	0.06	0.11
(1,529)	1:773:A:CYS:H	1:789:A:CYS:H	4	0.14	0.04	0.14
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB2	4	0.14	0.02	0.14
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB3	4	0.14	0.02	0.14
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB2	4	0.14	0.02	0.14
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB3	4	0.14	0.02	0.14
(1,1185)	1:802:A:PHE:HE1	1:803:A:SER:H	4	0.14	0.0	0.14
(1,1185)	1:802:A:PHE:HE2	1:803:A:SER:H	4	0.14	0.0	0.14
(1,2567)	1:811:A:LYS:HG2	1:812:A:GLU:H	4	0.14	0.02	0.13
(1,2567)	1:811:A:LYS:HG3	1:812:A:GLU:H	4	0.14	0.02	0.13
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG11	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG12	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG13	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG21	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG22	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG23	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG11	4	0.13	0.03	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG12	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG13	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG21	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG22	4	0.13	0.03	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG23	4	0.13	0.03	0.12
(1,1443)	1:745:A:MET:HA	1:755:A:TYR:HB3	4	0.13	0.02	0.12
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB2	4	0.13	0.03	0.12
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB3	4	0.13	0.03	0.12
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG2	4	0.13	0.02	0.12
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG3	4	0.13	0.02	0.12
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG2	4	0.13	0.02	0.12
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG3	4	0.13	0.02	0.12
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG2	4	0.13	0.02	0.12
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG3	4	0.13	0.02	0.12
(1,268)	1:690:A:SER:HA	1:691:A:HIS:H	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB1	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB2	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB3	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB1	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB2	4	0.12	0.01	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB3	4	0.12	0.01	0.12
(1,109)	1:794:A:ALA:H	1:795:A:SER:HA	4	0.12	0.02	0.11
(1,532)	1:773:A:CYS:H	1:773:A:CYS:HB2	4	0.12	0.02	0.11
(1,1095)	1:727:A:VAL:HG11	1:835:A:ILE:HA	4	0.12	0.01	0.12
(1,1095)	1:727:A:VAL:HG12	1:835:A:ILE:HA	4	0.12	0.01	0.12
(1,1095)	1:727:A:VAL:HG13	1:835:A:ILE:HA	4	0.12	0.01	0.12
(1,1782)	1:822:A:ALA:HB1	1:825:A:CYS:HB3	4	0.12	0.02	0.11
(1,1782)	1:822:A:ALA:HB2	1:825:A:CYS:HB3	4	0.12	0.02	0.11
(1,1782)	1:822:A:ALA:HB3	1:825:A:CYS:HB3	4	0.12	0.02	0.11
(1,114)	1:775:A:ALA:H	1:776:A:CYS:H	4	0.11	0.01	0.12
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG12	4	0.11	0.0	0.11
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG13	4	0.11	0.0	0.11
(1,878)	1:841:A:GLU:H	1:842:A:THR:H	3	0.21	0.03	0.22
(1,1354)	1:738:A:LEU:HG	1:740:A:LEU:HG	3	0.21	0.0	0.21
(1,149)	1:729:A:ALA:H	1:738:A:LEU:HG	3	0.2	0.03	0.18
(1,1633)	1:742:A:VAL:HG21	1:835:A:ILE:HA	3	0.19	0.07	0.2
(1,1633)	1:742:A:VAL:HG22	1:835:A:ILE:HA	3	0.19	0.07	0.2
(1,1633)	1:742:A:VAL:HG23	1:835:A:ILE:HA	3	0.19	0.07	0.2
(1,1886)	1:727:A:VAL:HB	1:741:A:THR:HA	3	0.18	0.03	0.17
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB2	3	0.17	0.07	0.13
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB3	3	0.17	0.07	0.13
(1,1107)	1:738:A:LEU:HD11	1:739:A:PRO:HD2	3	0.16	0.02	0.17

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1107)	1:738:A:LEU:HD12	1:739:A:PRO:HD2	3	0.16	0.02	0.17
(1,1107)	1:738:A:LEU:HD13	1:739:A:PRO:HD2	3	0.16	0.02	0.17
(1,2480)	1:799:A:GLU:HG2	1:801:A:GLY:H	3	0.16	0.03	0.15
(1,2480)	1:799:A:GLU:HG3	1:801:A:GLY:H	3	0.16	0.03	0.15
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD11	3	0.16	0.02	0.17
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD12	3	0.16	0.02	0.17
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD13	3	0.16	0.02	0.17
(1,2588)	1:816:A:SER:HB2	1:819:A:GLU:HB3	3	0.15	0.01	0.16
(1,2588)	1:816:A:SER:HB3	1:819:A:GLU:HB3	3	0.15	0.01	0.16
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD11	3	0.14	0.02	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD12	3	0.14	0.02	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD13	3	0.14	0.02	0.13
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB2	3	0.14	0.02	0.14
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB3	3	0.14	0.02	0.14
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB2	3	0.14	0.02	0.14
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB3	3	0.14	0.02	0.14
(1,1270)	1:794:A:ALA:HB1	1:819:A:GLU:HB2	3	0.14	0.02	0.15
(1,1270)	1:794:A:ALA:HB2	1:819:A:GLU:HB2	3	0.14	0.02	0.15
(1,1270)	1:794:A:ALA:HB3	1:819:A:GLU:HB2	3	0.14	0.02	0.15
(1,1058)	1:829:A:SER:HB2	1:830:A:ILE:HA	3	0.13	0.02	0.15
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG2	3	0.13	0.0	0.13
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG3	3	0.13	0.0	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG2	3	0.13	0.0	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG3	3	0.13	0.0	0.13
(1,579)	1:841:A:GLU:HA	1:842:A:THR:H	3	0.13	0.01	0.14
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE2	3	0.13	0.0	0.13
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE3	3	0.13	0.0	0.13
(1,309)	1:824:A:ARG:H	1:824:A:ARG:HE	3	0.12	0.01	0.12
(1,1050)	1:705:A:TRP:HD1	1:750:A:CYS:HA	3	0.12	0.01	0.12
(1,1771)	1:778:A:LEU:HD21	1:779:A:TRP:HZ2	3	0.12	0.01	0.11
(1,1771)	1:778:A:LEU:HD22	1:779:A:TRP:HZ2	3	0.12	0.01	0.11
(1,1771)	1:778:A:LEU:HD23	1:779:A:TRP:HZ2	3	0.12	0.01	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD11	3	0.12	0.0	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD12	3	0.12	0.0	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD13	3	0.12	0.0	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD21	3	0.12	0.0	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD22	3	0.12	0.0	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD23	3	0.12	0.0	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD11	3	0.12	0.01	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD12	3	0.12	0.01	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD13	3	0.12	0.01	0.12
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD11	3	0.12	0.01	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD12	3	0.12	0.01	0.12
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD13	3	0.12	0.01	0.12
(1,585)	1:735:A:LYS:H	1:735:A:LYS:HD2	3	0.11	0.01	0.1
(1,1079)	1:842:A:THR:HB	1:843:A:GLN:H	3	0.11	0.0	0.11
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD2	3	0.11	0.0	0.11
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD3	3	0.11	0.0	0.11
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG2	3	0.1	0.0	0.1
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG3	3	0.1	0.0	0.1
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB1	2	0.31	0.01	0.31
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB2	2	0.31	0.01	0.31
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB3	2	0.31	0.01	0.31
(1,1706)	1:782:A:CYS:HA	1:789:A:CYS:HA	2	0.25	0.03	0.25
(1,987)	1:709:A:GLN:HG3	1:712:A:ARG:H	2	0.2	0.09	0.2
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB1	2	0.19	0.02	0.19
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB2	2	0.19	0.02	0.19
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB3	2	0.19	0.02	0.19
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB1	2	0.19	0.02	0.19
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB2	2	0.19	0.02	0.19
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB3	2	0.19	0.02	0.19
(1,572)	1:816:A:SER:H	1:819:A:GLU:HB2	2	0.18	0.06	0.18
(1,2423)	1:788:A:LYS:HE2	1:790:A:VAL:HA	2	0.18	0.01	0.18
(1,2423)	1:788:A:LYS:HE3	1:790:A:VAL:HA	2	0.18	0.01	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB1	2	0.18	0.0	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB2	2	0.18	0.0	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB3	2	0.18	0.0	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB1	2	0.18	0.0	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB2	2	0.18	0.0	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB3	2	0.18	0.0	0.18
(1,2411)	1:781:A:LYS:HG2	1:782:A:CYS:H	2	0.16	0.05	0.16
(1,2411)	1:781:A:LYS:HG3	1:782:A:CYS:H	2	0.16	0.05	0.16
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG2	2	0.15	0.04	0.15
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG3	2	0.15	0.04	0.15
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG2	2	0.15	0.04	0.15
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG3	2	0.15	0.04	0.15
(1,2039)	1:716:A:LYS:HE2	1:717:A:MET:H	2	0.14	0.02	0.14
(1,2039)	1:716:A:LYS:HE3	1:717:A:MET:H	2	0.14	0.02	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG11	2	0.14	0.03	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG12	2	0.14	0.03	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG13	2	0.14	0.03	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG21	2	0.14	0.03	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG22	2	0.14	0.03	0.14
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG23	2	0.14	0.03	0.14

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,782)	1:760:A:ARG:HE	1:761:A:ASP:HA	2	0.14	0.02	0.14
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG21	2	0.14	0.02	0.14
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG22	2	0.14	0.02	0.14
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG23	2	0.14	0.02	0.14
(1,1313)	1:742:A:VAL:HG11	1:835:A:ILE:HB	2	0.13	0.01	0.13
(1,1313)	1:742:A:VAL:HG12	1:835:A:ILE:HB	2	0.13	0.01	0.13
(1,1313)	1:742:A:VAL:HG13	1:835:A:ILE:HB	2	0.13	0.01	0.13
(1,1476)	1:813:A:GLN:HA	1:840:A:ALA:HA	2	0.13	0.0	0.13
(1,2424)	1:788:A:LYS:HE2	1:790:A:VAL:HB	2	0.13	0.02	0.13
(1,2424)	1:788:A:LYS:HE3	1:790:A:VAL:HB	2	0.13	0.02	0.13
(1,519)	1:767:A:ALA:HA	1:768:A:SER:H	2	0.12	0.02	0.12
(1,818)	1:717:A:MET:HE1	1:751:A:GLN:HE22	2	0.12	0.02	0.12
(1,818)	1:717:A:MET:HE2	1:751:A:GLN:HE22	2	0.12	0.02	0.12
(1,818)	1:717:A:MET:HE3	1:751:A:GLN:HE22	2	0.12	0.02	0.12
(1,1098)	1:709:A:GLN:HG3	1:712:A:ARG:HG2	2	0.12	0.02	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG11	2	0.12	0.01	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG12	2	0.12	0.01	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG13	2	0.12	0.01	0.12
(1,1410)	1:725:A:LEU:HD11	1:817:A:GLU:HB3	2	0.12	0.01	0.12
(1,1410)	1:725:A:LEU:HD12	1:817:A:GLU:HB3	2	0.12	0.01	0.12
(1,1410)	1:725:A:LEU:HD13	1:817:A:GLU:HB3	2	0.12	0.01	0.12
(1,1869)	1:741:A:THR:HG21	1:742:A:VAL:HA	2	0.12	0.02	0.12
(1,1869)	1:741:A:THR:HG22	1:742:A:VAL:HA	2	0.12	0.02	0.12
(1,1869)	1:741:A:THR:HG23	1:742:A:VAL:HA	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB1	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB2	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB3	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB1	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB2	2	0.12	0.02	0.12
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB3	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG11	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG12	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG13	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG21	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG22	2	0.12	0.02	0.12
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG23	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD11	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD12	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD13	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD21	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD22	2	0.12	0.02	0.12
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD23	2	0.12	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,298)	1:702:A:CYS:HB3	1:706:A:GLU:H	2	0.12	0.02	0.12
(1,863)	1:795:A:SER:H	1:797:A:CYS:H	2	0.12	0.0	0.12
(1,967)	1:815:A:MET:HG3	1:820:A:ALA:H	2	0.12	0.01	0.12
(1,407)	1:704:A:ARG:H	1:705:A:TRP:HZ2	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE21	2	0.12	0.02	0.12
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE22	2	0.12	0.02	0.12
(1,533)	1:772:A:ALA:HB1	1:773:A:CYS:H	2	0.12	0.0	0.12
(1,533)	1:772:A:ALA:HB2	1:773:A:CYS:H	2	0.12	0.0	0.12
(1,533)	1:772:A:ALA:HB3	1:773:A:CYS:H	2	0.12	0.0	0.12
(1,9)	1:765:A:LEU:H	1:766:A:PRO:HD3	2	0.11	0.0	0.11
(1,260)	1:809:A:ASN:HB3	1:811:A:LYS:H	2	0.11	0.01	0.11
(1,921)	1:767:A:ALA:HB1	1:768:A:SER:H	2	0.11	0.0	0.11
(1,921)	1:767:A:ALA:HB2	1:768:A:SER:H	2	0.11	0.0	0.11
(1,921)	1:767:A:ALA:HB3	1:768:A:SER:H	2	0.11	0.0	0.11
(1,1672)	1:726:A:ASP:HB3	1:727:A:VAL:HA	2	0.11	0.01	0.11
(1,2337)	1:760:A:ARG:HG2	1:761:A:ASP:H	2	0.11	0.0	0.11
(1,2337)	1:760:A:ARG:HG3	1:761:A:ASP:H	2	0.11	0.0	0.11
(1,544)	1:751:A:GLN:H	1:751:A:GLN:HE21	2	0.11	0.0	0.11
(1,803)	1:809:A:ASN:HA	1:809:A:ASN:HD22	2	0.11	0.0	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD11	2	0.11	0.0	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD12	2	0.11	0.0	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD13	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD1	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD2	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD1	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD2	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD1	2	0.11	0.0	0.11
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD2	2	0.11	0.0	0.11
(1,1540)	1:791:A:CYS:HA	1:825:A:CYS:HB2	2	0.11	0.0	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB1	2	0.11	0.0	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB2	2	0.11	0.0	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB3	2	0.11	0.0	0.11

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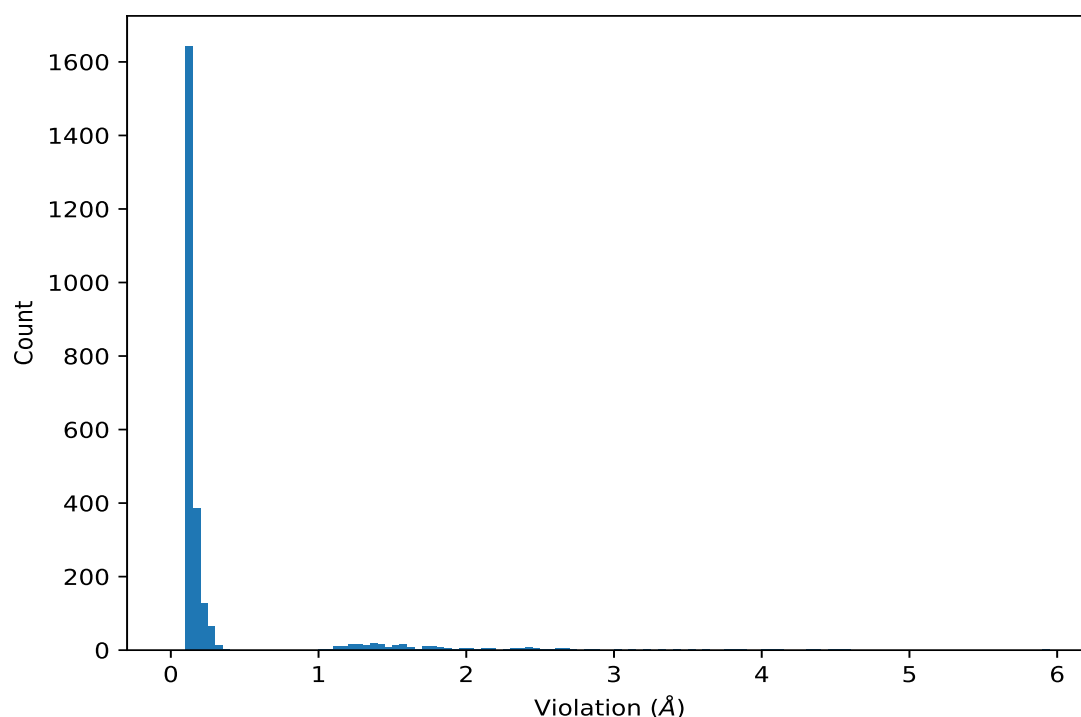
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG2	2	0.11	0.0	0.11
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG3	2	0.11	0.0	0.11
(1,1779)	1:771:A:LYS:HA	1:771:A:LYS:HD2	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	25	5.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	28	4.58
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	26	4.53
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	27	4.49
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	31	4.38
(1,2704)	1:789:A:CYS:SG	1:773:A:CYS:SG	25	4.33
(1,2701)	1:773:A:CYS:SG	1:789:A:CYS:SG	25	4.33
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	33	4.14
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	27	4.08
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	27	4.08
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	27	4.08
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	30	4.03
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	45	3.9
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	29	3.83
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	34	3.76
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	40	3.63
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	37	3.52
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	30	3.51
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	38	3.43
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	30	3.41
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	35	3.33
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	37	3.22
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	32	3.15
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	28	3.14
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	42	3.02
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	28	3.01
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	48	2.9
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	34	2.89
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	29	2.83
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	46	2.81
(1,2702)	1:776:A:CYS:SG	1:782:A:CYS:SG	39	2.81
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	27	2.73
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	26	2.72
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	47	2.68
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	37	2.68
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	37	2.68
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	37	2.68
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	42	2.66
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	30	2.63
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	41	2.63
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	41	2.6
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	46	2.6
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	28	2.57

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	24	2.56
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	31	2.55
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	48	2.49
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	39	2.46
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	31	2.46
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	45	2.46
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	41	2.44
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	45	2.43
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	24	2.41
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	44	2.41
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	24	2.41
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	24	2.41
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	44	2.41
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	29	2.4
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	38	2.38
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	42	2.38
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	36	2.36
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	44	2.34
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	30	2.34
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	30	2.34
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	30	2.34
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	46	2.3
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	29	2.25
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	43	2.19
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	39	2.18
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	42	2.18
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	38	2.18
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	39	2.14
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	32	2.14
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	34	2.11
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	33	2.1
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	44	2.06
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	30	2.02
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	37	2.02
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	38	2.02
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	32	2.02
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	40	2.01
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	32	1.99
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	39	1.98
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	39	1.98
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	39	1.98
(1,811)	1:709:A:GLN:HG3	1:710:A:ASN:HD21	31	1.94

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	31	1.91
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	29	1.9
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	26	1.88
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	42	1.86
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	37	1.85
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	39	1.83
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	36	1.82
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	36	1.82
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	36	1.82
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	47	1.81
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	36	1.8
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	37	1.8
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	45	1.79
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	44	1.78
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	32	1.76
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	32	1.76
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	32	1.76
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	47	1.75
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	48	1.75
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	43	1.75
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	43	1.75
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	43	1.75
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	40	1.73
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	33	1.73
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	28	1.72
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	28	1.72
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	28	1.72
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	28	1.71
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	47	1.71
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	47	1.71
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	47	1.71
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	35	1.66
(1,2703)	1:782:A:CYS:SG	1:776:A:CYS:SG	44	1.66
(1,2702)	1:776:A:CYS:SG	1:782:A:CYS:SG	44	1.66
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	29	1.63
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	38	1.63
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	38	1.63
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	38	1.63
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	40	1.6
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	40	1.6
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	40	1.6
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	34	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2703)	1:782:A:CYS:SG	1:776:A:CYS:SG	48	1.59
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	25	1.59
(1,2702)	1:776:A:CYS:SG	1:782:A:CYS:SG	48	1.59
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	35	1.58
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	35	1.58
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	28	1.57
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	38	1.57
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	43	1.57
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	26	1.56
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	33	1.55
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	46	1.55
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	46	1.55
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	33	1.55
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	33	1.55
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	46	1.55
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	36	1.54
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	31	1.54
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	46	1.53
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	30	1.52
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	43	1.52
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	45	1.52
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	37	1.51
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	47	1.51
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	27	1.5
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	43	1.5
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	42	1.5
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	42	1.5
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	42	1.5
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	42	1.49
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	30	1.47
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	45	1.47
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	37	1.47
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	41	1.47
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	41	1.47
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	41	1.47
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	35	1.46
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	41	1.44
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	26	1.44
(1,2704)	1:789:A:CYS:SG	1:773:A:CYS:SG	48	1.44
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	27	1.44
(1,2701)	1:773:A:CYS:SG	1:789:A:CYS:SG	48	1.44
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	34	1.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	38	1.43
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	46	1.42
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	31	1.41
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	33	1.41
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	35	1.41
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	45	1.41
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	35	1.41
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	47	1.41
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	40	1.41
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	48	1.4
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	27	1.39
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	37	1.39
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	41	1.39
(1,2704)	1:782:A:CYS:SG	1:773:A:CYS:SG	45	1.39
(1,2703)	1:782:A:CYS:SG	1:773:A:CYS:SG	45	1.39
(1,2701)	1:773:A:CYS:SG	1:782:A:CYS:SG	45	1.39
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	32	1.38
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	48	1.38
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	36	1.38
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	27	1.37
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	29	1.37
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	27	1.36
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	46	1.36
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	34	1.36
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	47	1.35
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	33	1.35
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	36	1.35
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	44	1.34
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	43	1.34
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	35	1.33
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	40	1.33
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	41	1.32
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	36	1.32
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	44	1.32
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	36	1.32
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	39	1.31
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	46	1.31
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	47	1.31
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	39	1.3
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	45	1.29
(1,2703)	1:782:A:CYS:SG	1:789:A:CYS:SG	26	1.29
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	43	1.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	47	1.28
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	40	1.28
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	41	1.27
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	42	1.27
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	40	1.26
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	44	1.26
(1,2702)	1:776:A:CYS:SG	1:789:A:CYS:SG	42	1.26
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	48	1.25
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	48	1.25
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	46	1.25
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	32	1.25
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	35	1.25
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	26	1.24
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	33	1.24
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	29	1.24
(1,2703)	1:782:A:CYS:SG	1:776:A:CYS:SG	35	1.24
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	29	1.24
(1,2702)	1:776:A:CYS:SG	1:782:A:CYS:SG	35	1.24
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	29	1.24
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	38	1.23
(3,6)	1:797:A:CYS:SG	1:818:A:CYS:SG	44	1.23
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	32	1.23
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	33	1.23
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	31	1.22
(3,2)	1:715:A:CYS:SG	1:750:A:CYS:SG	39	1.21
(3,1)	1:702:A:CYS:SG	1:713:A:CYS:SG	27	1.21
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	34	1.21
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	34	1.21
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	34	1.21
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	29	1.2
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	33	1.2
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	43	1.2
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	31	1.2
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	31	1.2
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	31	1.2
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	38	1.19
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	30	1.18
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	36	1.17
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	28	1.16
(3,3)	1:721:A:CYS:SG	1:743:A:CYS:SG	28	1.16
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	26	1.15
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	31	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	34	1.14
(3,4)	1:728:A:CYS:SG	1:763:A:CYS:SG	34	1.14
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	41	1.13
(1,2704)	1:776:A:CYS:SG	1:773:A:CYS:SG	26	1.12
(1,2702)	1:776:A:CYS:SG	1:773:A:CYS:SG	26	1.12
(1,2701)	1:773:A:CYS:SG	1:776:A:CYS:SG	26	1.12
(3,7)	1:838:A:CYS:SG	1:805:A:CYS:SG	32	1.1
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	40	1.07
(3,5)	1:791:A:CYS:SG	1:825:A:CYS:SG	43	1.04
(1,1290)	1:709:A:GLN:HG2	1:714:A:VAL:HG21	45	0.39
(1,1290)	1:709:A:GLN:HG2	1:714:A:VAL:HG22	45	0.39
(1,1290)	1:709:A:GLN:HG2	1:714:A:VAL:HG23	45	0.39
(1,2413)	1:782:A:CYS:HB2	1:789:A:CYS:HA	22	0.33
(1,2413)	1:782:A:CYS:HB3	1:789:A:CYS:HA	22	0.33
(1,2240)	1:742:A:VAL:HG11	1:746:A:HIS:HA	28	0.32
(1,2240)	1:742:A:VAL:HG12	1:746:A:HIS:HA	28	0.32
(1,2240)	1:742:A:VAL:HG13	1:746:A:HIS:HA	28	0.32
(1,2240)	1:742:A:VAL:HG21	1:746:A:HIS:HA	28	0.32
(1,2240)	1:742:A:VAL:HG22	1:746:A:HIS:HA	28	0.32
(1,2240)	1:742:A:VAL:HG23	1:746:A:HIS:HA	28	0.32
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB1	27	0.32
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB2	27	0.32
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB3	27	0.32
(1,1000)	1:709:A:GLN:HB2	1:710:A:ASN:HB2	14	0.32
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	4	0.31
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	1	0.31
(1,2240)	1:742:A:VAL:HG11	1:746:A:HIS:HA	5	0.3
(1,2240)	1:742:A:VAL:HG12	1:746:A:HIS:HA	5	0.3
(1,2240)	1:742:A:VAL:HG13	1:746:A:HIS:HA	5	0.3
(1,2240)	1:742:A:VAL:HG21	1:746:A:HIS:HA	5	0.3
(1,2240)	1:742:A:VAL:HG22	1:746:A:HIS:HA	5	0.3
(1,2240)	1:742:A:VAL:HG23	1:746:A:HIS:HA	5	0.3
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	18	0.3
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	23	0.3
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	31	0.3
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB1	28	0.3
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB2	28	0.3
(1,1366)	1:819:A:GLU:HB3	1:820:A:ALA:HB3	28	0.3
(1,987)	1:709:A:GLN:HG3	1:712:A:ARG:H	14	0.3
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	13	0.29
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	30	0.28
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	30	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	30	0.28
(1,1706)	1:782:A:CYS:HA	1:789:A:CYS:HA	21	0.28
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	26	0.28
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	6	0.27
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	6	0.27
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB2	21	0.27
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB3	21	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	12	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	12	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	12	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	21	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	21	0.27
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	21	0.27
(1,1633)	1:742:A:VAL:HG21	1:835:A:ILE:HA	2	0.27
(1,1633)	1:742:A:VAL:HG22	1:835:A:ILE:HA	2	0.27
(1,1633)	1:742:A:VAL:HG23	1:835:A:ILE:HA	2	0.27
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	45	0.27
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	23	0.27
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	30	0.27
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	43	0.27
(1,2628)	1:823:A:LEU:HD11	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD11	1:828:A:GLN:HE22	47	0.26
(1,2628)	1:823:A:LEU:HD12	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD12	1:828:A:GLN:HE22	47	0.26
(1,2628)	1:823:A:LEU:HD13	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD13	1:828:A:GLN:HE22	47	0.26
(1,2628)	1:823:A:LEU:HD21	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD21	1:828:A:GLN:HE22	47	0.26
(1,2628)	1:823:A:LEU:HD22	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD22	1:828:A:GLN:HE22	47	0.26
(1,2628)	1:823:A:LEU:HD23	1:828:A:GLN:HE21	47	0.26
(1,2628)	1:823:A:LEU:HD23	1:828:A:GLN:HE22	47	0.26
(1,2339)	1:760:A:ARG:HG2	1:762:A:SER:H	21	0.26
(1,2339)	1:760:A:ARG:HG3	1:762:A:SER:H	21	0.26
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	25	0.26
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	22	0.25
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	23	0.25
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	23	0.25
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	23	0.25
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	23	0.25
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	23	0.25
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	20	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	40	0.25
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	2	0.25
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	29	0.25
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	34	0.25
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	46	0.25
(1,572)	1:816:A:SER:H	1:819:A:GLU:HB2	28	0.25
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	1	0.25
(1,80)	1:808:A:VAL:H	1:808:A:VAL:HB	35	0.25
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	12	0.24
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	12	0.24
(1,2402)	1:781:A:LYS:H	1:789:A:CYS:HB2	30	0.24
(1,2402)	1:781:A:LYS:H	1:789:A:CYS:HB3	30	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	32	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	32	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	32	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	33	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	33	0.24
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	33	0.24
(1,1741)	1:738:A:LEU:HA	1:738:A:LEU:HG	4	0.24
(1,1741)	1:738:A:LEU:HA	1:738:A:LEU:HG	13	0.24
(1,1741)	1:738:A:LEU:HA	1:738:A:LEU:HG	21	0.24
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	11	0.24
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	36	0.24
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	47	0.24
(1,149)	1:729:A:ALA:H	1:738:A:LEU:HG	4	0.24
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	34	0.23
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	4	0.23
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	21	0.23
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	37	0.23
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	24	0.23
(1,878)	1:841:A:GLU:H	1:842:A:THR:H	16	0.23
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	20	0.22
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	20	0.22
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	20	0.22
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	20	0.22
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	20	0.22
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	20	0.22
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	38	0.22
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	38	0.22
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	13	0.22
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	13	0.22
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	28	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	28	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	3	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	47	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	47	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	47	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	47	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	47	0.22
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	47	0.22
(1,1886)	1:727:A:VAL:HB	1:741:A:THR:HA	10	0.22
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	24	0.22
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	24	0.22
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	24	0.22
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	23	0.22
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	28	0.22
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	28	0.22
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	28	0.22
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	28	0.22
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	28	0.22
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	28	0.22
(1,1706)	1:782:A:CYS:HA	1:789:A:CYS:HA	24	0.22
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	12	0.22
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	20	0.22
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	5	0.22
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	16	0.22
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	24	0.22
(1,878)	1:841:A:GLU:H	1:842:A:THR:H	31	0.22
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	38	0.21
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	38	0.21
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	38	0.21
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	38	0.21
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	38	0.21
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	38	0.21
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	8	0.21
(1,1401)	1:808:A:VAL:HB	1:830:A:ILE:HA	18	0.21
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	18	0.21
(1,1354)	1:738:A:LEU:HG	1:740:A:LEU:HG	15	0.21
(1,1354)	1:738:A:LEU:HG	1:740:A:LEU:HG	36	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB1	21	0.21
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB2	21	0.21
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB3	21	0.21
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB1	21	0.21
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB2	21	0.21
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB3	21	0.21
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	33	0.21
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	48	0.21
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	1	0.2
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	1	0.2
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	1	0.2
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	1	0.2
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	1	0.2
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	1	0.2
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	26	0.2
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	26	0.2
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	26	0.2
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	26	0.2
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	26	0.2
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	26	0.2
(1,2480)	1:799:A:GLU:HG2	1:801:A:GLY:H	20	0.2
(1,2480)	1:799:A:GLU:HG3	1:801:A:GLY:H	20	0.2
(1,2411)	1:781:A:LYS:HG2	1:782:A:CYS:H	43	0.2
(1,2411)	1:781:A:LYS:HG3	1:782:A:CYS:H	43	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	9	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	9	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	9	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	9	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	9	0.2
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	9	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	15	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	15	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	15	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	15	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	15	0.2
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	15	0.2
(1,1633)	1:742:A:VAL:HG21	1:835:A:ILE:HA	29	0.2
(1,1633)	1:742:A:VAL:HG22	1:835:A:ILE:HA	29	0.2
(1,1633)	1:742:A:VAL:HG23	1:835:A:ILE:HA	29	0.2
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	3	0.2
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	22	0.2
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	30	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	35	0.2
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	35	0.2
(1,1354)	1:738:A:LEU:HG	1:740:A:LEU:HG	9	0.2
(1,1201)	1:725:A:LEU:HG	1:779:A:TRP:HZ2	18	0.2
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	13	0.2
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	45	0.2
(1,529)	1:773:A:CYS:H	1:789:A:CYS:H	31	0.2
(1,34)	1:709:A:GLN:H	1:709:A:GLN:HG2	14	0.2
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG2	36	0.19
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG3	36	0.19
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG2	36	0.19
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG3	36	0.19
(1,2423)	1:788:A:LYS:HE2	1:790:A:VAL:HA	23	0.19
(1,2423)	1:788:A:LYS:HE3	1:790:A:VAL:HA	23	0.19
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	40	0.19
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	40	0.19
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	9	0.19
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	9	0.19
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	9	0.19
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	9	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	17	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	42	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	43	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	43	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	43	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	43	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	43	0.19
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	43	0.19
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	41	0.19
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	41	0.19
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	41	0.19
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	41	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	41	0.19
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	41	0.19
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	13	0.19
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	13	0.19
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	13	0.19
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	6	0.19
(1,1813)	1:725:A:LEU:HG	1:817:A:GLU:HG3	18	0.19
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	45	0.19
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	45	0.19
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	45	0.19
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	45	0.19
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	45	0.19
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	45	0.19
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	5	0.19
(1,1471)	1:767:A:ALA:HA	1:768:A:SER:HB2	30	0.19
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	47	0.19
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	17	0.19
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	17	0.19
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	17	0.19
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	18	0.19
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	18	0.19
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	18	0.19
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	29	0.19
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	29	0.19
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	29	0.19
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	22	0.18
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	22	0.18
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	22	0.18
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	22	0.18
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	22	0.18
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	22	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB1	28	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB2	28	0.18
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB3	28	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB1	28	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB2	28	0.18
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB3	28	0.18
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	22	0.18
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	22	0.18
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG11	21	0.18
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG12	21	0.18
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG13	21	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG21	21	0.18
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG22	21	0.18
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG23	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG11	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG12	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG13	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG21	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG22	21	0.18
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG23	21	0.18
(1,2365)	1:771:A:LYS:HB2	1:776:A:CYS:HB2	34	0.18
(1,2365)	1:771:A:LYS:HB2	1:776:A:CYS:HB3	34	0.18
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	47	0.18
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	47	0.18
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	47	0.18
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	27	0.18
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	27	0.18
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	27	0.18
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	25	0.18
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	1	0.18
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	1	0.18
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	1	0.18
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	1	0.18
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	1	0.18
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	1	0.18
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	23	0.18
(1,1555)	1:725:A:LEU:HA	1:725:A:LEU:HG	43	0.18
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	18	0.18
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD11	35	0.18
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD12	35	0.18
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD13	35	0.18
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	5	0.18
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	20	0.18
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	39	0.18
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	7	0.18
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	7	0.18
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	7	0.18
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	44	0.18
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	44	0.18
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	44	0.18
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	26	0.18
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	26	0.18
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	26	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	7	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	7	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	7	0.18
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	19	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	19	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	19	0.18
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	23	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	23	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	23	0.18
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	31	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	31	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	31	0.18
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	37	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	37	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	37	0.18
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	42	0.18
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	42	0.18
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	42	0.18
(1,1107)	1:738:A:LEU:HD11	1:739:A:PRO:HD2	4	0.18
(1,1107)	1:738:A:LEU:HD12	1:739:A:PRO:HD2	4	0.18
(1,1107)	1:738:A:LEU:HD13	1:739:A:PRO:HD2	4	0.18
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	15	0.18
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	35	0.18
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	35	0.18
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	35	0.18
(1,149)	1:729:A:ALA:H	1:738:A:LEU:HG	13	0.18
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	24	0.17
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	31	0.17
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	31	0.17
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	31	0.17
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	31	0.17
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	31	0.17
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	31	0.17
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB1	27	0.17
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB2	27	0.17
(1,2602)	1:819:A:GLU:HG2	1:822:A:ALA:HB3	27	0.17
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB1	27	0.17
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB2	27	0.17
(1,2602)	1:819:A:GLU:HG3	1:822:A:ALA:HB3	27	0.17
(1,2567)	1:811:A:LYS:HG2	1:812:A:GLU:H	45	0.17
(1,2567)	1:811:A:LYS:HG3	1:812:A:GLU:H	45	0.17
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	1	0.17
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	1	0.17
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	1	0.17
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	1	0.17
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	1	0.17
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	30	0.17
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	30	0.17
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	30	0.17
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	30	0.17
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	30	0.17
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	30	0.17
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	17	0.17
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	17	0.17
(1,2423)	1:788:A:LYS:HE2	1:790:A:VAL:HA	30	0.17
(1,2423)	1:788:A:LYS:HE3	1:790:A:VAL:HA	30	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	16	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	18	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	18	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	18	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	18	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	18	0.17
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	18	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG11	38	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG12	38	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG13	38	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG21	38	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG22	38	0.17
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG23	38	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	6	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	6	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	6	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	6	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	6	0.17
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	6	0.17
(1,1886)	1:727:A:VAL:HB	1:741:A:THR:HA	14	0.17
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	20	0.17
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	26	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1443)	1:745:A:MET:HA	1:755:A:TYR:HB3	41	0.17
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD11	41	0.17
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD12	41	0.17
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD13	41	0.17
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	39	0.17
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	39	0.17
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	39	0.17
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	31	0.17
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	31	0.17
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	31	0.17
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	46	0.17
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	46	0.17
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	16	0.17
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	16	0.17
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	16	0.17
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	33	0.17
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	33	0.17
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	33	0.17
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	44	0.17
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	44	0.17
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	44	0.17
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	47	0.17
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	47	0.17
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	47	0.17
(1,1107)	1:738:A:LEU:HD11	1:739:A:PRO:HD2	13	0.17
(1,1107)	1:738:A:LEU:HD12	1:739:A:PRO:HD2	13	0.17
(1,1107)	1:738:A:LEU:HD13	1:739:A:PRO:HD2	13	0.17
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD11	15	0.17
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD12	15	0.17
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD13	15	0.17
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	20	0.17
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	20	0.17
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	20	0.17
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	29	0.17
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	29	0.17
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	29	0.17
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB1	25	0.17
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB2	25	0.17
(1,919)	1:766:A:PRO:HG2	1:767:A:ALA:HB3	25	0.17
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB1	25	0.17
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB2	25	0.17
(1,919)	1:766:A:PRO:HG3	1:767:A:ALA:HB3	25	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,880)	1:742:A:VAL:HG11	1:802:A:PHE:HE1	2	0.17
(1,880)	1:742:A:VAL:HG11	1:802:A:PHE:HE2	2	0.17
(1,880)	1:742:A:VAL:HG12	1:802:A:PHE:HE1	2	0.17
(1,880)	1:742:A:VAL:HG12	1:802:A:PHE:HE2	2	0.17
(1,880)	1:742:A:VAL:HG13	1:802:A:PHE:HE1	2	0.17
(1,880)	1:742:A:VAL:HG13	1:802:A:PHE:HE2	2	0.17
(1,878)	1:841:A:GLU:H	1:842:A:THR:H	8	0.17
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	18	0.17
(1,149)	1:729:A:ALA:H	1:738:A:LEU:HG	21	0.17
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	25	0.16
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	14	0.16
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	24	0.16
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	24	0.16
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	24	0.16
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	24	0.16
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	24	0.16
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	24	0.16
(1,2588)	1:816:A:SER:HB2	1:819:A:GLU:HB3	9	0.16
(1,2588)	1:816:A:SER:HB3	1:819:A:GLU:HB3	9	0.16
(1,2588)	1:816:A:SER:HB2	1:819:A:GLU:HB3	24	0.16
(1,2588)	1:816:A:SER:HB3	1:819:A:GLU:HB3	24	0.16
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	43	0.16
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	43	0.16
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	43	0.16
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	43	0.16
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	43	0.16
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	43	0.16
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	4	0.16
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	4	0.16
(1,2483)	1:800:A:GLU:H	1:800:A:GLU:HG2	38	0.16
(1,2483)	1:800:A:GLU:H	1:800:A:GLU:HG3	38	0.16
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB2	39	0.16
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB3	39	0.16
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB2	39	0.16
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB3	39	0.16
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	18	0.16
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	18	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	18	0.16
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	18	0.16
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG2	47	0.16
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG3	47	0.16
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG2	47	0.16
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG3	47	0.16
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG2	47	0.16
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG3	47	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	14	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	31	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	41	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	41	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	41	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	41	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	41	0.16
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	41	0.16
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB2	4	0.16
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB3	4	0.16
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB2	18	0.16
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB3	18	0.16
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB2	18	0.16
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB3	18	0.16
(1,2039)	1:716:A:LYS:HE2	1:717:A:MET:H	5	0.16
(1,2039)	1:716:A:LYS:HE3	1:717:A:MET:H	5	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	46	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	46	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	46	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	48	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	48	0.16
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	48	0.16
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	4	0.16
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	4	0.16
(1,1820)	1:824:A:ARG:HD2	1:830:A:ILE:HG13	29	0.16
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	38	0.16
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	40	0.16
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	43	0.16
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	43	0.16
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	43	0.16
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	43	0.16
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	43	0.16
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	43	0.16
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	32	0.16
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	18	0.16
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	18	0.16
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	18	0.16
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG21	2	0.16
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG22	2	0.16
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG23	2	0.16
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	14	0.16
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	14	0.16
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	19	0.16
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	19	0.16
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	32	0.16
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	32	0.16
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	32	0.16
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	32	0.16
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	32	0.16
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	32	0.16
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	34	0.16
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	34	0.16
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	34	0.16
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	34	0.16
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	34	0.16
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	34	0.16
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	1	0.16
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	1	0.16
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	1	0.16
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	3	0.16
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	3	0.16
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	3	0.16
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	43	0.16
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	43	0.16
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	43	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1057)	1:743:A:CYS:HA	1:802:A:PHE:HD1	2	0.16
(1,1057)	1:743:A:CYS:HA	1:802:A:PHE:HD2	2	0.16
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	33	0.16
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	43	0.16
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	2	0.16
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	2	0.16
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	2	0.16
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	5	0.16
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	5	0.16
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	5	0.16
(1,918)	1:766:A:PRO:HB2	1:767:A:ALA:HB1	21	0.16
(1,918)	1:766:A:PRO:HB2	1:767:A:ALA:HB2	21	0.16
(1,918)	1:766:A:PRO:HB2	1:767:A:ALA:HB3	21	0.16
(1,529)	1:773:A:CYS:H	1:789:A:CYS:H	33	0.16
(1,192)	1:728:A:CYS:HB3	1:763:A:CYS:H	43	0.16
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	17	0.15
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	17	0.15
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	40	0.15
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	40	0.15
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	48	0.15
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	48	0.15
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	48	0.15
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	48	0.15
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	48	0.15
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	48	0.15
(1,2480)	1:799:A:GLU:HG2	1:801:A:GLY:H	5	0.15
(1,2480)	1:799:A:GLU:HG3	1:801:A:GLY:H	5	0.15
(1,2424)	1:788:A:LYS:HE2	1:790:A:VAL:HB	11	0.15
(1,2424)	1:788:A:LYS:HE3	1:790:A:VAL:HB	11	0.15
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	44	0.15
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	44	0.15
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	44	0.15
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	44	0.15
(1,2240)	1:742:A:VAL:HG11	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG12	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG13	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG21	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG22	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG23	1:746:A:HIS:HA	2	0.15
(1,2240)	1:742:A:VAL:HG11	1:746:A:HIS:HA	29	0.15
(1,2240)	1:742:A:VAL:HG12	1:746:A:HIS:HA	29	0.15
(1,2240)	1:742:A:VAL:HG13	1:746:A:HIS:HA	29	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2240)	1:742:A:VAL:HG21	1:746:A:HIS:HA	29	0.15
(1,2240)	1:742:A:VAL:HG22	1:746:A:HIS:HA	29	0.15
(1,2240)	1:742:A:VAL:HG23	1:746:A:HIS:HA	29	0.15
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB2	30	0.15
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB3	30	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	17	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	25	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	25	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	25	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	25	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	25	0.15
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	25	0.15
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB2	5	0.15
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB3	5	0.15
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB2	5	0.15
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB3	5	0.15
(1,1925)	1:700:A:PRO:HA	1:701:A:LYS:HG2	39	0.15
(1,1925)	1:700:A:PRO:HA	1:701:A:LYS:HG3	39	0.15
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	16	0.15
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	16	0.15
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	16	0.15
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	16	0.15
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	16	0.15
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	16	0.15
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	12	0.15
(1,1782)	1:822:A:ALA:HB1	1:825:A:CYS:HB3	39	0.15
(1,1782)	1:822:A:ALA:HB2	1:825:A:CYS:HB3	39	0.15
(1,1782)	1:822:A:ALA:HB3	1:825:A:CYS:HB3	39	0.15
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	18	0.15
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	18	0.15
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	18	0.15
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	18	0.15
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	18	0.15
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	18	0.15
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG2	27	0.15
(1,1777)	1:765:A:LEU:HD21	1:766:A:PRO:HG3	27	0.15
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG2	27	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1777)	1:765:A:LEU:HD22	1:766:A:PRO:HG3	27	0.15
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG2	27	0.15
(1,1777)	1:765:A:LEU:HD23	1:766:A:PRO:HG3	27	0.15
(1,1751)	1:747:A:VAL:HG21	1:802:A:PHE:HD1	15	0.15
(1,1751)	1:747:A:VAL:HG21	1:802:A:PHE:HD2	15	0.15
(1,1751)	1:747:A:VAL:HG22	1:802:A:PHE:HD1	15	0.15
(1,1751)	1:747:A:VAL:HG22	1:802:A:PHE:HD2	15	0.15
(1,1751)	1:747:A:VAL:HG23	1:802:A:PHE:HD1	15	0.15
(1,1751)	1:747:A:VAL:HG23	1:802:A:PHE:HD2	15	0.15
(1,1720)	1:811:A:LYS:HA	1:811:A:LYS:HG2	19	0.15
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	14	0.15
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	10	0.15
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	12	0.15
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	24	0.15
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	4	0.15
(1,1422)	1:709:A:GLN:HA	1:709:A:GLN:HG3	45	0.15
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	2	0.15
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	28	0.15
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	29	0.15
(1,1270)	1:794:A:ALA:HB1	1:819:A:GLU:HB2	9	0.15
(1,1270)	1:794:A:ALA:HB2	1:819:A:GLU:HB2	9	0.15
(1,1270)	1:794:A:ALA:HB3	1:819:A:GLU:HB2	9	0.15
(1,1270)	1:794:A:ALA:HB1	1:819:A:GLU:HB2	33	0.15
(1,1270)	1:794:A:ALA:HB2	1:819:A:GLU:HB2	33	0.15
(1,1270)	1:794:A:ALA:HB3	1:819:A:GLU:HB2	33	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	3	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	3	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	16	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	16	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	17	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	17	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	31	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	31	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	41	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	41	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	42	0.15
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	42	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	38	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	38	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	38	0.15
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	38	0.15
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	38	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	38	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	45	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	45	0.15
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	45	0.15
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	45	0.15
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	45	0.15
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	45	0.15
(1,1201)	1:725:A:LEU:HG	1:779:A:TRP:HZ2	3	0.15
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	20	0.15
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	20	0.15
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	20	0.15
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	28	0.15
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	28	0.15
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	28	0.15
(1,1058)	1:829:A:SER:HB2	1:830:A:ILE:HA	11	0.15
(1,1058)	1:829:A:SER:HB2	1:830:A:ILE:HA	29	0.15
(1,1026)	1:698:A:ALA:HA	1:699:A:VAL:H	6	0.15
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	3	0.15
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	3	0.15
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	3	0.15
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	22	0.15
(1,802)	1:709:A:GLN:HE22	1:714:A:VAL:HG21	14	0.15
(1,802)	1:709:A:GLN:HE22	1:714:A:VAL:HG22	14	0.15
(1,802)	1:709:A:GLN:HE22	1:714:A:VAL:HG23	14	0.15
(1,782)	1:760:A:ARG:HE	1:761:A:ASP:HA	7	0.15
(1,531)	1:773:A:CYS:H	1:773:A:CYS:HB3	21	0.15
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD11	28	0.14
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD12	28	0.14
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD13	28	0.14
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD21	28	0.14
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD22	28	0.14
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD23	28	0.14
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG2	24	0.14
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG3	24	0.14
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG2	24	0.14
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG3	24	0.14
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	35	0.14
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	35	0.14
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	35	0.14
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	35	0.14
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	35	0.14
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	35	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	25	0.14
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	25	0.14
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	39	0.14
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	39	0.14
(1,2480)	1:799:A:GLU:HG2	1:801:A:GLY:H	43	0.14
(1,2480)	1:799:A:GLU:HG3	1:801:A:GLY:H	43	0.14
(1,2454)	1:793:A:GLU:HG2	1:822:A:ALA:HB1	39	0.14
(1,2454)	1:793:A:GLU:HG2	1:822:A:ALA:HB2	39	0.14
(1,2454)	1:793:A:GLU:HG2	1:822:A:ALA:HB3	39	0.14
(1,2454)	1:793:A:GLU:HG3	1:822:A:ALA:HB1	39	0.14
(1,2454)	1:793:A:GLU:HG3	1:822:A:ALA:HB2	39	0.14
(1,2454)	1:793:A:GLU:HG3	1:822:A:ALA:HB3	39	0.14
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB2	23	0.14
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB3	23	0.14
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB2	23	0.14
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB3	23	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG11	29	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG12	29	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG13	29	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG21	29	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG22	29	0.14
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG23	29	0.14
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB1	24	0.14
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB2	24	0.14
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB3	24	0.14
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB1	24	0.14
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB2	24	0.14
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB3	24	0.14
(1,2338)	1:760:A:ARG:HG2	1:761:A:ASP:HB2	21	0.14
(1,2338)	1:760:A:ARG:HG2	1:761:A:ASP:HB3	21	0.14
(1,2338)	1:760:A:ARG:HG3	1:761:A:ASP:HB2	21	0.14
(1,2338)	1:760:A:ARG:HG3	1:761:A:ASP:HB3	21	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	14	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	26	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	26	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	26	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	26	0.14
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	26	0.14
(1,2007)	1:707:A:LYS:HG2	1:716:A:LYS:HA	25	0.14
(1,2007)	1:707:A:LYS:HG3	1:716:A:LYS:HA	25	0.14
(1,1954)	1:703:A:GLN:H	1:713:A:CYS:HB2	20	0.14
(1,1954)	1:703:A:GLN:H	1:713:A:CYS:HB3	20	0.14
(1,1886)	1:727:A:VAL:HB	1:741:A:THR:HA	16	0.14
(1,1869)	1:741:A:THR:HG21	1:742:A:VAL:HA	34	0.14
(1,1869)	1:741:A:THR:HG22	1:742:A:VAL:HA	34	0.14
(1,1869)	1:741:A:THR:HG23	1:742:A:VAL:HA	34	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	7	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	7	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	7	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	10	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	10	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	10	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	14	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	14	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	14	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	22	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	22	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	22	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	34	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	34	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	34	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	36	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	36	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	36	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	37	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	37	0.14
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	37	0.14
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	26	0.14
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	31	0.14
(1,1564)	1:736:A:ARG:HA	1:737:A:ILE:HD11	4	0.14
(1,1564)	1:736:A:ARG:HA	1:737:A:ILE:HD12	4	0.14
(1,1564)	1:736:A:ARG:HA	1:737:A:ILE:HD13	4	0.14
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	30	0.14
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	33	0.14
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	39	0.14
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	19	0.14
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	10	0.14
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	26	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	33	0.14
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	48	0.14
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	12	0.14
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	15	0.14
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	44	0.14
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	5	0.14
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	36	0.14
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	12	0.14
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	8	0.14
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	8	0.14
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	8	0.14
(1,1313)	1:742:A:VAL:HG11	1:835:A:ILE:HB	3	0.14
(1,1313)	1:742:A:VAL:HG12	1:835:A:ILE:HB	3	0.14
(1,1313)	1:742:A:VAL:HG13	1:835:A:ILE:HB	3	0.14
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	41	0.14
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	41	0.14
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	41	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	12	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	12	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	12	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	33	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	33	0.14
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	33	0.14
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	4	0.14
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	4	0.14
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	4	0.14
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	4	0.14
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	4	0.14
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	4	0.14
(1,1201)	1:725:A:LEU:HG	1:779:A:TRP:HZ2	35	0.14
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	30	0.14
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	30	0.14
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	30	0.14
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	30	0.14
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	30	0.14
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	30	0.14
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	47	0.14
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	47	0.14
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	47	0.14
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	47	0.14
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	47	0.14
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	47	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:802:A:PHE:HE1	1:803:A:SER:H	16	0.14
(1,1185)	1:802:A:PHE:HE2	1:803:A:SER:H	16	0.14
(1,1185)	1:802:A:PHE:HE1	1:803:A:SER:H	19	0.14
(1,1185)	1:802:A:PHE:HE2	1:803:A:SER:H	19	0.14
(1,1185)	1:802:A:PHE:HE1	1:803:A:SER:H	21	0.14
(1,1185)	1:802:A:PHE:HE2	1:803:A:SER:H	21	0.14
(1,1171)	1:812:A:GLU:HA	1:815:A:MET:HE1	37	0.14
(1,1171)	1:812:A:GLU:HA	1:815:A:MET:HE2	37	0.14
(1,1171)	1:812:A:GLU:HA	1:815:A:MET:HE3	37	0.14
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	30	0.14
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	30	0.14
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	30	0.14
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	32	0.14
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	32	0.14
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	32	0.14
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	38	0.14
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	38	0.14
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	38	0.14
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	40	0.14
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	40	0.14
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	40	0.14
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	46	0.14
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	46	0.14
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	46	0.14
(1,1107)	1:738:A:LEU:HD11	1:739:A:PRO:HD2	21	0.14
(1,1107)	1:738:A:LEU:HD12	1:739:A:PRO:HD2	21	0.14
(1,1107)	1:738:A:LEU:HD13	1:739:A:PRO:HD2	21	0.14
(1,1102)	1:731:A:ASP:H	1:736:A:ARG:HG2	29	0.14
(1,1098)	1:709:A:GLN:HG3	1:712:A:ARG:HG2	31	0.14
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	2	0.14
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	5	0.14
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	31	0.14
(1,993)	1:800:A:GLU:H	1:800:A:GLU:HG3	43	0.14
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	7	0.14
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	7	0.14
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	7	0.14
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	33	0.14
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	45	0.14
(1,818)	1:717:A:MET:HE1	1:751:A:GLN:HE22	41	0.14
(1,818)	1:717:A:MET:HE2	1:751:A:GLN:HE22	41	0.14
(1,818)	1:717:A:MET:HE3	1:751:A:GLN:HE22	41	0.14
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:841:A:GLU:HA	1:842:A:THR:H	5	0.14
(1,579)	1:841:A:GLU:HA	1:842:A:THR:H	10	0.14
(1,532)	1:773:A:CYS:H	1:773:A:CYS:HB2	23	0.14
(1,519)	1:767:A:ALA:HA	1:768:A:SER:H	22	0.14
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	12	0.14
(1,453)	1:741:A:THR:HG21	1:744:A:LYS:H	7	0.14
(1,453)	1:741:A:THR:HG22	1:744:A:LYS:H	7	0.14
(1,453)	1:741:A:THR:HG23	1:744:A:LYS:H	7	0.14
(1,298)	1:702:A:CYS:HB3	1:706:A:GLU:H	45	0.14
(1,294)	1:706:A:GLU:H	1:716:A:LYS:H	25	0.14
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	26	0.14
(1,109)	1:794:A:ALA:H	1:795:A:SER:HA	42	0.14
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD11	42	0.13
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD12	42	0.13
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD13	42	0.13
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD11	42	0.13
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD12	42	0.13
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD13	42	0.13
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	35	0.13
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	35	0.13
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	43	0.13
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	43	0.13
(1,2635)	1:824:A:ARG:HB2	1:830:A:ILE:HD11	37	0.13
(1,2635)	1:824:A:ARG:HB2	1:830:A:ILE:HD12	37	0.13
(1,2635)	1:824:A:ARG:HB2	1:830:A:ILE:HD13	37	0.13
(1,2635)	1:824:A:ARG:HB3	1:830:A:ILE:HD11	37	0.13
(1,2635)	1:824:A:ARG:HB3	1:830:A:ILE:HD12	37	0.13
(1,2635)	1:824:A:ARG:HB3	1:830:A:ILE:HD13	37	0.13
(1,2588)	1:816:A:SER:HB2	1:819:A:GLU:HB3	15	0.13
(1,2588)	1:816:A:SER:HB3	1:819:A:GLU:HB3	15	0.13
(1,2584)	1:816:A:SER:HB2	1:817:A:GLU:HB2	32	0.13
(1,2584)	1:816:A:SER:HB3	1:817:A:GLU:HB2	32	0.13
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG2	9	0.13
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG3	9	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG2	9	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG3	9	0.13
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG2	15	0.13
(1,2579)	1:815:A:MET:HB2	1:819:A:GLU:HG3	15	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG2	15	0.13
(1,2579)	1:815:A:MET:HB3	1:819:A:GLU:HG3	15	0.13
(1,2567)	1:811:A:LYS:HG2	1:812:A:GLU:H	17	0.13
(1,2567)	1:811:A:LYS:HG3	1:812:A:GLU:H	17	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2567)	1:811:A:LYS:HG2	1:812:A:GLU:H	32	0.13
(1,2567)	1:811:A:LYS:HG3	1:812:A:GLU:H	32	0.13
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE22	2	0.13
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE22	2	0.13
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE22	2	0.13
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE22	2	0.13
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE22	2	0.13
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE21	2	0.13
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE22	2	0.13
(1,2539)	1:808:A:VAL:HG11	1:809:A:ASN:HA	23	0.13
(1,2539)	1:808:A:VAL:HG12	1:809:A:ASN:HA	23	0.13
(1,2539)	1:808:A:VAL:HG13	1:809:A:ASN:HA	23	0.13
(1,2539)	1:808:A:VAL:HG21	1:809:A:ASN:HA	23	0.13
(1,2539)	1:808:A:VAL:HG22	1:809:A:ASN:HA	23	0.13
(1,2539)	1:808:A:VAL:HG23	1:809:A:ASN:HA	23	0.13
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG2	40	0.13
(1,2487)	1:801:A:GLY:H	1:817:A:GLU:HG3	40	0.13
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB1	14	0.13
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB2	14	0.13
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB3	14	0.13
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB1	14	0.13
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB2	14	0.13
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB3	14	0.13
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB2	24	0.13
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB3	24	0.13
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE2	14	0.13
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE3	14	0.13
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE2	34	0.13
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE3	34	0.13
(1,2360)	1:771:A:LYS:H	1:771:A:LYS:HG2	40	0.13
(1,2360)	1:771:A:LYS:H	1:771:A:LYS:HG3	40	0.13
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	39	0.13
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	39	0.13
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	39	0.13
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	39	0.13
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	21	0.13
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	21	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG2	33	0.13
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG3	33	0.13
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG2	33	0.13
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG3	33	0.13
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG2	33	0.13
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG3	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD11	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD12	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD13	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD21	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD22	33	0.13
(1,2224)	1:740:A:LEU:HA	1:748:A:LEU:HD23	33	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	43	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	45	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	45	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	45	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	45	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	45	0.13
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	45	0.13
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB2	21	0.13
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB3	21	0.13
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB2	21	0.13
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB3	21	0.13
(1,2041)	1:717:A:MET:HA	1:720:A:GLU:HB2	33	0.13
(1,2041)	1:717:A:MET:HA	1:720:A:GLU:HB3	33	0.13
(1,1963)	1:703:A:GLN:HG2	1:705:A:TRP:HE1	16	0.13
(1,1963)	1:703:A:GLN:HG3	1:705:A:TRP:HE1	16	0.13
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	4	0.13
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	4	0.13
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	4	0.13
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	40	0.13
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	40	0.13
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	40	0.13
(1,1821)	1:824:A:ARG:HD3	1:830:A:ILE:HG13	30	0.13
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	22	0.13
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	32	0.13
(1,1771)	1:778:A:LEU:HD21	1:779:A:TRP:HZ2	10	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:778:A:LEU:HD22	1:779:A:TRP:HZ2	10	0.13
(1,1771)	1:778:A:LEU:HD23	1:779:A:TRP:HZ2	10	0.13
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	31	0.13
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	31	0.13
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	31	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	7	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	9	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	17	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	18	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	21	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	36	0.13
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	48	0.13
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	16	0.13
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	17	0.13
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	20	0.13
(1,1476)	1:813:A:GLN:HA	1:840:A:ALA:HA	9	0.13
(1,1476)	1:813:A:GLN:HA	1:840:A:ALA:HA	13	0.13
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	28	0.13
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	7	0.13
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	14	0.13
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	20	0.13
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	40	0.13
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	23	0.13
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD11	37	0.13
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD12	37	0.13
(1,1438)	1:728:A:CYS:HB3	1:737:A:ILE:HD13	37	0.13
(1,1428)	1:709:A:GLN:HG3	1:710:A:ASN:HB3	14	0.13
(1,1410)	1:725:A:LEU:HD11	1:817:A:GLU:HB3	12	0.13
(1,1410)	1:725:A:LEU:HD12	1:817:A:GLU:HB3	12	0.13
(1,1410)	1:725:A:LEU:HD13	1:817:A:GLU:HB3	12	0.13
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	17	0.13
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	41	0.13
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	44	0.13
(1,1325)	1:742:A:VAL:HG21	1:835:A:ILE:HB	20	0.13
(1,1325)	1:742:A:VAL:HG22	1:835:A:ILE:HB	20	0.13
(1,1325)	1:742:A:VAL:HG23	1:835:A:ILE:HB	20	0.13
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG11	32	0.13
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG12	32	0.13
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG13	32	0.13
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	3	0.13
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	3	0.13
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	47	0.13
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	47	0.13
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	47	0.13
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	46	0.13
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	46	0.13
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	46	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	4	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	4	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	33	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	33	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	34	0.13
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	34	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	21	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	21	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	21	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	21	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	21	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	21	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	23	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	23	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	23	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	23	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	23	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	23	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	31	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	31	0.13
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	31	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	31	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	31	0.13
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	31	0.13
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	11	0.13
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	11	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	11	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	11	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	11	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	11	0.13
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	23	0.13
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	23	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	23	0.13
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	23	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	23	0.13
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	23	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1185)	1:802:A:PHE:HE1	1:803:A:SER:H	29	0.13
(1,1185)	1:802:A:PHE:HE2	1:803:A:SER:H	29	0.13
(1,1122)	1:724:A:SER:HA	1:778:A:LEU:HD21	39	0.13
(1,1122)	1:724:A:SER:HA	1:778:A:LEU:HD22	39	0.13
(1,1122)	1:724:A:SER:HA	1:778:A:LEU:HD23	39	0.13
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	5	0.13
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	5	0.13
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	5	0.13
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	6	0.13
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	6	0.13
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	6	0.13
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	35	0.13
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	35	0.13
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	35	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD11	9	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD12	9	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD13	9	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD11	36	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD12	36	0.13
(1,1085)	1:738:A:LEU:HG	1:740:A:LEU:HD13	36	0.13
(1,1050)	1:705:A:TRP:HD1	1:750:A:CYS:HA	31	0.13
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	1	0.13
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	10	0.13
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	16	0.13
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	20	0.13
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	41	0.13
(1,1016)	1:811:A:LYS:HE2	1:812:A:GLU:H	42	0.13
(1,967)	1:815:A:MET:HG3	1:820:A:ALA:H	28	0.13
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	47	0.13
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	14	0.13
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	21	0.13
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	29	0.13
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	30	0.13
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	47	0.13
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	1	0.13
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	10	0.13
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	36	0.13
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	40	0.13
(1,727)	1:709:A:GLN:HG3	1:710:A:ASN:H	14	0.13
(1,585)	1:735:A:LYS:H	1:735:A:LYS:HD2	9	0.13
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	24	0.13
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	33	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,407)	1:704:A:ARG:H	1:705:A:TRP:HZ2	17	0.13
(1,309)	1:824:A:ARG:H	1:824:A:ARG:HE	5	0.13
(1,268)	1:690:A:SER:HA	1:691:A:HIS:H	31	0.13
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	18	0.13
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	19	0.13
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	21	0.12
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	12	0.12
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	12	0.12
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	32	0.12
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	32	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD11	48	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD12	48	0.12
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD13	48	0.12
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD11	48	0.12
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD12	48	0.12
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD13	48	0.12
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	44	0.12
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	44	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	29	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	29	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	48	0.12
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	48	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD11	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD12	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD13	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD21	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD22	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD23	2	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD11	47	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD12	47	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD13	47	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD21	47	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD22	47	0.12
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD23	47	0.12
(1,2594)	1:818:A:CYS:HB2	1:822:A:ALA:HB1	21	0.12
(1,2594)	1:818:A:CYS:HB2	1:822:A:ALA:HB2	21	0.12
(1,2594)	1:818:A:CYS:HB2	1:822:A:ALA:HB3	21	0.12
(1,2594)	1:818:A:CYS:HB3	1:822:A:ALA:HB1	21	0.12
(1,2594)	1:818:A:CYS:HB3	1:822:A:ALA:HB2	21	0.12
(1,2594)	1:818:A:CYS:HB3	1:822:A:ALA:HB3	21	0.12
(1,2567)	1:811:A:LYS:HG2	1:812:A:GLU:H	15	0.12
(1,2567)	1:811:A:LYS:HG3	1:812:A:GLU:H	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	34	0.12
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	34	0.12
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	34	0.12
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	34	0.12
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	34	0.12
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	34	0.12
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	32	0.12
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	32	0.12
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	32	0.12
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	32	0.12
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	32	0.12
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	32	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB1	25	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB2	25	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB3	25	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB1	25	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB2	25	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB3	25	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB1	47	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB2	47	0.12
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB3	47	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB1	47	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB2	47	0.12
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB3	47	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG11	23	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG12	23	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG13	23	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG21	23	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG22	23	0.12
(1,2425)	1:788:A:LYS:HE2	1:790:A:VAL:HG23	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG11	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG12	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG13	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG21	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG22	23	0.12
(1,2425)	1:788:A:LYS:HE3	1:790:A:VAL:HG23	23	0.12
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB2	25	0.12
(1,2420)	1:788:A:LYS:HG2	1:789:A:CYS:HB3	25	0.12
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB2	25	0.12
(1,2420)	1:788:A:LYS:HG3	1:789:A:CYS:HB3	25	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG11	22	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG12	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG13	22	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG21	22	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG22	22	0.12
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG23	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG11	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG12	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG13	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG21	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG22	22	0.12
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG23	22	0.12
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	16	0.12
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	16	0.12
(1,2392)	1:778:A:LEU:HD11	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD11	1:817:A:GLU:HG3	47	0.12
(1,2392)	1:778:A:LEU:HD12	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD12	1:817:A:GLU:HG3	47	0.12
(1,2392)	1:778:A:LEU:HD13	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD13	1:817:A:GLU:HG3	47	0.12
(1,2392)	1:778:A:LEU:HD21	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD21	1:817:A:GLU:HG3	47	0.12
(1,2392)	1:778:A:LEU:HD22	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD22	1:817:A:GLU:HG3	47	0.12
(1,2392)	1:778:A:LEU:HD23	1:817:A:GLU:HG2	47	0.12
(1,2392)	1:778:A:LEU:HD23	1:817:A:GLU:HG3	47	0.12
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB2	48	0.12
(1,2368)	1:772:A:ALA:HA	1:788:A:LYS:HB3	48	0.12
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE2	8	0.12
(1,2364)	1:771:A:LYS:HA	1:771:A:LYS:HE3	8	0.12
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	3	0.12
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	3	0.12
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	12	0.12
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	12	0.12
(1,2352)	1:769:A:ALA:HB1	1:771:A:LYS:HE2	46	0.12
(1,2352)	1:769:A:ALA:HB1	1:771:A:LYS:HE3	46	0.12
(1,2352)	1:769:A:ALA:HB2	1:771:A:LYS:HE2	46	0.12
(1,2352)	1:769:A:ALA:HB2	1:771:A:LYS:HE3	46	0.12
(1,2352)	1:769:A:ALA:HB3	1:771:A:LYS:HE2	46	0.12
(1,2352)	1:769:A:ALA:HB3	1:771:A:LYS:HE3	46	0.12
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG2	28	0.12
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG3	28	0.12
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG2	28	0.12
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG3	28	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG2	28	0.12
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG3	28	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD11	9	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD12	9	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD13	9	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD21	9	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD22	9	0.12
(1,2072)	1:724:A:SER:H	1:778:A:LEU:HD23	9	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	12	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	27	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	47	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	47	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	47	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	47	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	47	0.12
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	47	0.12
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB2	16	0.12
(1,2060)	1:721:A:CYS:HB2	1:743:A:CYS:HB3	16	0.12
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB2	16	0.12
(1,2060)	1:721:A:CYS:HB3	1:743:A:CYS:HB3	16	0.12
(1,2039)	1:716:A:LYS:HE2	1:717:A:MET:H	33	0.12
(1,2039)	1:716:A:LYS:HE3	1:717:A:MET:H	33	0.12
(1,1997)	1:706:A:GLU:HB2	1:713:A:CYS:HB2	16	0.12
(1,1997)	1:706:A:GLU:HB2	1:713:A:CYS:HB3	16	0.12
(1,1982)	1:704:A:ARG:HG2	1:802:A:PHE:HD1	15	0.12
(1,1982)	1:704:A:ARG:HG2	1:802:A:PHE:HD2	15	0.12
(1,1982)	1:704:A:ARG:HG3	1:802:A:PHE:HD1	15	0.12
(1,1982)	1:704:A:ARG:HG3	1:802:A:PHE:HD2	15	0.12
(1,1934)	1:701:A:LYS:HA	1:701:A:LYS:HD2	30	0.12
(1,1934)	1:701:A:LYS:HA	1:701:A:LYS:HD3	30	0.12
(1,1926)	1:700:A:PRO:HA	1:701:A:LYS:HD2	13	0.12
(1,1926)	1:700:A:PRO:HA	1:701:A:LYS:HD3	13	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	23	0.12
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	23	0.12
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	23	0.12
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	11	0.12
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	11	0.12
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	11	0.12
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	30	0.12
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	21	0.12
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	21	0.12
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	21	0.12
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	47	0.12
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	47	0.12
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	47	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	14	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	14	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	14	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	43	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	43	0.12
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	43	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	8	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	8	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	8	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	8	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	8	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	8	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	8	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	8	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	8	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	45	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	45	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	45	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	45	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	45	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	45	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	45	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	45	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	45	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	48	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	48	0.12
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	48	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	48	0.12
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	48	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	48	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	48	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	48	0.12
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	48	0.12
(1,1672)	1:726:A:ASP:HB3	1:727:A:VAL:HA	12	0.12
(1,1620)	1:721:A:CYS:HB2	1:744:A:LYS:HA	12	0.12
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	3	0.12
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	19	0.12
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	28	0.12
(1,1556)	1:736:A:ARG:HA	1:736:A:ARG:HD2	45	0.12
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	11	0.12
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	20	0.12
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	32	0.12
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	2	0.12
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	19	0.12
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	29	0.12
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	30	0.12
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	31	0.12
(1,1456)	1:836:A:ARG:HA	1:836:A:ARG:HD2	8	0.12
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	1	0.12
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	15	0.12
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	41	0.12
(1,1443)	1:745:A:MET:HA	1:755:A:TYR:HB3	9	0.12
(1,1410)	1:725:A:LEU:HD11	1:817:A:GLU:HB3	22	0.12
(1,1410)	1:725:A:LEU:HD12	1:817:A:GLU:HB3	22	0.12
(1,1410)	1:725:A:LEU:HD13	1:817:A:GLU:HB3	22	0.12
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	4	0.12
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	9	0.12
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	19	0.12
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	22	0.12
(1,1384)	1:724:A:SER:HA	1:742:A:VAL:HB	16	0.12
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	12	0.12
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	25	0.12
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	38	0.12
(1,1374)	1:745:A:MET:HG2	1:746:A:HIS:HB2	18	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG11	30	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG12	30	0.12
(1,1316)	1:724:A:SER:HA	1:742:A:VAL:HG13	30	0.12
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	4	0.12
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	4	0.12
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	4	0.12
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	35	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	35	0.12
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	35	0.12
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	46	0.12
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	46	0.12
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	46	0.12
(1,1313)	1:742:A:VAL:HG11	1:835:A:ILE:HB	9	0.12
(1,1313)	1:742:A:VAL:HG12	1:835:A:ILE:HB	9	0.12
(1,1313)	1:742:A:VAL:HG13	1:835:A:ILE:HB	9	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	10	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	10	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	10	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	11	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	11	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	11	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	16	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	16	0.12
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	16	0.12
(1,1294)	1:808:A:VAL:HG21	1:813:A:GLN:H	20	0.12
(1,1294)	1:808:A:VAL:HG22	1:813:A:GLN:H	20	0.12
(1,1294)	1:808:A:VAL:HG23	1:813:A:GLN:H	20	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	5	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	5	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	9	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	9	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	27	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	27	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	43	0.12
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	43	0.12
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	13	0.12
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	13	0.12
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	13	0.12
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	13	0.12
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	13	0.12
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	13	0.12
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	1	0.12
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	1	0.12
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	1	0.12
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	1	0.12
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	1	0.12
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	1	0.12
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	22	0.12
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	22	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	22	0.12
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	22	0.12
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	22	0.12
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	22	0.12
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	2	0.12
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	2	0.12
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	2	0.12
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	12	0.12
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	12	0.12
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	12	0.12
(1,1095)	1:727:A:VAL:HG11	1:835:A:ILE:HA	12	0.12
(1,1095)	1:727:A:VAL:HG12	1:835:A:ILE:HA	12	0.12
(1,1095)	1:727:A:VAL:HG13	1:835:A:ILE:HA	12	0.12
(1,1095)	1:727:A:VAL:HG11	1:835:A:ILE:HA	23	0.12
(1,1095)	1:727:A:VAL:HG12	1:835:A:ILE:HA	23	0.12
(1,1095)	1:727:A:VAL:HG13	1:835:A:ILE:HA	23	0.12
(1,1095)	1:727:A:VAL:HG11	1:835:A:ILE:HA	30	0.12
(1,1095)	1:727:A:VAL:HG12	1:835:A:ILE:HA	30	0.12
(1,1095)	1:727:A:VAL:HG13	1:835:A:ILE:HA	30	0.12
(1,1050)	1:705:A:TRP:HD1	1:750:A:CYS:HA	34	0.12
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	23	0.12
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	4	0.12
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	9	0.12
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	9	0.12
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	9	0.12
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	9	0.12
(1,917)	1:813:A:GLN:HG3	1:840:A:ALA:HB1	2	0.12
(1,917)	1:813:A:GLN:HG3	1:840:A:ALA:HB2	2	0.12
(1,917)	1:813:A:GLN:HG3	1:840:A:ALA:HB3	2	0.12
(1,863)	1:795:A:SER:H	1:797:A:CYS:H	13	0.12
(1,863)	1:795:A:SER:H	1:797:A:CYS:H	15	0.12
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	34	0.12
(1,811)	1:709:A:GLN:HG3	1:710:A:ASN:HD21	24	0.12
(1,782)	1:760:A:ARG:HE	1:761:A:ASP:HA	36	0.12
(1,572)	1:816:A:SER:H	1:819:A:GLU:HB2	27	0.12
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	24	0.12
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	24	0.12
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	24	0.12
(1,533)	1:772:A:ALA:HB1	1:773:A:CYS:H	31	0.12
(1,533)	1:772:A:ALA:HB2	1:773:A:CYS:H	31	0.12
(1,533)	1:772:A:ALA:HB3	1:773:A:CYS:H	31	0.12
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	10	0.12
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	40	0.12
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	15	0.12
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	48	0.12
(1,309)	1:824:A:ARG:H	1:824:A:ARG:HE	8	0.12
(1,268)	1:690:A:SER:HA	1:691:A:HIS:H	2	0.12
(1,268)	1:690:A:SER:HA	1:691:A:HIS:H	28	0.12
(1,260)	1:809:A:ASN:HB3	1:811:A:LYS:H	24	0.12
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	2	0.12
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	30	0.12
(1,114)	1:775:A:ALA:H	1:776:A:CYS:H	22	0.12
(1,114)	1:775:A:ALA:H	1:776:A:CYS:H	46	0.12
(1,5)	1:765:A:LEU:H	1:765:A:LEU:HD11	20	0.12
(1,5)	1:765:A:LEU:H	1:765:A:LEU:HD12	20	0.12
(1,5)	1:765:A:LEU:H	1:765:A:LEU:HD13	20	0.12
(2,17)	1:790:A:VAL:H	1:781:A:LYS:O	34	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	30	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	30	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	40	0.11
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	40	0.11
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	13	0.11
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	13	0.11
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	24	0.11
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	24	0.11
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	28	0.11
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	28	0.11
(1,2641)	1:826:A:ARG:H	1:826:A:ARG:HG2	14	0.11
(1,2641)	1:826:A:ARG:H	1:826:A:ARG:HG3	14	0.11
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	6	0.11
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	6	0.11
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	11	0.11
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	11	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD11	27	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD12	27	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD13	27	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD21	27	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD22	27	0.11
(1,2599)	1:819:A:GLU:HB3	1:823:A:LEU:HD23	27	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD11	6	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD12	6	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD13	6	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD21	6	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD22	6	0.11
(1,2598)	1:819:A:GLU:HB2	1:823:A:LEU:HD23	6	0.11
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG2	21	0.11
(1,2589)	1:816:A:SER:HB2	1:819:A:GLU:HG3	21	0.11
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG2	21	0.11
(1,2589)	1:816:A:SER:HB3	1:819:A:GLU:HG3	21	0.11
(1,2565)	1:811:A:LYS:HB2	1:812:A:GLU:HG2	1	0.11
(1,2565)	1:811:A:LYS:HB2	1:812:A:GLU:HG3	1	0.11
(1,2565)	1:811:A:LYS:HB3	1:812:A:GLU:HG2	1	0.11
(1,2565)	1:811:A:LYS:HB3	1:812:A:GLU:HG3	1	0.11
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	8	0.11
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	46	0.11
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	46	0.11
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	46	0.11
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	46	0.11
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	46	0.11
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	46	0.11
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	15	0.11
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	19	0.11
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	30	0.11
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	30	0.11
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	30	0.11
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	30	0.11
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	30	0.11
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	30	0.11
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB1	5	0.11
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB2	5	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2473)	1:797:A:CYS:HB2	1:822:A:ALA:HB3	5	0.11
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB1	5	0.11
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB2	5	0.11
(1,2473)	1:797:A:CYS:HB3	1:822:A:ALA:HB3	5	0.11
(1,2458)	1:794:A:ALA:HB1	1:819:A:GLU:HG2	27	0.11
(1,2458)	1:794:A:ALA:HB1	1:819:A:GLU:HG3	27	0.11
(1,2458)	1:794:A:ALA:HB2	1:819:A:GLU:HG2	27	0.11
(1,2458)	1:794:A:ALA:HB2	1:819:A:GLU:HG3	27	0.11
(1,2458)	1:794:A:ALA:HB3	1:819:A:GLU:HG2	27	0.11
(1,2458)	1:794:A:ALA:HB3	1:819:A:GLU:HG3	27	0.11
(1,2424)	1:788:A:LYS:HE2	1:790:A:VAL:HB	47	0.11
(1,2424)	1:788:A:LYS:HE3	1:790:A:VAL:HB	47	0.11
(1,2411)	1:781:A:LYS:HG2	1:782:A:CYS:H	39	0.11
(1,2411)	1:781:A:LYS:HG3	1:782:A:CYS:H	39	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG11	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG12	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG13	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG21	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG22	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG23	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG11	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG12	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG13	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG21	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG22	24	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG23	24	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG11	25	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG12	25	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG13	25	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG21	25	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG22	25	0.11
(1,2409)	1:781:A:LYS:HB2	1:790:A:VAL:HG23	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG11	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG12	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG13	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG21	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG22	25	0.11
(1,2409)	1:781:A:LYS:HB3	1:790:A:VAL:HG23	25	0.11
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	3	0.11
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	3	0.11
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE2	8	0.11
(1,2405)	1:781:A:LYS:HA	1:781:A:LYS:HE3	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG11	40	0.11
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG12	40	0.11
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG13	40	0.11
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG21	40	0.11
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG22	40	0.11
(1,2403)	1:781:A:LYS:H	1:790:A:VAL:HG23	40	0.11
(1,2370)	1:772:A:ALA:HB1	1:789:A:CYS:HB2	30	0.11
(1,2370)	1:772:A:ALA:HB1	1:789:A:CYS:HB3	30	0.11
(1,2370)	1:772:A:ALA:HB2	1:789:A:CYS:HB2	30	0.11
(1,2370)	1:772:A:ALA:HB2	1:789:A:CYS:HB3	30	0.11
(1,2370)	1:772:A:ALA:HB3	1:789:A:CYS:HB2	30	0.11
(1,2370)	1:772:A:ALA:HB3	1:789:A:CYS:HB3	30	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	31	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	31	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	31	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	31	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	36	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	36	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	36	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	36	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	42	0.11
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	42	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	42	0.11
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	42	0.11
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	29	0.11
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	29	0.11
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE2	32	0.11
(1,2357)	1:770:A:GLU:HA	1:771:A:LYS:HE3	32	0.11
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB1	45	0.11
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB2	45	0.11
(1,2348)	1:768:A:SER:HB2	1:769:A:ALA:HB3	45	0.11
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB1	45	0.11
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB2	45	0.11
(1,2348)	1:768:A:SER:HB3	1:769:A:ALA:HB3	45	0.11
(1,2339)	1:760:A:ARG:HG2	1:762:A:SER:H	9	0.11
(1,2339)	1:760:A:ARG:HG3	1:762:A:SER:H	9	0.11
(1,2339)	1:760:A:ARG:HG2	1:762:A:SER:H	27	0.11
(1,2339)	1:760:A:ARG:HG3	1:762:A:SER:H	27	0.11
(1,2339)	1:760:A:ARG:HG2	1:762:A:SER:H	28	0.11
(1,2339)	1:760:A:ARG:HG3	1:762:A:SER:H	28	0.11
(1,2337)	1:760:A:ARG:HG2	1:761:A:ASP:H	7	0.11
(1,2337)	1:760:A:ARG:HG3	1:761:A:ASP:H	7	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2337)	1:760:A:ARG:HG2	1:761:A:ASP:H	21	0.11
(1,2337)	1:760:A:ARG:HG3	1:761:A:ASP:H	21	0.11
(1,2335)	1:760:A:ARG:HB2	1:760:A:ARG:HD2	42	0.11
(1,2335)	1:760:A:ARG:HB2	1:760:A:ARG:HD3	42	0.11
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG2	5	0.11
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG3	5	0.11
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG12	9	0.11
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG13	9	0.11
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG12	28	0.11
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG13	28	0.11
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG2	19	0.11
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG3	19	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG11	43	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG12	43	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG13	43	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG21	43	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG22	43	0.11
(1,2073)	1:724:A:SER:HA	1:742:A:VAL:HG23	43	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	11	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	33	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	36	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	36	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	36	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	36	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	36	0.11
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	36	0.11
(1,2040)	1:717:A:MET:H	1:720:A:GLU:HB2	33	0.11
(1,2040)	1:717:A:MET:H	1:720:A:GLU:HB3	33	0.11
(1,1985)	1:704:A:ARG:HD2	1:802:A:PHE:HE1	12	0.11
(1,1985)	1:704:A:ARG:HD2	1:802:A:PHE:HE2	12	0.11
(1,1985)	1:704:A:ARG:HD3	1:802:A:PHE:HE1	12	0.11
(1,1985)	1:704:A:ARG:HD3	1:802:A:PHE:HE2	12	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD2	3	0.11
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD3	3	0.11
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD2	16	0.11
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD3	16	0.11
(1,1869)	1:741:A:THR:HG21	1:742:A:VAL:HA	17	0.11
(1,1869)	1:741:A:THR:HG22	1:742:A:VAL:HA	17	0.11
(1,1869)	1:741:A:THR:HG23	1:742:A:VAL:HA	17	0.11
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	24	0.11
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	24	0.11
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	24	0.11
(1,1835)	1:717:A:MET:HA	1:717:A:MET:HE1	9	0.11
(1,1835)	1:717:A:MET:HA	1:717:A:MET:HE2	9	0.11
(1,1835)	1:717:A:MET:HA	1:717:A:MET:HE3	9	0.11
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	5	0.11
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	5	0.11
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	5	0.11
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	36	0.11
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	36	0.11
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	36	0.11
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD11	47	0.11
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD12	47	0.11
(1,1822)	1:742:A:VAL:HB	1:835:A:ILE:HD13	47	0.11
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	3	0.11
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	5	0.11
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	9	0.11
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	24	0.11
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	24	0.11
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	24	0.11
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	46	0.11
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	46	0.11
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	46	0.11
(1,1789)	1:772:A:ALA:HA	1:788:A:LYS:HA	23	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB1	22	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB2	22	0.11
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB3	22	0.11
(1,1782)	1:822:A:ALA:HB1	1:825:A:CYS:HB3	28	0.11
(1,1782)	1:822:A:ALA:HB2	1:825:A:CYS:HB3	28	0.11
(1,1782)	1:822:A:ALA:HB3	1:825:A:CYS:HB3	28	0.11
(1,1780)	1:794:A:ALA:HA	1:822:A:ALA:HB1	36	0.11
(1,1780)	1:794:A:ALA:HA	1:822:A:ALA:HB2	36	0.11
(1,1780)	1:794:A:ALA:HA	1:822:A:ALA:HB3	36	0.11
(1,1771)	1:778:A:LEU:HD21	1:779:A:TRP:HZ2	24	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1771)	1:778:A:LEU:HD22	1:779:A:TRP:HZ2	24	0.11
(1,1771)	1:778:A:LEU:HD23	1:779:A:TRP:HZ2	24	0.11
(1,1771)	1:778:A:LEU:HD21	1:779:A:TRP:HZ2	29	0.11
(1,1771)	1:778:A:LEU:HD22	1:779:A:TRP:HZ2	29	0.11
(1,1771)	1:778:A:LEU:HD23	1:779:A:TRP:HZ2	29	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	18	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	18	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	18	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	41	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	41	0.11
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	41	0.11
(1,1544)	1:794:A:ALA:HA	1:819:A:GLU:HB2	42	0.11
(1,1540)	1:791:A:CYS:HA	1:825:A:CYS:HB2	43	0.11
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	2	0.11
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	6	0.11
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	11	0.11
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	37	0.11
(1,1472)	1:767:A:ALA:HA	1:768:A:SER:HB3	47	0.11
(1,1470)	1:698:A:ALA:HA	1:699:A:VAL:HB	32	0.11
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	18	0.11
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	43	0.11
(1,1443)	1:745:A:MET:HA	1:755:A:TYR:HB3	14	0.11
(1,1443)	1:745:A:MET:HA	1:755:A:TYR:HB3	16	0.11
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	15	0.11
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	31	0.11
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	40	0.11
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	48	0.11
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	18	0.11
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	26	0.11
(1,1379)	1:814:A:THR:HB	1:815:A:MET:HG2	35	0.11
(1,1314)	1:742:A:VAL:HG11	1:835:A:ILE:HA	16	0.11
(1,1314)	1:742:A:VAL:HG12	1:835:A:ILE:HA	16	0.11
(1,1314)	1:742:A:VAL:HG13	1:835:A:ILE:HA	16	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	15	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	15	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	15	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	33	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	33	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	33	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	40	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	40	0.11
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	40	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:794:A:ALA:HB1	1:819:A:GLU:HB2	24	0.11
(1,1270)	1:794:A:ALA:HB2	1:819:A:GLU:HB2	24	0.11
(1,1270)	1:794:A:ALA:HB3	1:819:A:GLU:HB2	24	0.11
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG21	25	0.11
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG22	25	0.11
(1,1264)	1:808:A:VAL:HB	1:830:A:ILE:HG23	25	0.11
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	18	0.11
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	18	0.11
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	30	0.11
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	30	0.11
(1,1201)	1:725:A:LEU:HG	1:779:A:TRP:HZ2	43	0.11
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	10	0.11
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	10	0.11
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	10	0.11
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	10	0.11
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	10	0.11
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	10	0.11
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD1	19	0.11
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD2	19	0.11
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD1	19	0.11
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD2	19	0.11
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD1	19	0.11
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD2	19	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	10	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	10	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	10	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	11	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	11	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	11	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	24	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	24	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	24	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	25	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	25	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	25	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	26	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	26	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	26	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	27	0.11
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	27	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	27	0.11
(1,1108)	1:738:A:LEU:HD21	1:739:A:PRO:HD2	41	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1108)	1:738:A:LEU:HD22	1:739:A:PRO:HD2	41	0.11
(1,1108)	1:738:A:LEU:HD23	1:739:A:PRO:HD2	41	0.11
(1,1098)	1:709:A:GLN:HG3	1:712:A:ARG:HG2	14	0.11
(1,1079)	1:842:A:THR:HB	1:843:A:GLN:H	18	0.11
(1,1079)	1:842:A:THR:HB	1:843:A:GLN:H	47	0.11
(1,1078)	1:842:A:THR:H	1:842:A:THR:HB	14	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD11	40	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD12	40	0.11
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD13	40	0.11
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	24	0.11
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	37	0.11
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	44	0.11
(1,987)	1:709:A:GLN:HG3	1:712:A:ARG:H	45	0.11
(1,967)	1:815:A:MET:HG3	1:820:A:ALA:H	27	0.11
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	6	0.11
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	23	0.11
(1,926)	1:741:A:THR:HG21	1:742:A:VAL:HB	46	0.11
(1,926)	1:741:A:THR:HG22	1:742:A:VAL:HB	46	0.11
(1,926)	1:741:A:THR:HG23	1:742:A:VAL:HB	46	0.11
(1,921)	1:767:A:ALA:HB1	1:768:A:SER:H	20	0.11
(1,921)	1:767:A:ALA:HB2	1:768:A:SER:H	20	0.11
(1,921)	1:767:A:ALA:HB3	1:768:A:SER:H	20	0.11
(1,921)	1:767:A:ALA:HB1	1:768:A:SER:H	32	0.11
(1,921)	1:767:A:ALA:HB2	1:768:A:SER:H	32	0.11
(1,921)	1:767:A:ALA:HB3	1:768:A:SER:H	32	0.11
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	28	0.11
(1,830)	1:697:A:GLN:HA	1:697:A:GLN:HE22	22	0.11
(1,818)	1:717:A:MET:HE1	1:751:A:GLN:HE22	29	0.11
(1,818)	1:717:A:MET:HE2	1:751:A:GLN:HE22	29	0.11
(1,818)	1:717:A:MET:HE3	1:751:A:GLN:HE22	29	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	7	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	8	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	12	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	27	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	29	0.11
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	38	0.11
(1,811)	1:709:A:GLN:HG3	1:710:A:ASN:HD21	14	0.11
(1,803)	1:809:A:ASN:HA	1:809:A:ASN:HD22	45	0.11
(1,579)	1:841:A:GLU:HA	1:842:A:THR:H	18	0.11
(1,576)	1:841:A:GLU:HG3	1:842:A:THR:H	47	0.11
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	15	0.11
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	15	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	15	0.11
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	34	0.11
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	34	0.11
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	34	0.11
(1,544)	1:751:A:GLN:H	1:751:A:GLN:HE21	37	0.11
(1,533)	1:772:A:ALA:HB1	1:773:A:CYS:H	33	0.11
(1,533)	1:772:A:ALA:HB2	1:773:A:CYS:H	33	0.11
(1,533)	1:772:A:ALA:HB3	1:773:A:CYS:H	33	0.11
(1,532)	1:773:A:CYS:H	1:773:A:CYS:HB2	31	0.11
(1,532)	1:773:A:CYS:H	1:773:A:CYS:HB2	33	0.11
(1,529)	1:773:A:CYS:H	1:789:A:CYS:H	27	0.11
(1,519)	1:767:A:ALA:HA	1:768:A:SER:H	45	0.11
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	2	0.11
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	13	0.11
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	17	0.11
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	27	0.11
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	1	0.11
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	5	0.11
(1,328)	1:840:A:ALA:HA	1:841:A:GLU:H	16	0.11
(1,323)	1:782:A:CYS:H	1:782:A:CYS:HB3	30	0.11
(1,309)	1:824:A:ARG:H	1:824:A:ARG:HE	9	0.11
(1,268)	1:690:A:SER:HA	1:691:A:HIS:H	25	0.11
(1,240)	1:798:A:GLU:H	1:799:A:GLU:H	42	0.11
(1,239)	1:736:A:ARG:H	1:737:A:ILE:HD11	29	0.11
(1,239)	1:736:A:ARG:H	1:737:A:ILE:HD12	29	0.11
(1,239)	1:736:A:ARG:H	1:737:A:ILE:HD13	29	0.11
(1,233)	1:699:A:VAL:H	1:699:A:VAL:HB	24	0.11
(1,159)	1:840:A:ALA:H	1:840:A:ALA:HB1	15	0.11
(1,159)	1:840:A:ALA:H	1:840:A:ALA:HB2	15	0.11
(1,159)	1:840:A:ALA:H	1:840:A:ALA:HB3	15	0.11
(1,114)	1:775:A:ALA:H	1:776:A:CYS:H	23	0.11
(1,109)	1:794:A:ALA:H	1:795:A:SER:HA	24	0.11
(1,109)	1:794:A:ALA:H	1:795:A:SER:HA	30	0.11
(1,72)	1:806:A:VAL:H	1:813:A:GLN:HG2	48	0.11
(1,9)	1:765:A:LEU:H	1:766:A:PRO:HD3	18	0.11
(1,9)	1:765:A:LEU:H	1:766:A:PRO:HD3	27	0.11
(1,2694)	1:840:A:ALA:HA	1:841:A:GLU:HG2	39	0.1
(1,2694)	1:840:A:ALA:HA	1:841:A:GLU:HG3	39	0.1
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD2	29	0.1
(1,2683)	1:836:A:ARG:HA	1:836:A:ARG:HD3	29	0.1
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD11	26	0.1
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD12	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2672)	1:834:A:SER:HB2	1:835:A:ILE:HD13	26	0.1
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD11	26	0.1
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD12	26	0.1
(1,2672)	1:834:A:SER:HB3	1:835:A:ILE:HD13	26	0.1
(1,2647)	1:826:A:ARG:HB2	1:828:A:GLN:H	46	0.1
(1,2647)	1:826:A:ARG:HB3	1:828:A:GLN:H	46	0.1
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	10	0.1
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	10	0.1
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG2	37	0.1
(1,2639)	1:825:A:CYS:H	1:826:A:ARG:HG3	37	0.1
(1,2625)	1:823:A:LEU:HD11	1:828:A:GLN:HA	2	0.1
(1,2625)	1:823:A:LEU:HD12	1:828:A:GLN:HA	2	0.1
(1,2625)	1:823:A:LEU:HD13	1:828:A:GLN:HA	2	0.1
(1,2625)	1:823:A:LEU:HD21	1:828:A:GLN:HA	2	0.1
(1,2625)	1:823:A:LEU:HD22	1:828:A:GLN:HA	2	0.1
(1,2625)	1:823:A:LEU:HD23	1:828:A:GLN:HA	2	0.1
(1,2623)	1:823:A:LEU:HD11	1:826:A:ARG:HE	1	0.1
(1,2623)	1:823:A:LEU:HD12	1:826:A:ARG:HE	1	0.1
(1,2623)	1:823:A:LEU:HD13	1:826:A:ARG:HE	1	0.1
(1,2623)	1:823:A:LEU:HD21	1:826:A:ARG:HE	1	0.1
(1,2623)	1:823:A:LEU:HD22	1:826:A:ARG:HE	1	0.1
(1,2623)	1:823:A:LEU:HD23	1:826:A:ARG:HE	1	0.1
(1,2607)	1:821:A:GLY:HA3	1:824:A:ARG:HB2	3	0.1
(1,2607)	1:821:A:GLY:HA3	1:824:A:ARG:HB3	3	0.1
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG11	1:813:A:GLN:HE22	5	0.1
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG12	1:813:A:GLN:HE22	5	0.1
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG13	1:813:A:GLN:HE22	5	0.1
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG21	1:813:A:GLN:HE22	5	0.1
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG22	1:813:A:GLN:HE22	5	0.1
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE21	5	0.1
(1,2546)	1:808:A:VAL:HG23	1:813:A:GLN:HE22	5	0.1
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	13	0.1
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	13	0.1
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	13	0.1
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	13	0.1
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	13	0.1
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	13	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2541)	1:808:A:VAL:HG11	1:809:A:ASN:HB3	25	0.1
(1,2541)	1:808:A:VAL:HG12	1:809:A:ASN:HB3	25	0.1
(1,2541)	1:808:A:VAL:HG13	1:809:A:ASN:HB3	25	0.1
(1,2541)	1:808:A:VAL:HG21	1:809:A:ASN:HB3	25	0.1
(1,2541)	1:808:A:VAL:HG22	1:809:A:ASN:HB3	25	0.1
(1,2541)	1:808:A:VAL:HG23	1:809:A:ASN:HB3	25	0.1
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	9	0.1
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	20	0.1
(1,2529)	1:806:A:VAL:HG11	1:831:A:SER:HB3	29	0.1
(1,2529)	1:806:A:VAL:HG12	1:831:A:SER:HB3	29	0.1
(1,2529)	1:806:A:VAL:HG13	1:831:A:SER:HB3	29	0.1
(1,2529)	1:806:A:VAL:HG21	1:831:A:SER:HB3	29	0.1
(1,2529)	1:806:A:VAL:HG22	1:831:A:SER:HB3	29	0.1
(1,2529)	1:806:A:VAL:HG23	1:831:A:SER:HB3	29	0.1
(1,2398)	1:780:A:GLY:H	1:781:A:LYS:HB2	43	0.1
(1,2398)	1:780:A:GLY:H	1:781:A:LYS:HB3	43	0.1
(1,2367)	1:771:A:LYS:HD2	1:772:A:ALA:H	20	0.1
(1,2367)	1:771:A:LYS:HD3	1:772:A:ALA:H	20	0.1
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	11	0.1
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	11	0.1
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	11	0.1
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	11	0.1
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE2	13	0.1
(1,2359)	1:770:A:GLU:HG2	1:771:A:LYS:HE3	13	0.1
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE2	13	0.1
(1,2359)	1:770:A:GLU:HG3	1:771:A:LYS:HE3	13	0.1
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG2	26	0.1
(1,2351)	1:769:A:ALA:HB1	1:770:A:GLU:HG3	26	0.1
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG2	26	0.1
(1,2351)	1:769:A:ALA:HB2	1:770:A:GLU:HG3	26	0.1
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG2	26	0.1
(1,2351)	1:769:A:ALA:HB3	1:770:A:GLU:HG3	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2349)	1:769:A:ALA:HA	1:770:A:GLU:HB2	18	0.1
(1,2349)	1:769:A:ALA:HA	1:770:A:GLU:HB3	18	0.1
(1,2347)	1:768:A:SER:HB2	1:769:A:ALA:H	45	0.1
(1,2347)	1:768:A:SER:HB3	1:769:A:ALA:H	45	0.1
(1,2342)	1:760:A:ARG:HE	1:761:A:ASP:HB2	9	0.1
(1,2342)	1:760:A:ARG:HE	1:761:A:ASP:HB3	9	0.1
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG2	10	0.1
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG3	10	0.1
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG2	24	0.1
(1,2299)	1:751:A:GLN:H	1:753:A:ARG:HG3	24	0.1
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG12	42	0.1
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG13	42	0.1
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG12	48	0.1
(1,2265)	1:746:A:HIS:H	1:835:A:ILE:HG13	48	0.1
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB2	15	0.1
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB3	15	0.1
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB2	21	0.1
(1,2205)	1:737:A:ILE:H	1:762:A:SER:HB3	21	0.1
(1,2202)	1:736:A:ARG:HB3	1:736:A:ARG:HD2	29	0.1
(1,2202)	1:736:A:ARG:HB3	1:736:A:ARG:HD3	29	0.1
(1,2099)	1:725:A:LEU:HD11	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD11	1:817:A:GLU:HG3	23	0.1
(1,2099)	1:725:A:LEU:HD12	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD12	1:817:A:GLU:HG3	23	0.1
(1,2099)	1:725:A:LEU:HD13	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD13	1:817:A:GLU:HG3	23	0.1
(1,2099)	1:725:A:LEU:HD21	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD21	1:817:A:GLU:HG3	23	0.1
(1,2099)	1:725:A:LEU:HD22	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD22	1:817:A:GLU:HG3	23	0.1
(1,2099)	1:725:A:LEU:HD23	1:817:A:GLU:HG2	23	0.1
(1,2099)	1:725:A:LEU:HD23	1:817:A:GLU:HG3	23	0.1
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG2	13	0.1
(1,2090)	1:725:A:LEU:HB3	1:817:A:GLU:HG3	13	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG11	48	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG12	48	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG13	48	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG21	48	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG22	48	0.1
(1,2071)	1:724:A:SER:H	1:742:A:VAL:HG23	48	0.1
(1,2023)	1:712:A:ARG:HD2	1:713:A:CYS:H	26	0.1
(1,2023)	1:712:A:ARG:HD3	1:713:A:CYS:H	26	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD2	22	0.1
(1,1957)	1:703:A:GLN:HA	1:704:A:ARG:HD3	22	0.1
(1,1900)	1:808:A:VAL:HA	1:815:A:MET:HE1	25	0.1
(1,1900)	1:808:A:VAL:HA	1:815:A:MET:HE2	25	0.1
(1,1900)	1:808:A:VAL:HA	1:815:A:MET:HE3	25	0.1
(1,1880)	1:746:A:HIS:HA	1:749:A:HIS:HD2	16	0.1
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE1	21	0.1
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE2	21	0.1
(1,1858)	1:805:A:CYS:HA	1:815:A:MET:HE3	21	0.1
(1,1828)	1:778:A:LEU:HD11	1:779:A:TRP:HZ2	14	0.1
(1,1828)	1:778:A:LEU:HD12	1:779:A:TRP:HZ2	14	0.1
(1,1828)	1:778:A:LEU:HD13	1:779:A:TRP:HZ2	14	0.1
(1,1815)	1:725:A:LEU:HG	1:817:A:GLU:HG2	39	0.1
(1,1804)	1:808:A:VAL:HG11	1:813:A:GLN:H	18	0.1
(1,1804)	1:808:A:VAL:HG12	1:813:A:GLN:H	18	0.1
(1,1804)	1:808:A:VAL:HG13	1:813:A:GLN:H	18	0.1
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB1	14	0.1
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB2	14	0.1
(1,1784)	1:791:A:CYS:HA	1:822:A:ALA:HB3	14	0.1
(1,1782)	1:822:A:ALA:HB1	1:825:A:CYS:HB3	27	0.1
(1,1782)	1:822:A:ALA:HB2	1:825:A:CYS:HB3	27	0.1
(1,1782)	1:822:A:ALA:HB3	1:825:A:CYS:HB3	27	0.1
(1,1782)	1:822:A:ALA:HB1	1:825:A:CYS:HB3	45	0.1
(1,1782)	1:822:A:ALA:HB2	1:825:A:CYS:HB3	45	0.1
(1,1782)	1:822:A:ALA:HB3	1:825:A:CYS:HB3	45	0.1
(1,1779)	1:771:A:LYS:HA	1:771:A:LYS:HD2	22	0.1
(1,1779)	1:771:A:LYS:HA	1:771:A:LYS:HD2	41	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	16	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	16	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	16	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD21	17	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD22	17	0.1
(1,1757)	1:745:A:MET:HB2	1:748:A:LEU:HD23	17	0.1
(1,1741)	1:738:A:LEU:HA	1:738:A:LEU:HG	15	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	22	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	22	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	22	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	22	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	22	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	22	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	22	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	22	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	22	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	34	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	34	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	34	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	34	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	34	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	34	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	34	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	34	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	34	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD11	39	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD12	39	0.1
(1,1734)	1:738:A:LEU:HD21	1:740:A:LEU:HD13	39	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD11	39	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD12	39	0.1
(1,1734)	1:738:A:LEU:HD22	1:740:A:LEU:HD13	39	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD11	39	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD12	39	0.1
(1,1734)	1:738:A:LEU:HD23	1:740:A:LEU:HD13	39	0.1
(1,1672)	1:726:A:ASP:HB3	1:727:A:VAL:HA	5	0.1
(1,1651)	1:830:A:ILE:HA	1:831:A:SER:HB3	29	0.1
(1,1633)	1:742:A:VAL:HG21	1:835:A:ILE:HA	20	0.1
(1,1633)	1:742:A:VAL:HG22	1:835:A:ILE:HA	20	0.1
(1,1633)	1:742:A:VAL:HG23	1:835:A:ILE:HA	20	0.1
(1,1625)	1:806:A:VAL:HB	1:814:A:THR:HA	7	0.1
(1,1559)	1:705:A:TRP:HA	1:747:A:VAL:HB	20	0.1
(1,1540)	1:791:A:CYS:HA	1:825:A:CYS:HB2	40	0.1
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	3	0.1
(1,1514)	1:702:A:CYS:HB2	1:706:A:GLU:HA	26	0.1
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	14	0.1
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	24	0.1
(1,1500)	1:805:A:CYS:HA	1:838:A:CYS:HA	43	0.1
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	6	0.1
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	26	0.1
(1,1444)	1:836:A:ARG:HA	1:836:A:ARG:HD3	39	0.1
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	14	0.1
(1,1400)	1:808:A:VAL:HB	1:809:A:ASN:HB2	20	0.1
(1,1347)	1:725:A:LEU:HD21	1:779:A:TRP:HE3	31	0.1
(1,1347)	1:725:A:LEU:HD22	1:779:A:TRP:HE3	31	0.1
(1,1347)	1:725:A:LEU:HD23	1:779:A:TRP:HE3	31	0.1
(1,1326)	1:725:A:LEU:HB2	1:742:A:VAL:HG21	9	0.1
(1,1326)	1:725:A:LEU:HB2	1:742:A:VAL:HG22	9	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1326)	1:725:A:LEU:HB2	1:742:A:VAL:HG23	9	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	13	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	13	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	13	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	17	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	17	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	17	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	20	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	20	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	20	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG21	43	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG22	43	0.1
(1,1301)	1:755:A:TYR:HB3	1:756:A:THR:HG23	43	0.1
(1,1292)	1:709:A:GLN:HA	1:714:A:VAL:HG21	45	0.1
(1,1292)	1:709:A:GLN:HA	1:714:A:VAL:HG22	45	0.1
(1,1292)	1:709:A:GLN:HA	1:714:A:VAL:HG23	45	0.1
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB1	27	0.1
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB2	27	0.1
(1,1279)	1:838:A:CYS:HB3	1:840:A:ALA:HB3	27	0.1
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE1	39	0.1
(1,1218)	1:745:A:MET:HA	1:755:A:TYR:HE2	39	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	28	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	28	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	28	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	28	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	28	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	28	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	29	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	29	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	29	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	29	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	29	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	29	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG11	35	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG12	35	0.1
(1,1215)	1:719:A:TYR:HD1	1:747:A:VAL:HG13	35	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG11	35	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG12	35	0.1
(1,1215)	1:719:A:TYR:HD2	1:747:A:VAL:HG13	35	0.1
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE1	33	0.1
(1,1192)	1:742:A:VAL:HG21	1:802:A:PHE:HE2	33	0.1
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE1	33	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1192)	1:742:A:VAL:HG22	1:802:A:PHE:HE2	33	0.1
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE1	33	0.1
(1,1192)	1:742:A:VAL:HG23	1:802:A:PHE:HE2	33	0.1
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD1	41	0.1
(1,1163)	1:717:A:MET:HE1	1:719:A:TYR:HD2	41	0.1
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD1	41	0.1
(1,1163)	1:717:A:MET:HE2	1:719:A:TYR:HD2	41	0.1
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD1	41	0.1
(1,1163)	1:717:A:MET:HE3	1:719:A:TYR:HD2	41	0.1
(1,1095)	1:727:A:VAL:HG11	1:835:A:ILE:HA	24	0.1
(1,1095)	1:727:A:VAL:HG12	1:835:A:ILE:HA	24	0.1
(1,1095)	1:727:A:VAL:HG13	1:835:A:ILE:HA	24	0.1
(1,1079)	1:842:A:THR:HB	1:843:A:GLN:H	24	0.1
(1,1058)	1:829:A:SER:HB2	1:830:A:ILE:HA	17	0.1
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD11	6	0.1
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD12	6	0.1
(1,1054)	1:764:A:THR:HA	1:765:A:LEU:HD13	6	0.1
(1,1050)	1:705:A:TRP:HD1	1:750:A:CYS:HA	32	0.1
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	40	0.1
(1,1035)	1:736:A:ARG:HA	1:736:A:ARG:HD3	47	0.1
(1,986)	1:709:A:GLN:HG3	1:714:A:VAL:HG11	45	0.1
(1,986)	1:709:A:GLN:HG3	1:714:A:VAL:HG12	45	0.1
(1,986)	1:709:A:GLN:HG3	1:714:A:VAL:HG13	45	0.1
(1,980)	1:748:A:LEU:HA	1:751:A:GLN:HG2	16	0.1
(1,966)	1:815:A:MET:HG3	1:820:A:ALA:HA	10	0.1
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	27	0.1
(1,953)	1:818:A:CYS:H	1:819:A:GLU:HB3	42	0.1
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	8	0.1
(1,864)	1:800:A:GLU:H	1:801:A:GLY:H	24	0.1
(1,812)	1:710:A:ASN:HB2	1:710:A:ASN:HD22	26	0.1
(1,811)	1:709:A:GLN:HG3	1:710:A:ASN:HD21	35	0.1
(1,809)	1:732:A:GLU:HB2	1:754:A:ASN:HD21	40	0.1
(1,806)	1:808:A:VAL:HB	1:809:A:ASN:HD21	33	0.1
(1,803)	1:809:A:ASN:HA	1:809:A:ASN:HD22	5	0.1
(1,783)	1:705:A:TRP:HE1	1:750:A:CYS:HB3	16	0.1
(1,772)	1:728:A:CYS:H	1:765:A:LEU:HD21	22	0.1
(1,772)	1:728:A:CYS:H	1:765:A:LEU:HD22	22	0.1
(1,772)	1:728:A:CYS:H	1:765:A:LEU:HD23	22	0.1
(1,585)	1:735:A:LYS:H	1:735:A:LYS:HD2	11	0.1
(1,585)	1:735:A:LYS:H	1:735:A:LYS:HD2	17	0.1
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	5	0.1
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	5	0.1
(1,552)	1:747:A:VAL:HG21	1:751:A:GLN:H	32	0.1
(1,552)	1:747:A:VAL:HG22	1:751:A:GLN:H	32	0.1
(1,552)	1:747:A:VAL:HG23	1:751:A:GLN:H	32	0.1
(1,544)	1:751:A:GLN:H	1:751:A:GLN:HE21	41	0.1
(1,540)	1:704:A:ARG:HD3	1:803:A:SER:H	34	0.1
(1,532)	1:773:A:CYS:H	1:773:A:CYS:HB2	48	0.1
(1,529)	1:773:A:CYS:H	1:789:A:CYS:H	22	0.1
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	30	0.1
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	38	0.1
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	42	0.1
(1,509)	1:733:A:ARG:H	1:733:A:ARG:HB3	44	0.1
(1,407)	1:704:A:ARG:H	1:705:A:TRP:HZ2	15	0.1
(1,373)	1:744:A:LYS:HB2	1:746:A:HIS:H	42	0.1
(1,298)	1:702:A:CYS:HB3	1:706:A:GLU:H	38	0.1
(1,281)	1:700:A:PRO:HB3	1:701:A:LYS:H	9	0.1
(1,260)	1:809:A:ASN:HB3	1:811:A:LYS:H	23	0.1
(1,156)	1:839:A:ALA:HA	1:840:A:ALA:H	15	0.1
(1,114)	1:775:A:ALA:H	1:776:A:CYS:H	28	0.1
(1,109)	1:794:A:ALA:H	1:795:A:SER:HA	19	0.1

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

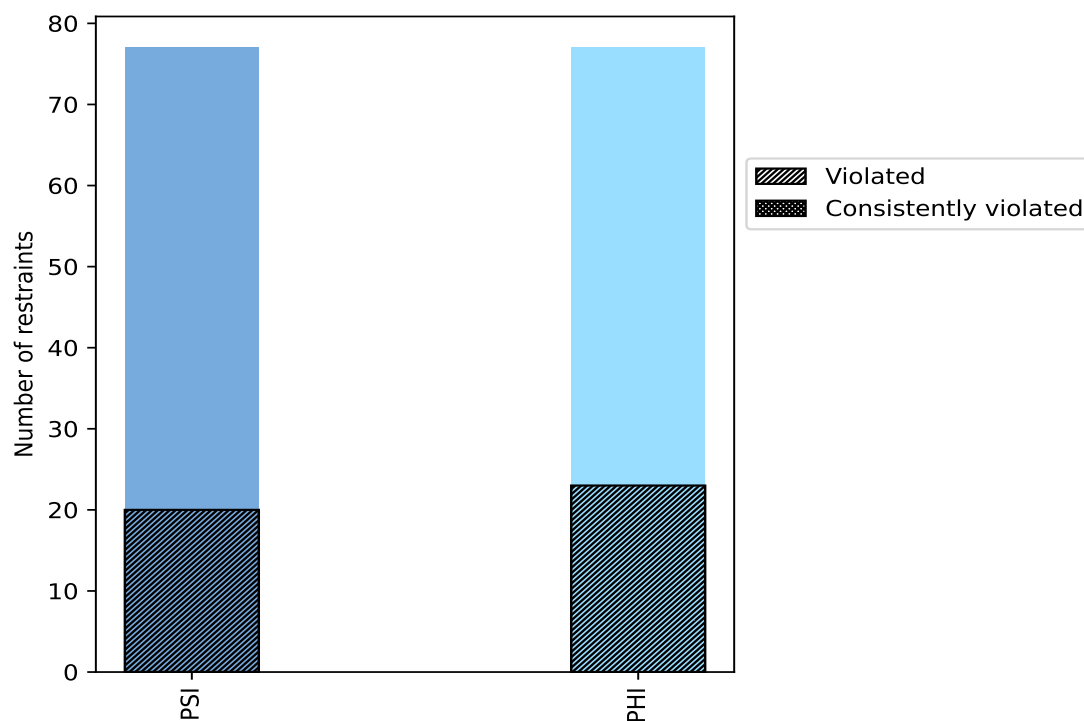
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	77	50.0	20	26.0	13.0	0	0.0	0.0
PHI	77	50.0	23	29.9	14.9	0	0.0	0.0
Total	154	100.0	43	27.9	27.9	0	0.0	0.0

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

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



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

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

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

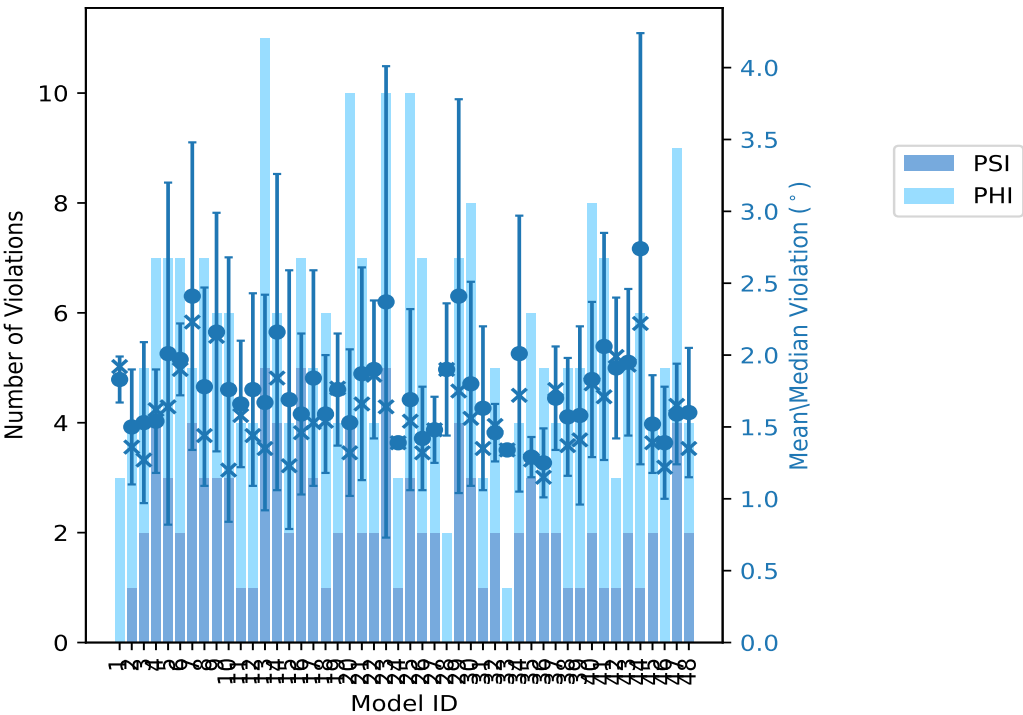
Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	0	3	3	1.83	1.96	0.16	1.92
2	1	3	4	1.5	2.17	0.4	1.36
3	2	3	5	1.53	2.62	0.56	1.27
4	4	3	7	1.54	2.15	0.36	1.62
5	3	4	7	2.01	4.84	1.19	1.64
6	2	5	7	1.97	2.51	0.25	1.9
7	4	1	5	2.41	4.17	1.07	2.23
8	3	4	7	1.78	2.85	0.69	1.44
9	3	3	6	2.16	3.62	0.83	2.13
10	3	3	6	1.76	3.52	0.92	1.2
11	1	3	4	1.66	2.31	0.44	1.58
12	1	3	4	1.76	2.92	0.67	1.44
13	5	6	11	1.67	3.19	0.75	1.35
14	4	2	6	2.16	3.79	1.1	1.84
15	2	2	4	1.69	3.24	0.9	1.23
16	5	2	7	1.59	2.88	0.56	1.46
17	3	2	5	1.84	3.28	0.75	1.53
18	1	5	6	1.59	2.38	0.41	1.54
19	2	2	4	1.76	2.28	0.39	1.77
20	4	6	10	1.53	2.54	0.51	1.32
21	2	5	7	1.87	3.53	0.74	1.66
22	2	2	4	1.9	2.47	0.48	1.86
23	5	5	10	2.37	6.71	1.64	1.64
24	1	2	3	1.39	1.43	0.03	1.39
25	3	7	10	1.69	2.9	0.63	1.54
26	2	5	7	1.42	2.0	0.36	1.32
27	2	2	4	1.48	1.74	0.23	1.48
28	0	2	2	1.9	2.36	0.46	1.9
29	4	3	7	2.41	4.9	1.37	1.75
30	3	5	8	1.8	2.88	0.71	1.56
31	1	2	3	1.63	2.42	0.57	1.35
32	2	3	5	1.46	1.66	0.2	1.51
33	0	1	1	1.34	1.34	0.0	1.34
34	2	2	4	2.01	3.59	0.96	1.72
35	3	3	6	1.29	1.47	0.14	1.27
36	2	3	5	1.25	1.71	0.24	1.15
37	2	2	4	1.7	2.06	0.36	1.76
38	1	4	5	1.57	2.34	0.41	1.37

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Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
39	1	4	5	1.58	2.73	0.62	1.41
40	2	6	8	1.83	2.76	0.54	1.8
41	1	6	7	2.06	3.61	0.79	1.71
42	1	2	3	1.91	2.46	0.49	1.99
43	2	3	5	1.95	2.61	0.51	1.93
44	1	5	6	2.74	5.3	1.5	2.22
45	2	2	4	1.52	2.09	0.34	1.39
46	0	5	5	1.39	2.11	0.39	1.22
47	4	5	9	1.59	2.33	0.35	1.65
48	2	2	4	1.6	2.38	0.45	1.35

10.2.1 Bar graph : Dihedral violation statistics for each model ⓘ



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

10.3 Dihedral-angle violation statistics for the ensemble ⓘ

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	%
5	4	9	1	2.1
4	3	7	2	4.2
2	3	5	3	6.2
0	1	1	4	8.3
2	2	4	5	10.4
1	3	4	6	12.5
0	0	0	7	14.6
2	1	3	8	16.7
0	2	2	9	18.8
1	0	1	10	20.8
1	1	2	11	22.9
0	0	0	12	25.0
0	1	1	13	27.1
1	0	1	14	29.2
0	0	0	15	31.2
0	0	0	16	33.3
0	0	0	17	35.4
0	0	0	18	37.5
0	0	0	19	39.6
1	0	1	20	41.7
0	0	0	21	43.8
0	1	1	22	45.8
0	0	0	23	47.9
0	0	0	24	50.0
0	0	0	25	52.1
0	0	0	26	54.2
0	0	0	27	56.2
0	0	0	28	58.3
0	0	0	29	60.4
0	0	0	30	62.5
0	0	0	31	64.6
0	0	0	32	66.7
0	0	0	33	68.8
0	0	0	34	70.8
0	0	0	35	72.9
0	0	0	36	75.0
0	0	0	37	77.1
0	0	0	38	79.2
0	0	0	39	81.2
0	1	1	40	83.3
0	0	0	41	85.4
0	0	0	42	87.5

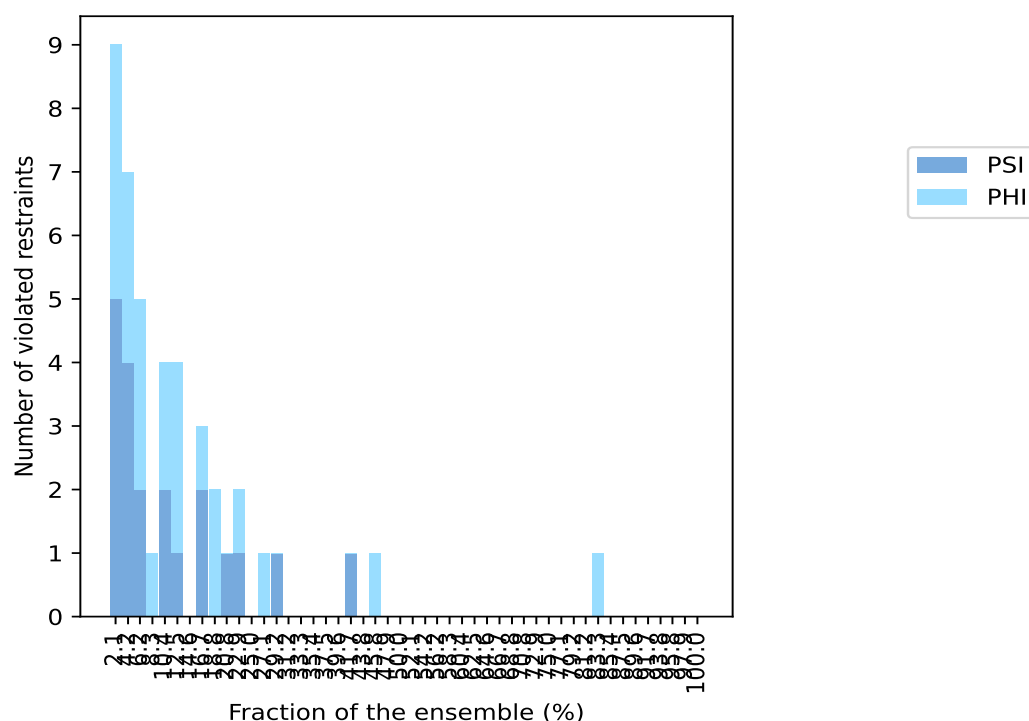
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	43	89.6
0	0	0	44	91.7
0	0	0	45	93.8
0	0	0	46	95.8
0	0	0	47	97.9
0	0	0	48	100.0

¹ Number of models with violations

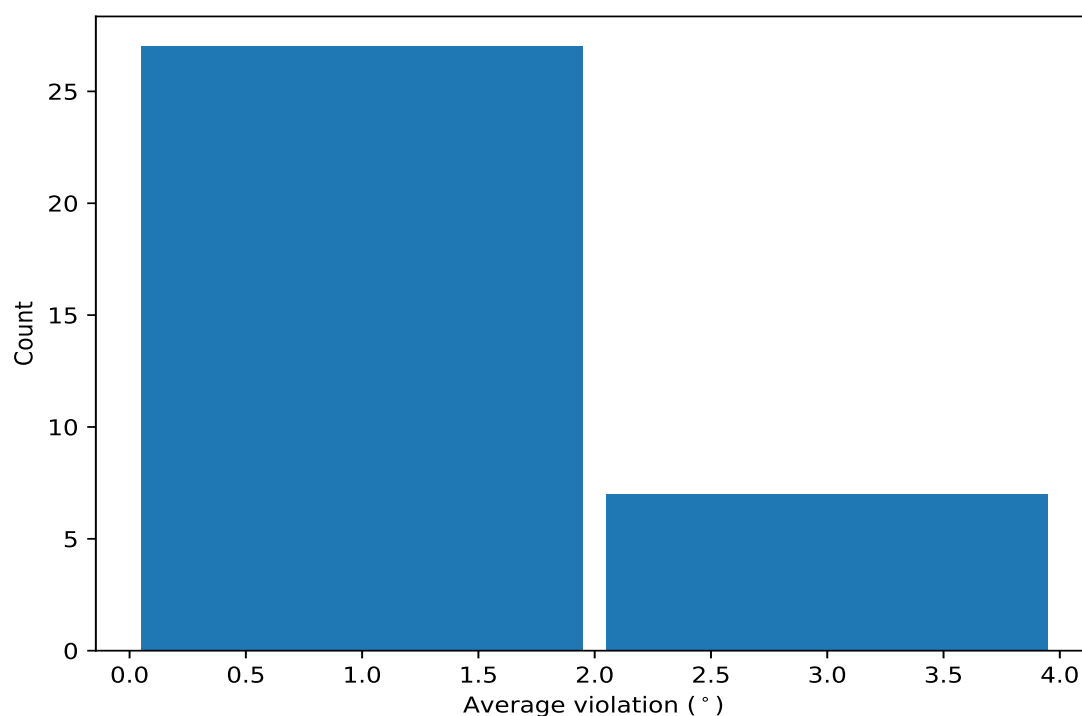
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	40	2.05	0.72	1.89
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	22	2.0	1.12	1.89
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	20	2.01	0.76	1.82
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	14	1.59	0.57	1.58
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	13	1.59	0.58	1.39
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	11	2.98	1.28	2.9
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	11	2.29	1.03	2.37
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	10	1.97	1.09	1.4
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	9	1.5	0.38	1.37
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	9	1.46	0.28	1.44
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	8	1.85	0.6	1.68
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	8	1.45	0.32	1.4
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	8	1.38	0.24	1.38
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	6	1.77	0.83	1.43
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	6	1.27	0.32	1.14
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	6	1.23	0.28	1.06
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	6	1.15	0.12	1.1
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	5	1.57	0.46	1.59
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	5	1.55	0.33	1.46
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	5	1.44	0.32	1.36
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	5	1.28	0.26	1.22

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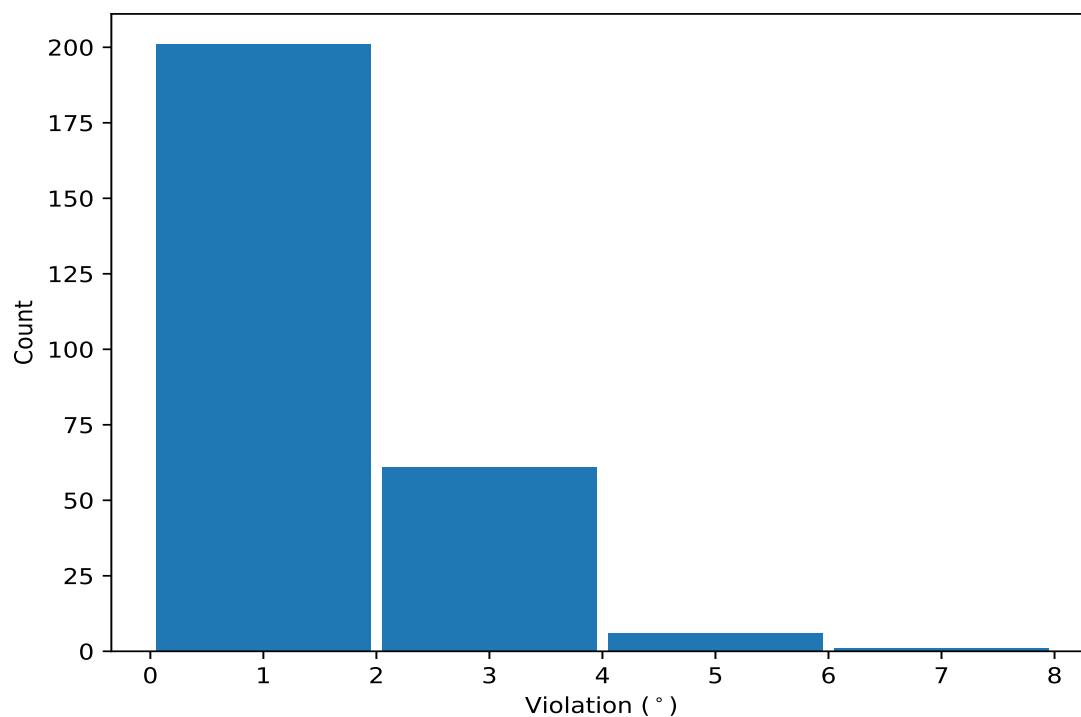
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,31)	1:727:A:VAL:C	1:728:A:CYS:N	1:728:A:CYS:CA	1:728:A:CYS:C	4	1.46	0.47	1.21
(1,91)	1:781:A:LYS:C	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	3	2.06	0.47	2.0
(1,19)	1:712:A:ARG:C	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	3	1.42	0.23	1.46
(1,83)	1:774:A:GLY:C	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	3	1.4	0.12	1.37
(1,8)	1:699:A:VAL:N	1:699:A:VAL:CA	1:699:A:VAL:C	1:700:A:PRO:N	3	1.35	0.11	1.35
(1,20)	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	1:714:A:VAL:N	3	1.21	0.16	1.18
(1,90)	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	1:782:A:CYS:N	2	2.49	0.01	2.49
(1,73)	1:763:A:CYS:C	1:764:A:THR:N	1:764:A:THR:CA	1:764:A:THR:C	2	1.92	0.69	1.92
(1,44)	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	1:739:A:PRO:N	2	1.48	0.18	1.48
(1,100)	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	1:792:A:ARG:N	2	1.42	0.28	1.42
(1,114)	1:808:A:VAL:N	1:808:A:VAL:CA	1:808:A:VAL:C	1:809:A:ASN:N	2	1.38	0.1	1.38
(1,139)	1:826:A:ARG:C	1:827:A:GLY:N	1:827:A:GLY:CA	1:827:A:GLY:C	2	1.25	0.02	1.25
(1,147)	1:830:A:ILE:C	1:831:A:SER:N	1:831:A:SER:CA	1:831:A:SER:C	2	1.11	0.01	1.11

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

10.5 All violated dihedral-angle restraints [i](#)

10.5.1 Histogram : Distribution of violations [i](#)

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



10.5.2 Table: All violated dihedral-angle restraints [\(i\)](#)

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	23	6.71
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	44	5.3
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	29	4.9
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	5	4.84
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	7	4.17
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	29	4.12
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	44	4.12
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	14	3.79
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	9	3.62
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	41	3.61
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	34	3.59
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	23	3.53
(1,78)	1:771:A:LYS:N	1:771:A:LYS:CA	1:771:A:LYS:C	1:772:A:ALA:N	21	3.53
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	10	3.52
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	14	3.43
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	17	3.28
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	15	3.24
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	13	3.19
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	13	3.17
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	23	3.11
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	7	2.97
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	12	2.92
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	25	2.9
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	41	2.9
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	16	2.88
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	30	2.88
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	8	2.85
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	40	2.76
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	39	2.73
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	25	2.69
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	8	2.68
(1,91)	1:781:A:LYS:C	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	30	2.66
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	3	2.62
(1,73)	1:763:A:CYS:C	1:764:A:THR:N	1:764:A:THR:CA	1:764:A:THR:C	43	2.61
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	44	2.58
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	9	2.57
(1,75)	1:764:A:THR:C	1:765:A:LEU:N	1:765:A:LEU:CA	1:765:A:LEU:C	20	2.54
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	6	2.51
(1,90)	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	1:782:A:CYS:N	30	2.5
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	20	2.48
(1,90)	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	1:782:A:CYS:N	22	2.47
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	42	2.46
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	10	2.43
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	31	2.42
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	18	2.38
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	48	2.38
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	9	2.37

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	40	2.37
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	28	2.36
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	43	2.34
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	38	2.34
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	47	2.33
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	11	2.31
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	19	2.28
(1,31)	1:727:A:VAL:C	1:728:A:CYS:N	1:728:A:CYS:CA	1:728:A:CYS:C	22	2.28
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	7	2.23
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	40	2.18
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	2	2.17
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	14	2.16
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	4	2.15
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	6	2.13
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	46	2.11
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	45	2.09
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	21	2.07
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	37	2.06
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	37	2.04
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	29	2.01
(1,91)	1:781:A:LYS:C	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	26	2.0
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	8	1.99
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	42	1.99
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	5	1.97
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	1	1.96
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	43	1.93
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	1	1.92
(1,98)	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	1:791:A:CYS:N	23	1.92
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	6	1.91
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	13	1.91
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	6	1.9
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	9	1.9
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	40	1.9
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	21	1.89
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	47	1.89
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	25	1.89
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	34	1.89
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	25	1.88
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	26	1.88
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	17	1.86
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	19	1.86
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	44	1.86
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	6	1.85
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	4	1.83
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	5	1.81
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	41	1.79
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	6	1.78
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	43	1.78
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	11	1.77
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	29	1.75
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	27	1.74

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	18	1.73
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	25	1.73
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	6	1.71
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	36	1.71
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	41	1.71
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	40	1.7
(1,100)	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	1:792:A:ARG:N	23	1.69
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	19	1.68
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	47	1.68
(1,19)	1:712:A:ARG:C	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	47	1.68
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	21	1.66
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	32	1.66
(1,44)	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	1:739:A:PRO:N	4	1.66
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	47	1.65
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	18	1.65
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	30	1.65
(1,80)	1:772:A:ALA:N	1:772:A:ALA:CA	1:772:A:ALA:C	1:773:A:CYS:N	27	1.65
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	39	1.65
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	16	1.64
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	5	1.64
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	38	1.63
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	4	1.62
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	1	1.6
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	16	1.59
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	20	1.59
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	23	1.59
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	32	1.58
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	5	1.56
(1,83)	1:774:A:GLY:C	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	13	1.56
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	34	1.56
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	41	1.55
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	17	1.53
(1,91)	1:781:A:LYS:C	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	32	1.51
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	14	1.51
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	13	1.5
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	29	1.5
(1,114)	1:808:A:VAL:N	1:808:A:VAL:CA	1:808:A:VAL:C	1:809:A:ASN:N	30	1.48
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	3	1.48
(1,8)	1:699:A:VAL:N	1:699:A:VAL:CA	1:699:A:VAL:C	1:700:A:PRO:N	37	1.48
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	21	1.47
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	35	1.47
(1,48)	1:740:A:LEU:N	1:740:A:LEU:CA	1:740:A:LEU:C	1:741:A:THR:N	16	1.46
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	32	1.46
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	26	1.46
(1,19)	1:712:A:ARG:C	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	46	1.46
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	41	1.46
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	35	1.46
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	12	1.45
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	12	1.44
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	8	1.44
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	8	1.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	22	1.43
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	24	1.43
(1,95)	1:788:A:LYS:C	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	18	1.43
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	28	1.43
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	9	1.43
(1,20)	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	1:714:A:VAL:N	45	1.42
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	2	1.41
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	39	1.41
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	11	1.4
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	22	1.4
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	29	1.4
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	24	1.39
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	44	1.39
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	4	1.39
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	40	1.39
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	23	1.39
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	41	1.37
(1,83)	1:774:A:GLY:C	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	47	1.37
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	38	1.37
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	48	1.36
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	45	1.36
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	24	1.36
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	31	1.35
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	13	1.35
(1,8)	1:699:A:VAL:N	1:699:A:VAL:CA	1:699:A:VAL:C	1:700:A:PRO:N	7	1.35
(1,93)	1:787:A:SER:C	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	33	1.34
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	38	1.34
(1,24)	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	1:716:A:LYS:N	25	1.34
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	23	1.34
(1,3)	1:692:A:MET:C	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	48	1.34
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	20	1.33
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	20	1.32
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	48	1.32
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	26	1.32
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	47	1.32
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	7	1.31
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	20	1.31
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	27	1.31
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	2	1.3
(1,44)	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	1:739:A:PRO:N	15	1.3
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	17	1.29
(1,4)	1:693:A:ASN:N	1:693:A:ASN:CA	1:693:A:ASN:C	1:694:A:PRO:N	20	1.29
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	42	1.28
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	5	1.28
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	18	1.28
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	13	1.27
(1,139)	1:826:A:ARG:C	1:827:A:GLY:N	1:827:A:GLY:CA	1:827:A:GLY:C	3	1.27
(1,114)	1:808:A:VAL:N	1:808:A:VAL:CA	1:808:A:VAL:C	1:809:A:ASN:N	35	1.27
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	35	1.27
(1,83)	1:774:A:GLY:C	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	21	1.26
(1,31)	1:727:A:VAL:C	1:728:A:CYS:N	1:728:A:CYS:CA	1:728:A:CYS:C	12	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,139)	1:826:A:ARG:C	1:827:A:GLY:N	1:827:A:GLY:CA	1:827:A:GLY:C	40	1.24
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	47	1.24
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	17	1.24
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	16	1.24
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	37	1.24
(1,73)	1:763:A:CYS:C	1:764:A:THR:N	1:764:A:THR:CA	1:764:A:THR:C	20	1.23
(1,27)	1:723:A:PRO:C	1:724:A:SER:N	1:724:A:SER:CA	1:724:A:SER:C	16	1.23
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	36	1.23
(1,5)	1:694:A:PRO:C	1:695:A:LEU:N	1:695:A:LEU:CA	1:695:A:LEU:C	13	1.23
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	46	1.22
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	23	1.22
(1,8)	1:699:A:VAL:N	1:699:A:VAL:CA	1:699:A:VAL:C	1:700:A:PRO:N	3	1.22
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	10	1.21
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	21	1.2
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	19	1.2
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	10	1.2
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	27	1.2
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	30	1.19
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	29	1.19
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	45	1.19
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	25	1.18
(1,20)	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	1:714:A:VAL:N	35	1.18
(1,31)	1:727:A:VAL:C	1:728:A:CYS:N	1:728:A:CYS:CA	1:728:A:CYS:C	25	1.17
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	23	1.16
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	38	1.16
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	10	1.16
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	44	1.16
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	26	1.15
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	36	1.15
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	4	1.15
(1,31)	1:727:A:VAL:C	1:728:A:CYS:N	1:728:A:CYS:CA	1:728:A:CYS:C	15	1.15
(1,9)	1:701:A:LYS:C	1:702:A:CYS:N	1:702:A:CYS:CA	1:702:A:CYS:C	11	1.15
(1,100)	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	1:792:A:ARG:N	20	1.14
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	36	1.13
(1,147)	1:830:A:ILE:C	1:831:A:SER:N	1:831:A:SER:CA	1:831:A:SER:C	46	1.12
(1,94)	1:788:A:LYS:N	1:788:A:LYS:CA	1:788:A:LYS:C	1:789:A:CYS:N	47	1.12
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	16	1.12
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	26	1.12
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	40	1.12
(1,102)	1:792:A:ARG:N	1:792:A:ARG:CA	1:792:A:ARG:C	1:793:A:GLU:N	43	1.11
(1,22)	1:714:A:VAL:N	1:714:A:VAL:CA	1:714:A:VAL:C	1:715:A:CYS:N	2	1.11
(1,19)	1:712:A:ARG:C	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	13	1.11
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	31	1.11
(1,147)	1:830:A:ILE:C	1:831:A:SER:N	1:831:A:SER:CA	1:831:A:SER:C	18	1.1
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	32	1.09
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	25	1.08
(1,123)	1:814:A:THR:C	1:815:A:MET:N	1:815:A:MET:CA	1:815:A:MET:C	35	1.08
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	25	1.08
(1,144)	1:829:A:SER:N	1:829:A:SER:CA	1:829:A:SER:C	1:830:A:ILE:N	14	1.07
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	9	1.06
(1,153)	1:837:A:PRO:C	1:838:A:CYS:N	1:838:A:CYS:CA	1:838:A:CYS:C	20	1.06

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	15	1.06
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	39	1.06
(1,97)	1:789:A:CYS:C	1:790:A:VAL:N	1:790:A:VAL:CA	1:790:A:VAL:C	30	1.05
(1,96)	1:789:A:CYS:N	1:789:A:CYS:CA	1:789:A:CYS:C	1:790:A:VAL:N	13	1.05
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	3	1.05
(1,84)	1:775:A:ALA:N	1:775:A:ALA:CA	1:775:A:ALA:C	1:776:A:CYS:N	36	1.05
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	8	1.05
(1,17)	1:708:A:LEU:C	1:709:A:GLN:N	1:709:A:GLN:CA	1:709:A:GLN:C	39	1.05
(1,43)	1:737:A:ILE:C	1:738:A:LEU:N	1:738:A:LEU:CA	1:738:A:LEU:C	10	1.04
(1,99)	1:790:A:VAL:C	1:791:A:CYS:N	1:791:A:CYS:CA	1:791:A:CYS:C	8	1.03
(1,23)	1:714:A:VAL:C	1:715:A:CYS:N	1:715:A:CYS:CA	1:715:A:CYS:C	46	1.03
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	34	1.02
(1,20)	1:713:A:CYS:N	1:713:A:CYS:CA	1:713:A:CYS:C	1:714:A:VAL:N	13	1.02
(1,92)	1:782:A:CYS:N	1:782:A:CYS:CA	1:782:A:CYS:C	1:783:A:ASP:N	4	1.01
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	26	1.01
(1,81)	1:773:A:CYS:C	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	30	1.01
(1,89)	1:780:A:GLY:C	1:781:A:LYS:N	1:781:A:LYS:CA	1:781:A:LYS:C	14	1.0
(1,82)	1:774:A:GLY:N	1:774:A:GLY:CA	1:774:A:GLY:C	1:775:A:ALA:N	5	1.0