



Full wwPDB NMR Structure Validation Report ⓘ

Mar 7, 2026 – 12:34 AM UTC

PDB ID : 2KVA / pdb_00002kva
BMRB ID : 16772
Title : SOLUTION STRUCTURE OF CI-MPR ligand-free domain 5
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Deposited on : 2010-03-10

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

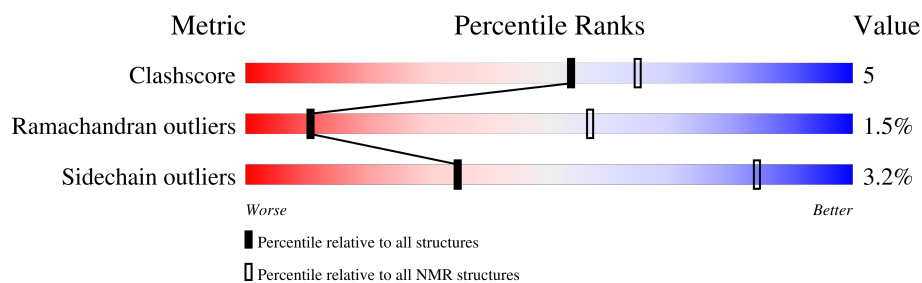
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 87%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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

Mol	Chain	Length	Quality of chain
1	A	148	

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:586-A:696, A:700-A:707, A:712-A:725 (133)	0.80	14

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 4 clusters and 5 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2134 atoms, of which 956 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2134	734	956	198	239	7	

There are 6 discrepancies between the modelled and reference sequences:

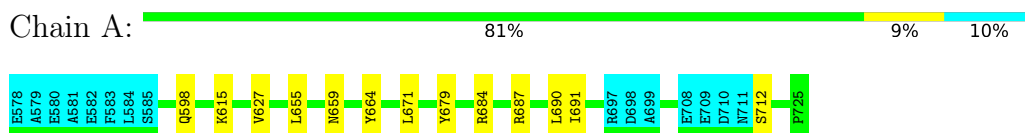
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	GLU	-	expression tag	UNP P08169
A	579	ALA	-	expression tag	UNP P08169
A	580	GLU	-	expression tag	UNP P08169
A	581	ALA	-	expression tag	UNP P08169
A	582	GLU	-	expression tag	UNP P08169
A	583	PHE	-	expression tag	UNP P08169

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Cation-independent mannose-6-phosphate receptor

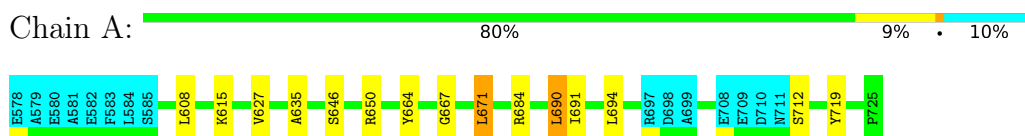


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

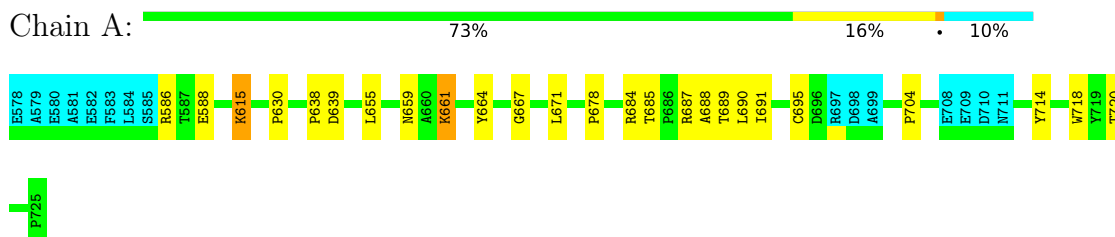
4.2.1 Score per residue for model 1

- Molecule 1: Cation-independent mannose-6-phosphate receptor



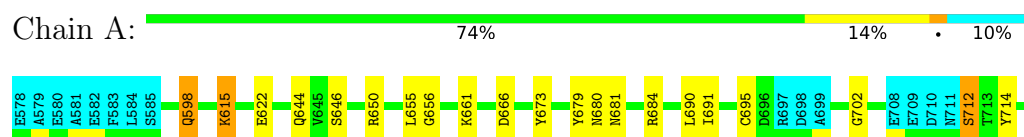
4.2.2 Score per residue for model 2

- Molecule 1: Cation-independent mannose-6-phosphate receptor



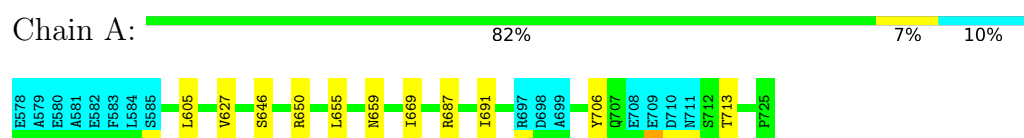
4.2.3 Score per residue for model 3

- Molecule 1: Cation-independent mannose-6-phosphate receptor



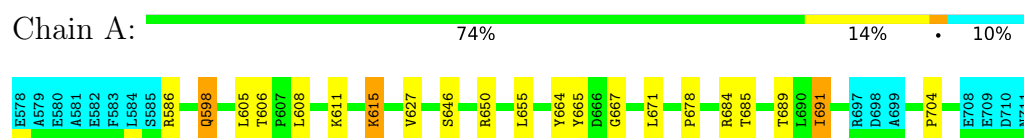
4.2.4 Score per residue for model 4

- Molecule 1: Cation-independent mannose-6-phosphate receptor



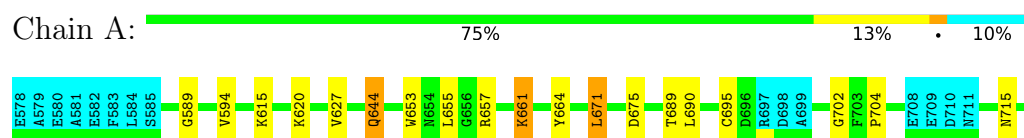
4.2.5 Score per residue for model 5

- Molecule 1: Cation-independent mannose-6-phosphate receptor



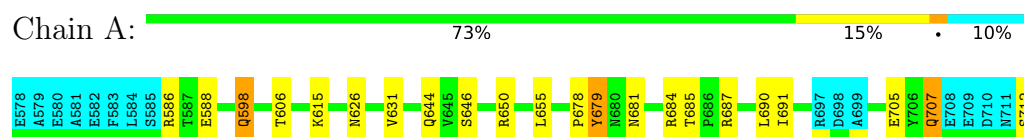
4.2.6 Score per residue for model 6

- Molecule 1: Cation-independent mannose-6-phosphate receptor



4.2.7 Score per residue for model 7

- Molecule 1: Cation-independent mannose-6-phosphate receptor

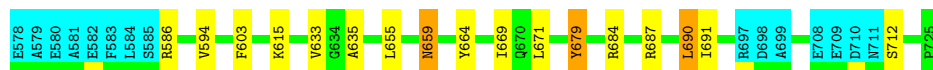




4.2.8 Score per residue for model 8

- Molecule 1: Cation-independent mannose-6-phosphate receptor

Chain A: 78% 9% 10%



4.2.9 Score per residue for model 9

- Molecule 1: Cation-independent mannose-6-phosphate receptor

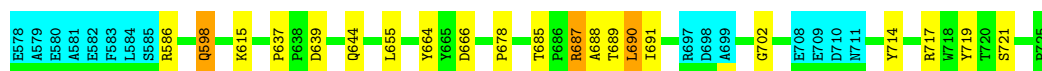
Chain A: 77% 9% 10%



4.2.10 Score per residue for model 10

- Molecule 1: Cation-independent mannose-6-phosphate receptor

Chain A: 76% 12% 10%



4.2.11 Score per residue for model 11

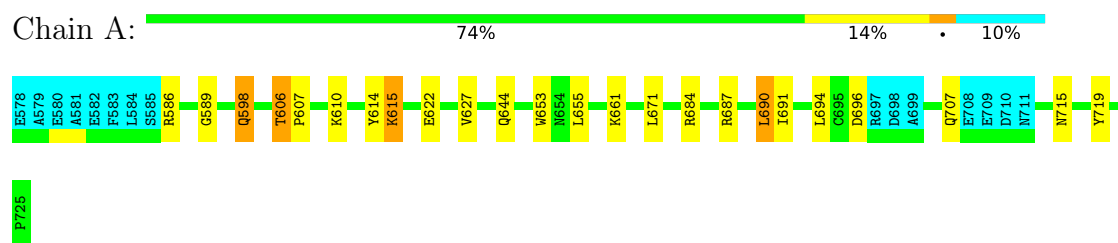
- Molecule 1: Cation-independent mannose-6-phosphate receptor

Chain A: 70% 15% 5% 10%



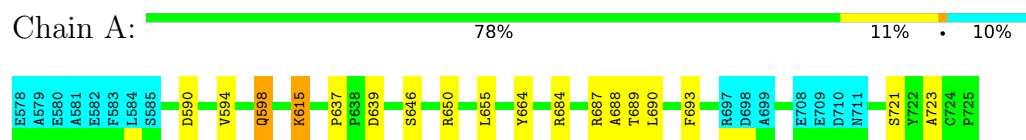
4.2.12 Score per residue for model 12

- Molecule 1: Cation-independent mannose-6-phosphate receptor



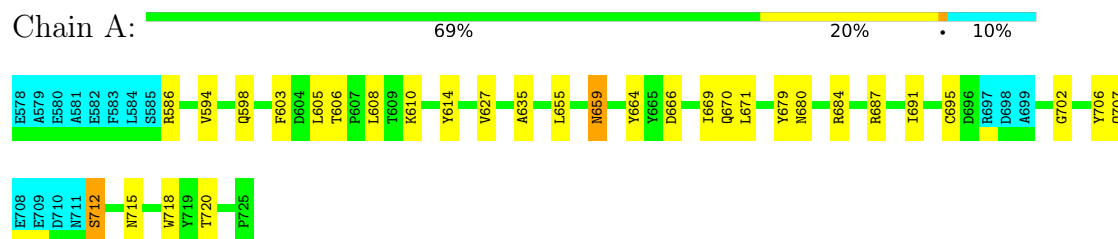
4.2.13 Score per residue for model 13

- Molecule 1: Cation-independent mannose-6-phosphate receptor



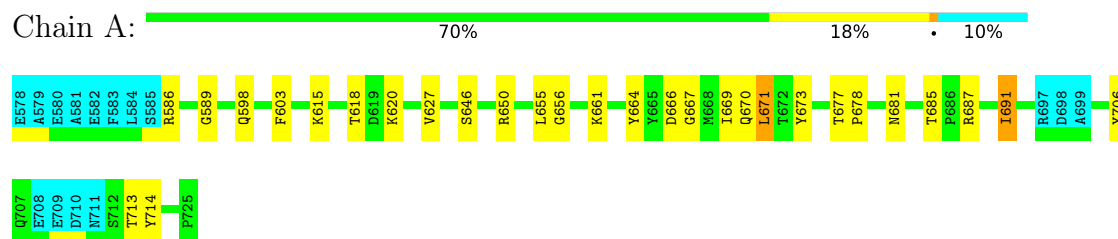
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Cation-independent mannose-6-phosphate receptor



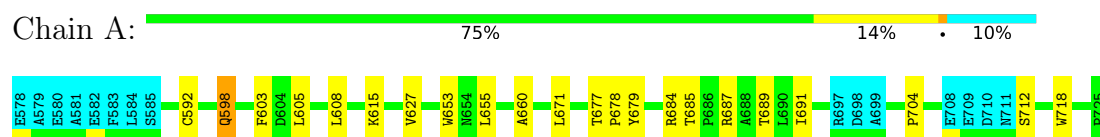
4.2.15 Score per residue for model 15

- Molecule 1: Cation-independent mannose-6-phosphate receptor



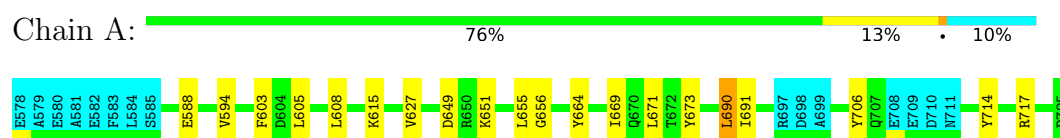
4.2.16 Score per residue for model 16

- Molecule 1: Cation-independent mannose-6-phosphate receptor



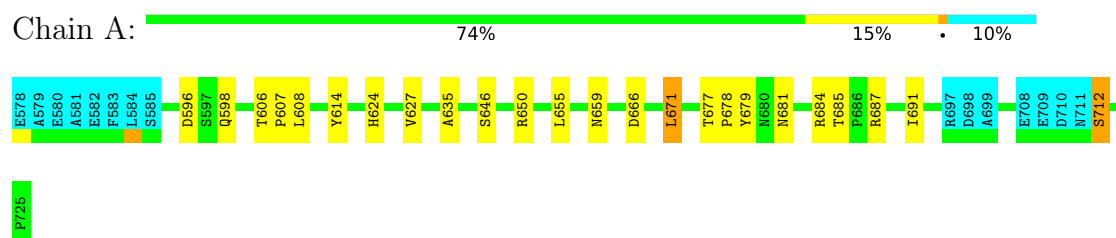
4.2.17 Score per residue for model 17

- Molecule 1: Cation-independent mannose-6-phosphate receptor



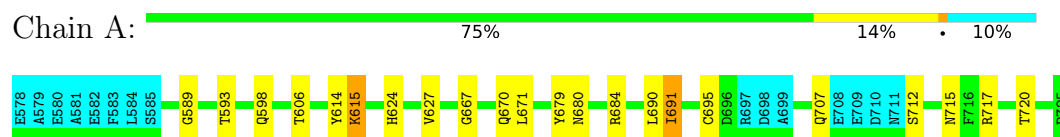
4.2.18 Score per residue for model 18

- Molecule 1: Cation-independent mannose-6-phosphate receptor



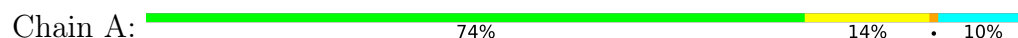
4.2.19 Score per residue for model 19

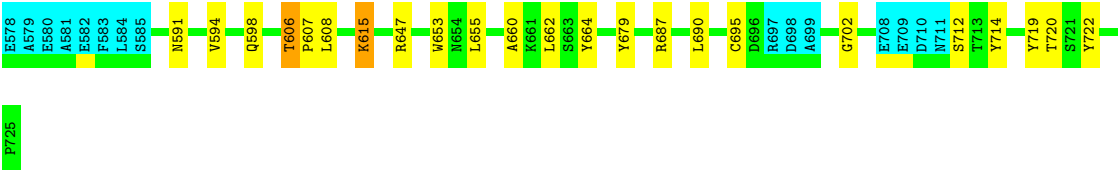
- Molecule 1: Cation-independent mannose-6-phosphate receptor



4.2.20 Score per residue for model 20

- Molecule 1: Cation-independent mannose-6-phosphate receptor





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5 Refinement protocol and experimental data overview

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
Xplor-NIH	refinement	2.9.3

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	1608
Number of shifts mapped to atoms	1498
Number of unparsed shifts	0
Number of shifts with mapping errors	110
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	1.16±0.03	2±1/1087 (0.1± 0.1%)	0.91±0.02	0±0/1475 (0.0± 0.0%)
All	All	1.17	30/21740 (0.1%)	0.91	6/29500 (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	0.1±0.3
All	All	0	2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	615	LYS	C-N	-6.66	1.25	1.33	11	1
1	A	627	VAL	C-N	-6.32	1.25	1.33	19	5
1	A	687	ARG	CZ-NH2	-6.09	1.25	1.33	9	1
1	A	606	THR	CA-C	6.09	1.59	1.52	5	6
1	A	690	LEU	N-CA	-6.01	1.39	1.46	10	9
1	A	615	LYS	N-CA	-5.75	1.39	1.46	17	1
1	A	717	ARG	C-N	-5.66	1.25	1.33	10	3
1	A	653	TRP	C-N	-5.50	1.25	1.33	20	2
1	A	659	ASN	C-N	-5.44	1.27	1.33	4	1
1	A	606	THR	C-N	5.05	1.39	1.34	5	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	603	PHE	CA-CB-CG	5.53	119.33	113.80	16	1
1	A	659	ASN	CA-CB-CG	5.25	117.85	112.60	14	3
1	A	608	LEU	N-CA-C	-5.09	106.91	113.23	1	1
1	A	647	ARG	N-CA-C	-5.03	107.70	113.88	20	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	647	ARG	Sidechain	1
1	A	586	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	1058	864	985	11±3
All	All	21160	17280	19700	211

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:679:TYR:OH	1:A:712:SER:HA	0.70	1.87	16	6
1:A:676:GLY:HA3	1:A:687:ARG:NH2	0.69	2.03	9	1
1:A:586:ARG:HA	1:A:664:TYR:O	0.62	1.94	5	8
1:A:655:LEU:HA	1:A:687:ARG:NH2	0.62	2.10	9	1
1:A:655:LEU:HD23	1:A:714:TYR:CD1	0.60	2.32	17	4
1:A:695:CYS:HA	1:A:720:THR:O	0.59	1.97	3	7
1:A:707:GLN:HG2	1:A:715:ASN:HB3	0.59	1.74	7	1
1:A:646:SER:O	1:A:650:ARG:HA	0.58	1.97	3	9
1:A:655:LEU:HB3	1:A:689:THR:OG1	0.57	1.99	10	8
1:A:655:LEU:HG	1:A:687:ARG:HD3	0.56	1.77	20	7
1:A:687:ARG:HA	1:A:687:ARG:CZ	0.56	2.30	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:627:VAL:HA	1:A:671:LEU:HD11	0.56	1.75	9	6
1:A:664:TYR:CZ	1:A:667:GLY:HA2	0.55	2.36	9	5
1:A:615:LYS:HD3	1:A:615:LYS:O	0.54	2.02	9	8
1:A:687:ARG:NE	1:A:688:ALA:H	0.53	2.01	10	3
1:A:687:ARG:HA	1:A:687:ARG:NH1	0.53	2.18	10	1
1:A:661:LYS:HD2	1:A:661:LYS:C	0.53	2.28	6	2
1:A:678:PRO:HA	1:A:685:THR:O	0.53	2.04	10	8
1:A:707:GLN:HG3	1:A:715:ASN:HB3	0.52	1.81	12	2
1:A:622:GLU:O	1:A:644:GLN:HA	0.52	2.04	3	2
1:A:605:LEU:O	1:A:608:LEU:HB2	0.52	2.05	16	4
1:A:670:GLN:HA	1:A:691:ILE:O	0.52	2.05	15	3
1:A:608:LEU:HB3	1:A:627:VAL:HG21	0.51	1.83	5	2
1:A:630:PRO:HB2	1:A:638:PRO:O	0.51	2.06	2	1
1:A:589:GLY:O	1:A:661:LYS:HA	0.51	2.06	15	1
1:A:655:LEU:HG	1:A:687:ARG:CD	0.50	2.35	15	6
1:A:594:VAL:CG2	1:A:664:TYR:HB2	0.50	2.37	17	4
1:A:644:GLN:OE1	1:A:653:TRP:HB2	0.49	2.07	6	1
1:A:669:ILE:HB	1:A:693:PHE:HB2	0.49	1.83	11	1
1:A:649:ASP:OD1	1:A:651:LYS:HG3	0.48	2.07	17	1
1:A:671:LEU:O	1:A:690:LEU:HA	0.48	2.07	19	7
1:A:702:GLY:HA2	1:A:719:TYR:O	0.48	2.09	6	5
1:A:704:PRO:HB3	1:A:718:TRP:CE3	0.48	2.44	2	4
1:A:610:LYS:HE2	1:A:614:TYR:CZ	0.48	2.43	9	3
1:A:605:LEU:HD21	1:A:669:ILE:HG21	0.48	1.84	4	1
1:A:679:TYR:OH	1:A:687:ARG:HG3	0.47	2.09	20	1
1:A:594:VAL:HG21	1:A:664:TYR:HB2	0.47	1.85	14	4
1:A:598:GLN:NE2	1:A:598:GLN:H	0.47	2.08	12	7
1:A:591:ASN:HA	1:A:660:ALA:CB	0.47	2.39	20	1
1:A:603:PHE:CD2	1:A:669:ILE:HD11	0.47	2.45	17	5
1:A:671:LEU:HB3	1:A:691:ILE:HB	0.46	1.88	5	1
1:A:702:GLY:HA3	1:A:718:TRP:NE1	0.46	2.26	14	1
1:A:614:TYR:O	1:A:624:HIS:HA	0.46	2.11	19	4
1:A:681:ASN:O	1:A:684:ARG:HD2	0.45	2.12	3	1
1:A:677:THR:HB	1:A:687:ARG:NH1	0.45	2.27	15	4
1:A:679:TYR:CZ	1:A:712:SER:HA	0.45	2.47	8	1
1:A:592:CYS:H	1:A:660:ALA:HB1	0.44	1.72	16	1
1:A:691:ILE:HG21	1:A:718:TRP:CE3	0.44	2.48	11	1
1:A:693:PHE:HB3	1:A:723:ALA:HB2	0.44	1.89	13	1
1:A:659:ASN:HD21	1:A:661:LYS:HB3	0.44	1.72	2	1
1:A:589:GLY:O	1:A:661:LYS:HG2	0.44	2.12	12	2
1:A:694:LEU:O	1:A:719:TYR:HA	0.43	2.13	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:656:GLY:HA3	1:A:673:TYR:HB3	0.43	1.90	3	3
1:A:657:ARG:HD2	1:A:675:ASP:OD2	0.43	2.13	6	1
1:A:589:GLY:HA3	1:A:593:THR:O	0.43	2.14	19	1
1:A:690:LEU:O	1:A:715:ASN:HA	0.43	2.14	6	1
1:A:707:GLN:CG	1:A:715:ASN:HB3	0.43	2.43	14	1
1:A:591:ASN:HA	1:A:660:ALA:HB3	0.42	1.91	20	1
1:A:594:VAL:HB	1:A:662:LEU:HB2	0.42	1.90	20	1
1:A:687:ARG:HD3	1:A:714:TYR:CE2	0.42	2.49	10	2
1:A:592:CYS:N	1:A:660:ALA:HB1	0.42	2.29	16	1
1:A:683:LYS:HD2	1:A:683:LYS:N	0.42	2.30	11	1
1:A:661:LYS:HB3	1:A:661:LYS:NZ	0.42	2.29	6	1
1:A:606:THR:N	1:A:607:PRO:HD2	0.42	2.29	18	3
1:A:690:LEU:HD23	1:A:690:LEU:C	0.41	2.41	19	5
1:A:707:GLN:HG3	1:A:715:ASN:O	0.41	2.15	7	1
1:A:627:VAL:HA	1:A:671:LEU:CD2	0.41	2.45	16	1
1:A:608:LEU:CB	1:A:627:VAL:HG21	0.41	2.46	18	1
1:A:633:VAL:HG12	1:A:635:ALA:H	0.41	1.76	8	1
1:A:687:ARG:HD2	1:A:712:SER:O	0.41	2.16	9	1
1:A:626:ASN:HB2	1:A:631:VAL:HG12	0.41	1.91	7	1
1:A:644:GLN:HG2	1:A:655:LEU:HD11	0.41	1.93	7	2
1:A:659:ASN:HD22	1:A:659:ASN:C	0.41	2.23	8	1
1:A:696:ASP:HB3	1:A:719:TYR:CD1	0.41	2.50	12	1
1:A:653:TRP:HB3	1:A:687:ARG:NH1	0.41	2.31	16	1
1:A:637:PRO:C	1:A:639:ASP:H	0.40	2.24	10	2
1:A:690:LEU:C	1:A:690:LEU:HD23	0.40	2.42	1	1
1:A:596:ASP:OD1	1:A:598:GLN:HB2	0.40	2.17	18	1
1:A:586:ARG:C	1:A:586:ARG:HD2	0.40	2.40	5	1
1:A:608:LEU:HD11	1:A:722:TYR:CG	0.40	2.52	20	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	132/148 (89%)	120±2 (91±1%)	10±2 (7±2%)	2±1 (1±1%)	11	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2640/2960 (89%)	2405 (91%)	196 (7%)	39 (1%)	11	57

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	684	ARG	11
1	A	712	SER	7
1	A	666	ASP	5
1	A	667	GLY	4
1	A	635	ALA	3
1	A	680	ASN	3
1	A	681	ASN	3
1	A	639	ASP	1
1	A	679	TYR	1
1	A	590	ASP	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	116/128 (91%)	112±2 (97±1%)	4±2 (3±1%)	35	84
All	All	2320/2560 (91%)	2246 (97%)	74 (3%)	35	84

All 17 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	615	LYS	16
1	A	691	ILE	15
1	A	598	GLN	12
1	A	671	LEU	6
1	A	659	ASN	5
1	A	588	GLU	3
1	A	661	LYS	3
1	A	687	ARG	3
1	A	620	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	679	TYR	2
1	A	684	ARG	1
1	A	611	LYS	1
1	A	644	GLN	1
1	A	586	ARG	1
1	A	705	GLU	1
1	A	707	GLN	1
1	A	618	THR	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 87% for the well-defined parts and 83% 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	1608
Number of shifts mapped to atoms	1498
Number of unparsed shifts	0
Number of shifts with mapping errors	110
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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

- No matching atom found in the structure. All 110 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	584	LEU	HD11	0.924	0.005	2
1	A	584	LEU	HD12	0.924	0.005	2
1	A	584	LEU	HD22	0.893	0.020	2
1	A	584	LEU	HD23	0.893	0.020	2
1	A	587	THR	HG22	1.442	0.020	1
1	A	587	THR	HG23	1.442	0.020	1
1	A	593	THR	HG22	1.269	0.020	1
1	A	593	THR	HG23	1.269	0.020	1
1	A	594	VAL	HG11	0.907	0.020	2
1	A	594	VAL	HG12	0.907	0.020	2
1	A	594	VAL	HG22	1.016	0.020	2
1	A	594	VAL	HG23	1.016	0.020	2
1	A	598	GLN	HE22	6.855	0.020	2
1	A	605	LEU	HD11	-0.058	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	605	LEU	HD12	-0.058	0.020	2
1	A	605	LEU	HD22	-0.107	0.020	2
1	A	605	LEU	HD23	-0.107	0.020	2
1	A	606	THR	HG22	1.417	0.001	1
1	A	606	THR	HG23	1.417	0.001	1
1	A	608	LEU	HD11	0.608	0.020	2
1	A	608	LEU	HD12	0.608	0.020	2
1	A	608	LEU	HD22	0.35	0.020	2
1	A	608	LEU	HD23	0.35	0.020	2
1	A	609	THR	HG22	1.286	0.020	1
1	A	609	THR	HG23	1.286	0.020	1
1	A	616	VAL	HG11	1.292	0.020	2
1	A	616	VAL	HG12	1.292	0.020	2
1	A	616	VAL	HG22	0.979	0.020	2
1	A	616	VAL	HG23	0.979	0.020	2
1	A	618	THR	HG22	1.485	0.020	1
1	A	618	THR	HG23	1.485	0.020	1
1	A	625	ILE	HD12	0.003	0.020	1
1	A	625	ILE	HD13	0.003	0.020	1
1	A	625	ILE	HG13	0.828	0.020	2
1	A	625	ILE	HG21	0.665	0.020	1
1	A	625	ILE	HG22	0.665	0.020	1
1	A	626	ASN	HD22	7.174	0.020	2
1	A	627	VAL	HG11	0.665	0.020	2
1	A	627	VAL	HG12	0.665	0.020	2
1	A	627	VAL	HG22	0.66	0.020	2
1	A	627	VAL	HG23	0.66	0.020	2
1	A	631	VAL	HG11	0.89	0.020	2
1	A	631	VAL	HG12	0.89	0.020	2
1	A	631	VAL	HG22	0.911	0.020	2
1	A	631	VAL	HG23	0.911	0.020	2
1	A	633	VAL	HG11	0.467	0.020	2
1	A	633	VAL	HG12	0.467	0.020	2
1	A	633	VAL	HG22	0.562	0.001	2
1	A	633	VAL	HG23	0.562	0.001	2
1	A	644	GLN	HE22	3.719	0.020	2
1	A	645	VAL	HG11	0.908	0.020	2
1	A	645	VAL	HG12	0.908	0.020	2
1	A	645	VAL	HG22	0.859	0.020	2
1	A	645	VAL	HG23	0.859	0.020	2
1	A	654	ASN	HD22	6.287	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	655	LEU	HD11	0.244	0.020	2
1	A	655	LEU	HD12	0.244	0.020	2
1	A	655	LEU	HD22	0.604	0.020	2
1	A	655	LEU	HD23	0.604	0.020	2
1	A	659	ASN	HD22	7.872	0.020	2
1	A	662	LEU	HD11	0.673	0.020	2
1	A	662	LEU	HD12	0.673	0.020	2
1	A	662	LEU	HD22	0.559	0.020	2
1	A	662	LEU	HD23	0.559	0.020	2
1	A	669	ILE	HD12	0.083	0.020	1
1	A	669	ILE	HD13	0.083	0.020	1
1	A	669	ILE	HG13	0.628	0.020	2
1	A	669	ILE	HG21	0.831	0.001	1
1	A	669	ILE	HG22	0.831	0.001	1
1	A	670	GLN	HE22	6.869	0.020	2
1	A	671	LEU	HD11	1.083	0.020	2
1	A	671	LEU	HD12	1.083	0.020	2
1	A	671	LEU	HD22	1.068	0.020	2
1	A	671	LEU	HD23	1.068	0.020	2
1	A	672	THR	HG22	1.167	0.020	1
1	A	672	THR	HG23	1.167	0.020	1
1	A	677	THR	HG22	1.767	0.020	1
1	A	677	THR	HG23	1.767	0.020	1
1	A	680	ASN	HD22	6.951	0.020	2
1	A	681	ASN	HD22	6.873	0.020	2
1	A	685	THR	HG22	1.459	0.020	1
1	A	685	THR	HG23	1.459	0.020	1
1	A	689	THR	HG22	1.206	0.020	1
1	A	689	THR	HG23	1.206	0.020	1
1	A	690	LEU	HD11	0.825	0.020	2
1	A	690	LEU	HD12	0.825	0.020	2
1	A	690	LEU	HD22	0.813	0.020	2
1	A	690	LEU	HD23	0.813	0.020	2
1	A	691	ILE	HD12	0.634	0.020	1
1	A	691	ILE	HD13	0.634	0.020	1
1	A	691	ILE	HG13	0.555	0.003	2
1	A	691	ILE	HG21	0.018	0.004	1
1	A	691	ILE	HG22	0.018	0.004	1
1	A	692	THR	HG22	1.146	0.020	1
1	A	692	THR	HG23	1.146	0.020	1
1	A	694	LEU	HD11	0.868	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	694	LEU	HD12	0.868	0.020	2
1	A	694	LEU	HD22	0.517	0.020	2
1	A	694	LEU	HD23	0.517	0.020	2
1	A	701	VAL	HG11	1.633	0.020	2
1	A	701	VAL	HG12	1.633	0.020	2
1	A	701	VAL	HG22	1.454	0.020	2
1	A	701	VAL	HG23	1.454	0.020	2
1	A	707	GLN	HE22	6.693	0.020	2
1	A	711	ASN	HD22	6.78	0.020	2
1	A	713	THR	HG22	1.117	0.020	1
1	A	713	THR	HG23	1.117	0.020	1
1	A	715	ASN	HD22	6.87	0.020	2
1	A	720	THR	HG22	1.194	0.020	1
1	A	720	THR	HG23	1.194	0.020	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	141	-0.44 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	-0.61 ± 0.10	Should be applied
$^{13}\text{C}'$	135	0.07 ± 0.13	None needed (< 0.5 ppm)
^{15}N	135	-0.31 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 87%, i.e. 1511 atoms were assigned a chemical shift out of a possible 1743. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	649/659 (98%)	268/268 (100%)	256/266 (96%)	125/125 (100%)
Sidechain	748/892 (84%)	498/573 (87%)	237/277 (86%)	13/42 (31%)
Aromatic	114/192 (59%)	70/91 (77%)	42/97 (43%)	2/4 (50%)
Overall	1511/1743 (87%)	836/932 (90%)	535/640 (84%)	140/171 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1604 atoms were assigned a chemical shift out of a possible 1927. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	698/734 (95%)	287/298 (96%)	276/296 (93%)	135/140 (96%)
Sidechain	792/991 (80%)	527/634 (83%)	251/311 (81%)	14/46 (30%)
Aromatic	114/202 (56%)	70/96 (73%)	42/102 (41%)	2/4 (50%)
Overall	1604/1927 (83%)	884/1028 (86%)	569/709 (80%)	151/190 (79%)

7.1.4 Statistically unusual chemical shifts [i](#)

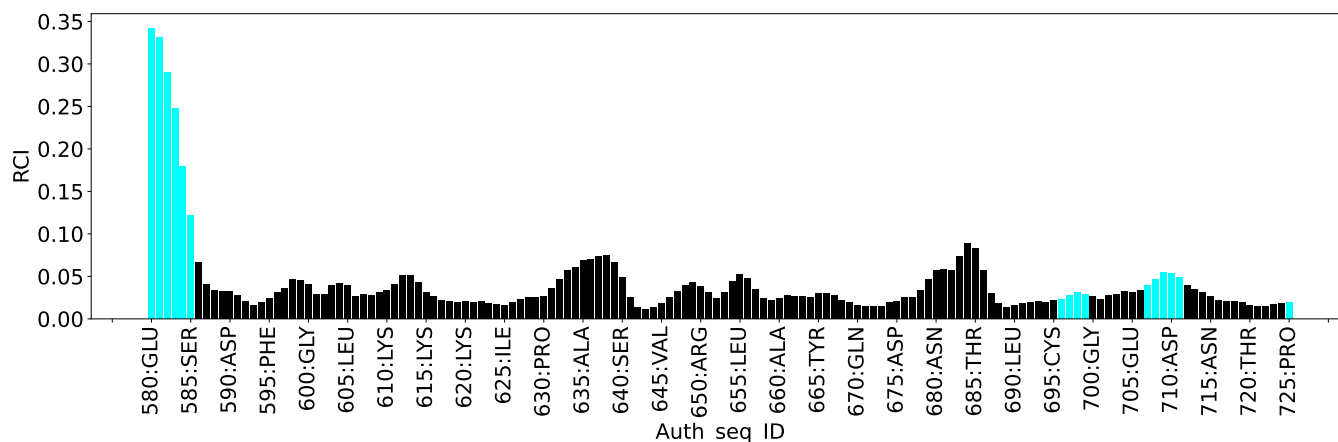
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	618	THR	HG1	5.85	0.08 – 2.19	22.3
1	A	720	THR	HG1	5.34	0.08 – 2.19	19.9
1	A	644	GLN	HE22	3.72	4.88 – 9.19	-7.7
1	A	704	PRO	HD3	0.86	1.76 – 5.48	-7.4

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 [i](#)

8.1 Conformationally restricting restraints [i](#)

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

Description	Value
Total distance restraints	1763
Intra-residue ($ i-j =0$)	329
Sequential ($ i-j =1$)	389
Medium range ($ i-j >1$ and $ i-j <5$)	170
Long range ($ i-j \geq 5$)	872
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	3
Total dihedral-angle restraints	165
Number of unmapped restraints	0
Number of restraints per residue	13.0
Number of long range restraints per residue ¹	5.9

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 [i](#)

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

8.2.1 Average number of distance violations per model [i](#)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	15.3	0.2
0.2-0.5 (Medium)	8.2	0.5
>0.5 (Large)	3.4	1.36

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)	24.3	5.63
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

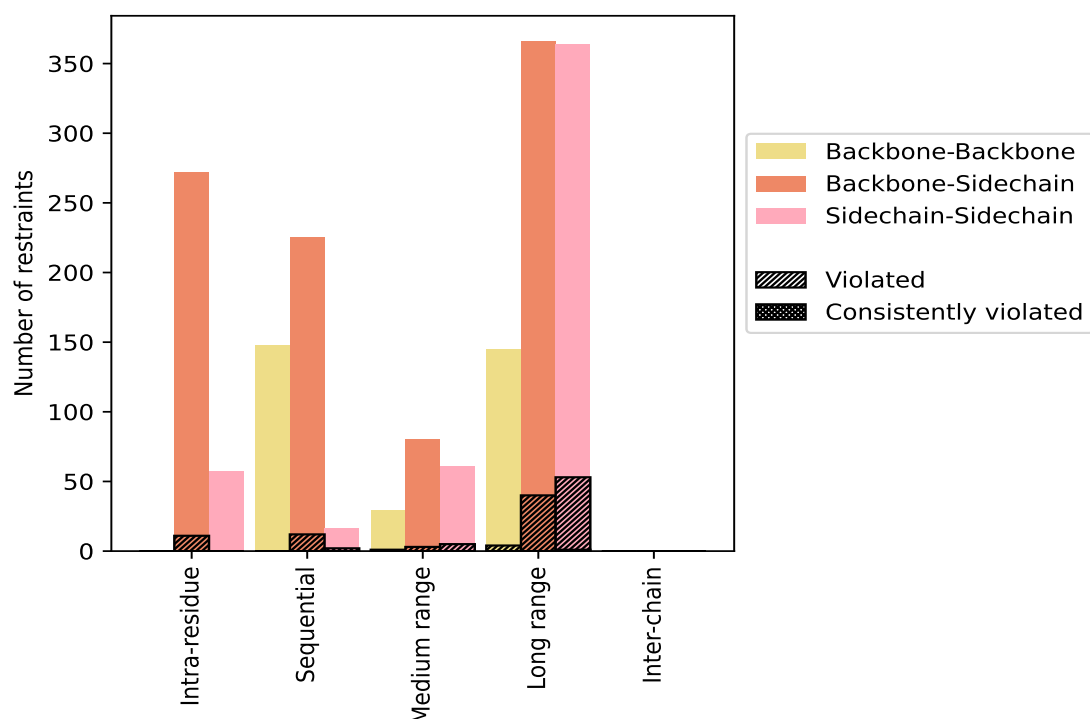
9.1 Summary of distance violations

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 ($i-j =0$)	329	18.7	11	3.3	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	272	15.4	11	4.0	0.6	0	0.0	0.0
Sidechain-Sidechain	57	3.2	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	389	22.1	14	3.6	0.8	0	0.0	0.0
Backbone-Backbone	148	8.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	225	12.8	12	5.3	0.7	0	0.0	0.0
Sidechain-Sidechain	16	0.9	2	12.5	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	170	9.6	9	5.3	0.5	0	0.0	0.0
Backbone-Backbone	29	1.6	1	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	80	4.5	3	3.8	0.2	0	0.0	0.0
Sidechain-Sidechain	61	3.5	5	8.2	0.3	0	0.0	0.0
Long range ($i-j \geq 5$)	872	49.5	97	11.1	5.5	1	0.1	0.1
Backbone-Backbone	145	8.2	4	2.8	0.2	0	0.0	0.0
Backbone-Sidechain	366	20.8	40	10.9	2.3	0	0.0	0.0
Sidechain-Sidechain	361	20.5	53	14.7	3.0	1	0.3	0.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	3	0.2	0	0.0	0.0	0	0.0	0.0
Total	1763	100.0	131	7.4	7.4	1	0.1	0.1
Backbone-Backbone	322	18.3	5	1.6	0.3	0	0.0	0.0
Backbone-Sidechain	943	53.5	66	7.0	3.7	0	0.0	0.0
Sidechain-Sidechain	498	28.2	60	12.0	3.4	1	0.2	0.1

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

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



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfid 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	3	2	1	24	0	30	0.28	1.26	0.26	0.16
2	5	2	2	22	0	31	0.27	0.91	0.21	0.14
3	3	0	2	16	0	21	0.23	0.92	0.18	0.16
4	4	3	3	23	0	33	0.26	1.36	0.25	0.18
5	3	1	2	21	0	27	0.23	0.74	0.19	0.14
6	3	0	0	25	0	28	0.25	0.82	0.19	0.17
7	5	2	3	22	0	32	0.22	0.96	0.18	0.16
8	3	2	0	22	0	27	0.27	0.82	0.22	0.15
9	3	0	3	20	0	26	0.24	0.98	0.21	0.15
10	3	3	0	22	0	28	0.24	0.91	0.18	0.16

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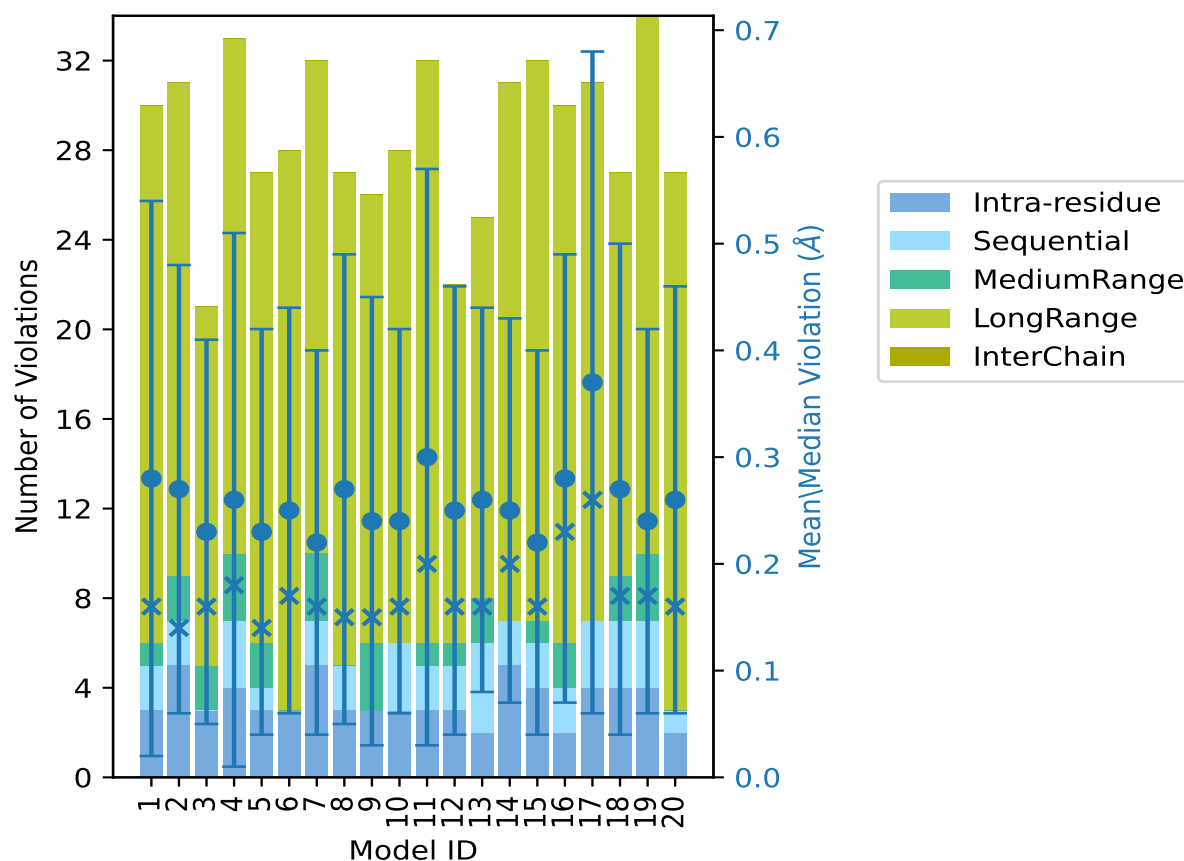
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	3	2	1	26	0	32	0.3	1.25	0.27	0.2
12	3	2	1	16	0	22	0.25	0.96	0.21	0.16
13	2	4	2	17	0	25	0.26	0.87	0.18	0.16
14	5	2	0	24	0	31	0.25	0.8	0.18	0.2
15	4	2	1	25	0	32	0.22	0.77	0.18	0.16
16	2	2	2	24	0	30	0.28	0.86	0.21	0.23
17	4	3	0	24	0	31	0.37	1.35	0.31	0.26
18	4	3	2	18	0	27	0.27	1.14	0.23	0.17
19	4	3	3	24	0	34	0.24	0.87	0.18	0.17
20	2	1	0	24	0	27	0.26	0.82	0.2	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 ⓘ



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

9.3 Distance violation statistics for the ensemble

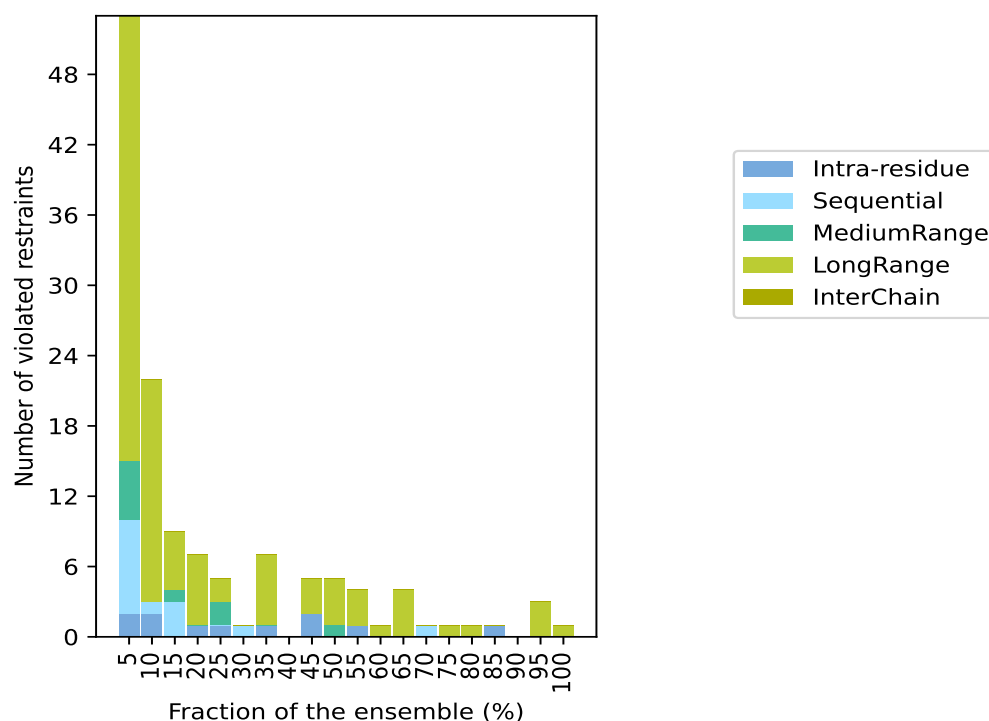
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1629(IR:318, SQ:375, MR:161, LR:775, IC:0) restraints are 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	%
2	8	5	38	0	53	1	5.0
2	1	0	19	0	22	2	10.0
0	3	1	5	0	9	3	15.0
1	0	0	6	0	7	4	20.0
1	0	2	2	0	5	5	25.0
0	1	0	0	0	1	6	30.0
1	0	0	6	0	7	7	35.0
0	0	0	0	0	0	8	40.0
2	0	0	3	0	5	9	45.0
0	0	1	4	0	5	10	50.0
1	0	0	3	0	4	11	55.0
0	0	0	1	0	1	12	60.0
0	0	0	4	0	4	13	65.0
0	1	0	0	0	1	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	1	0	1	16	80.0
1	0	0	0	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	3	0	3	19	95.0
0	0	0	1	0	1	20	100.0

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

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

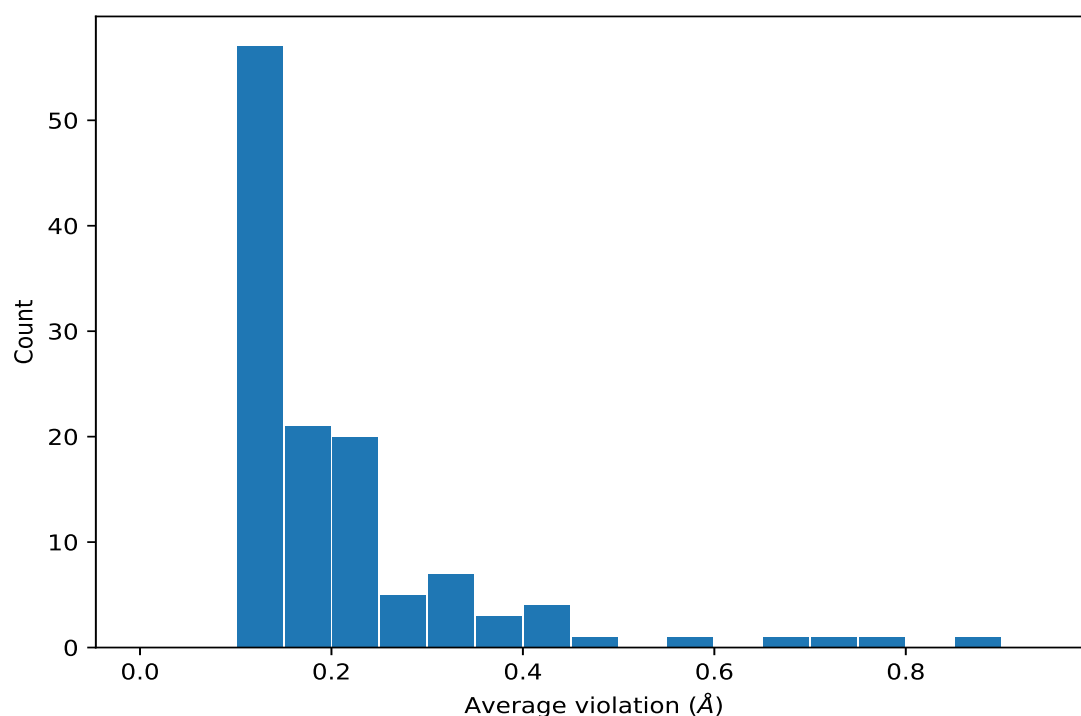
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	19	0.79	0.17	0.85
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	19	0.24	0.07	0.26
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	19	0.21	0.07	0.17
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	17	0.13	0.01	0.14
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	16	0.14	0.03	0.13
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	16	0.14	0.03	0.13
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	15	0.24	0.06	0.26
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	14	0.27	0.05	0.28
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	13	0.87	0.39	0.82
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	13	0.67	0.14	0.7
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	13	0.44	0.16	0.43
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	13	0.44	0.29	0.5
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	12	0.12	0.02	0.12
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	11	0.29	0.11	0.28
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	11	0.21	0.05	0.21
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	11	0.21	0.05	0.21

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	11	0.2	0.03	0.2
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	11	0.2	0.03	0.2
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	11	0.11	0.01	0.11
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	10	0.58	0.23	0.7
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	10	0.36	0.2	0.32
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	10	0.36	0.2	0.32
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	10	0.19	0.05	0.17
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	10	0.15	0.05	0.13
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	10	0.15	0.05	0.13
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	10	0.13	0.02	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	10	0.13	0.02	0.12
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	9	0.32	0.11	0.3
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	9	0.32	0.11	0.3
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	9	0.22	0.08	0.21
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	9	0.22	0.08	0.21
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	9	0.22	0.08	0.21
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	9	0.22	0.08	0.21
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	9	0.19	0.03	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	9	0.19	0.03	0.2
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	9	0.13	0.05	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	9	0.13	0.05	0.11
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	9	0.11	0.01	0.11
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	9	0.11	0.01	0.11
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	7	0.37	0.17	0.25
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	7	0.3	0.11	0.33
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	7	0.3	0.11	0.33
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	7	0.2	0.08	0.23
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	7	0.2	0.08	0.23
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	7	0.18	0.05	0.19
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	7	0.18	0.05	0.19
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	7	0.13	0.02	0.14
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	7	0.13	0.02	0.14
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	7	0.13	0.02	0.12
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	5	0.23	0.07	0.24
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	5	0.23	0.04	0.25
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	5	0.23	0.04	0.25
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	5	0.18	0.02	0.17
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	5	0.18	0.02	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	5	0.18	0.02	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	5	0.18	0.02	0.17
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	5	0.13	0.02	0.12
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	5	0.13	0.02	0.12

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	5	0.11	0.02	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	5	0.11	0.02	0.1
(1,301)	1:608:A:LEU:HD21	1:720:A:THR:HG21	4	0.74	0.08	0.73
(1,302)	1:608:A:LEU:HD21	1:722:A:TYR:H	4	0.47	0.04	0.48
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD1	4	0.43	0.19	0.5
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD2	4	0.43	0.19	0.5
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD1	4	0.31	0.11	0.36
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD2	4	0.31	0.11	0.36
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD1	4	0.17	0.08	0.12
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD2	4	0.17	0.08	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG2	4	0.12	0.01	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG3	4	0.12	0.01	0.12
(1,293)	1:608:A:LEU:HD13	1:720:A:THR:HG21	3	0.34	0.09	0.38
(1,469)	1:615:A:LYS:HE2	1:616:A:VAL:H	3	0.27	0.06	0.25
(1,469)	1:615:A:LYS:HE3	1:616:A:VAL:H	3	0.27	0.06	0.25
(1,766)	1:631:A:VAL:HG13	1:641:A:GLY:H	3	0.17	0.03	0.15
(1,233)	1:605:A:LEU:HG	1:606:A:THR:H	3	0.15	0.02	0.15
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB2	3	0.14	0.03	0.15
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB3	3	0.14	0.03	0.15
(1,287)	1:608:A:LEU:HB3	1:718:A:TRP:HZ2	3	0.13	0.02	0.13
(1,164)	1:596:A:ASP:HB2	1:600:A:GLY:H	3	0.13	0.01	0.12
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB2	3	0.12	0.03	0.1
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB3	3	0.12	0.03	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB2	3	0.12	0.03	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB3	3	0.12	0.03	0.1
(1,1381)	1:684:A:ARG:HG2	1:685:A:THR:H	3	0.11	0.02	0.1
(1,1381)	1:684:A:ARG:HG3	1:685:A:THR:H	3	0.11	0.02	0.1
(1,300)	1:608:A:LEU:HD21	1:718:A:TRP:HZ2	2	0.25	0.07	0.25
(1,1347)	1:679:A:TYR:HD1	1:685:A:THR:HG21	2	0.24	0.01	0.24
(1,1347)	1:679:A:TYR:HD2	1:685:A:THR:HG21	2	0.24	0.01	0.24
(1,290)	1:608:A:LEU:HD13	1:701:A:VAL:HA	2	0.22	0.1	0.22
(1,299)	1:608:A:LEU:HD21	1:718:A:TRP:HE1	2	0.22	0.06	0.22
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE1	2	0.18	0.04	0.18
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE2	2	0.18	0.04	0.18
(1,903)	1:645:A:VAL:HG13	1:652:A:SER:H	2	0.16	0.04	0.16
(1,903)	1:645:A:VAL:HG21	1:652:A:SER:H	2	0.16	0.04	0.16
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB2	2	0.16	0.05	0.16
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB3	2	0.16	0.05	0.16
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD13	2	0.14	0.02	0.14
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD21	2	0.14	0.02	0.14
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE1	2	0.14	0.03	0.14
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE2	2	0.14	0.03	0.14

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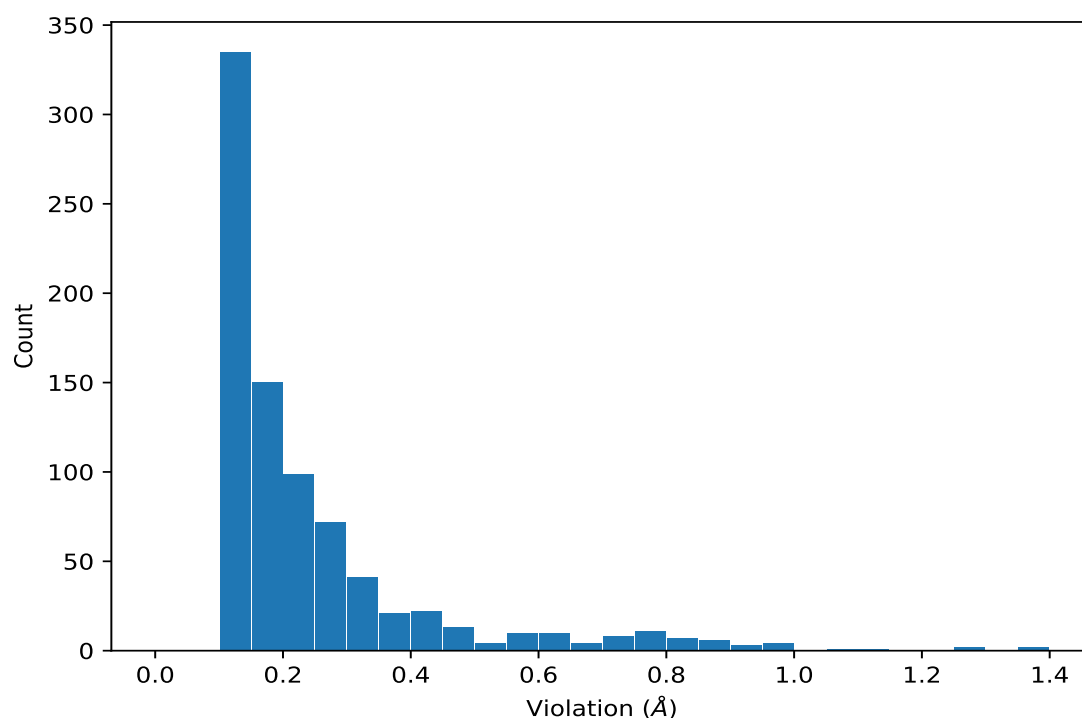
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE1	2	0.14	0.03	0.14
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE2	2	0.14	0.03	0.14
(1,718)	1:627:A:VAL:HG21	1:673:A:TYR:HH	2	0.14	0.0	0.14
(1,1184)	1:669:A:ILE:HD11	1:724:A:CYS:H	2	0.13	0.01	0.13
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD2	2	0.12	0.02	0.12
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD3	2	0.12	0.02	0.12
(1,1585)	1:701:A:VAL:HB	1:702:A:GLY:H	2	0.12	0.01	0.12
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD1	2	0.12	0.01	0.12
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD2	2	0.12	0.01	0.12
(1,298)	1:608:A:LEU:HD21	1:701:A:VAL:HA	2	0.12	0.01	0.12
(1,419)	1:614:A:TYR:H	1:632:A:SER:H	2	0.12	0.01	0.12
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD1	2	0.12	0.01	0.12
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD2	2	0.12	0.01	0.12
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE2	2	0.12	0.0	0.12
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE3	2	0.12	0.0	0.12
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE1	2	0.11	0.01	0.11
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE2	2	0.11	0.01	0.11
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE1	2	0.11	0.0	0.11
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE2	2	0.11	0.0	0.11
(1,1509)	1:693:A:PHE:HD1	1:723:A:ALA:H	2	0.11	0.0	0.11
(1,1509)	1:693:A:PHE:HD2	1:723:A:ALA:H	2	0.11	0.0	0.11
(1,724)	1:627:A:VAL:HG13	1:673:A:TYR:HH	2	0.11	0.0	0.11
(1,724)	1:627:A:VAL:HG21	1:673:A:TYR:HH	2	0.11	0.0	0.11

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	4	1.36
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	17	1.35
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	1	1.26
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	11	1.25
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	18	1.14
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	11	1.05
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	9	0.98
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	17	0.97
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	12	0.96
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	7	0.96
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	3	0.92
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	2	0.91
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	10	0.91
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	19	0.87
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	13	0.87
(1,301)	1:608:A:LEU:HD21	1:720:A:THR:HG21	16	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	17	0.85
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	1	0.85
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	4	0.85
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	16	0.84
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	16	0.83
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	17	0.83
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	20	0.82
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	8	0.82
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	6	0.82
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	14	0.8
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	8	0.78
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	18	0.78
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	19	0.78
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	15	0.77
(1,301)	1:608:A:LEU:HD21	1:720:A:THR:HG21	17	0.77
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	7	0.76
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	20	0.76
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	15	0.76
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	2	0.76
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	14	0.75
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	9	0.75
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	5	0.74
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	5	0.74
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	5	0.74
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	2	0.73
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	2	0.73
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	17	0.71
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	15	0.7
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	11	0.7
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	8	0.69
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	6	0.68
(1,301)	1:608:A:LEU:HD21	1:720:A:THR:HG21	14	0.68
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	6	0.66
(1,301)	1:608:A:LEU:HD21	1:720:A:THR:HG21	1	0.64
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	2	0.64
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	11	0.62
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	8	0.62
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD1	16	0.61
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD2	16	0.61
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	5	0.61
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	10	0.6
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	18	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	9	0.6
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	19	0.59
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	8	0.59
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	17	0.59
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	4	0.59
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	12	0.58
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	12	0.58
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	20	0.57
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD1	17	0.57
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD2	17	0.57
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	1	0.56
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	11	0.53
(1,302)	1:608:A:LEU:HD21	1:722:A:TYR:H	3	0.52
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	8	0.5
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	6	0.5
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	20	0.49
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	20	0.49
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	5	0.49
(1,884)	1:644:A:GLN:HE21	1:653:A:TRP:HA	13	0.49
(1,302)	1:608:A:LEU:HD21	1:722:A:TYR:H	10	0.49
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	13	0.49
(1,302)	1:608:A:LEU:HD21	1:722:A:TYR:H	1	0.48
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	18	0.45
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	18	0.45
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	2	0.45
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	19	0.45
(1,1008)	1:655:A:LEU:HD13	1:714:A:TYR:HE1	6	0.45
(1,1008)	1:655:A:LEU:HD13	1:714:A:TYR:HE2	6	0.45
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	2	0.44
(1,485)	1:616:A:VAL:HG13	1:703:A:PHE:HZ	13	0.44
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	10	0.43
(1,489)	1:616:A:VAL:HG21	1:706:A:TYR:H	17	0.43
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	1	0.43
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	1	0.43
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD1	14	0.43
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD2	14	0.43
(1,293)	1:608:A:LEU:HD13	1:720:A:THR:HG21	20	0.43
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	17	0.42
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	11	0.41
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	11	0.41
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	18	0.41
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	18	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	7	0.4
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	7	0.4
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	7	0.4
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	7	0.4
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	10	0.4
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	10	0.4
(1,302)	1:608:A:LEU:HD21	1:722:A:TYR:H	11	0.4
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	13	0.4
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD1	13	0.39
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD2	13	0.39
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	13	0.38
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	13	0.38
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	20	0.38
(1,969)	1:653:A:TRP:HA	1:677:A:THR:HG21	4	0.38
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	19	0.38
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	19	0.38
(1,293)	1:608:A:LEU:HD13	1:720:A:THR:HG21	13	0.38
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD1	4	0.37
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD2	4	0.37
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	16	0.36
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	18	0.36
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	9	0.36
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	9	0.36
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD1	19	0.36
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD2	19	0.36
(1,469)	1:615:A:LYS:HE2	1:616:A:VAL:H	11	0.35
(1,469)	1:615:A:LYS:HE3	1:616:A:VAL:H	11	0.35
(1,240)	1:605:A:LEU:HD21	1:693:A:PHE:HD1	1	0.35
(1,240)	1:605:A:LEU:HD21	1:693:A:PHE:HD2	1	0.35
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	2	0.34
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	12	0.34
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	20	0.34
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	10	0.34
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	10	0.34
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	14	0.33
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	14	0.33
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	20	0.33
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	7	0.33
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	15	0.33
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	20	0.33
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	4	0.33
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	19	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	3	0.33
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	3	0.33
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	1	0.33
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	1	0.33
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	17	0.32
(1,300)	1:608:A:LEU:HD21	1:718:A:TRP:HZ2	16	0.32
(1,290)	1:608:A:LEU:HD13	1:701:A:VAL:HA	2	0.32
(1,1436)	1:690:A:LEU:HD13	1:692:A:THR:H	5	0.31
(1,1436)	1:690:A:LEU:HD21	1:692:A:THR:H	5	0.31
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	3	0.31
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	3	0.31
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD1	16	0.31
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD2	16	0.31
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	4	0.31
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	11	0.31
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	11	0.31
(1,263)	1:606:A:THR:H	1:662:A:LEU:HD13	11	0.31
(1,263)	1:606:A:THR:H	1:662:A:LEU:HD21	11	0.31
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	13	0.3
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	6	0.3
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	15	0.3
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	10	0.3
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	10	0.3
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	14	0.3
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	12	0.3
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	7	0.3
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	17	0.3
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	17	0.3
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	1	0.29
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	2	0.29
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	15	0.29
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	15	0.29
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	8	0.29
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	18	0.29
(1,299)	1:608:A:LEU:HD21	1:718:A:TRP:HE1	16	0.29
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	20	0.29
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	8	0.28
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	8	0.28
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	10	0.28
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	12	0.28
(1,980)	1:653:A:TRP:HD1	1:677:A:THR:HG21	11	0.28
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	4	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	5	0.28
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	7	0.28
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	10	0.28
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	11	0.28
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	6	0.28
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	9	0.27
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	17	0.27
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	17	0.27
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	17	0.27
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	17	0.27
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	17	0.27
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	16	0.27
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	16	0.27
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	16	0.27
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	2	0.27
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	12	0.27
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	10	0.27
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	16	0.27
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	16	0.27
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	4	0.26
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	9	0.26
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	19	0.26
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	16	0.26
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	16	0.26
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	19	0.26
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	14	0.26
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	17	0.26
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	7	0.26
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	7	0.26
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	7	0.26
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	17	0.26
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	17	0.26
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	17	0.26
(1,1347)	1:679:A:TYR:HD1	1:685:A:THR:HG21	19	0.25
(1,1347)	1:679:A:TYR:HD2	1:685:A:THR:HG21	19	0.25
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	2	0.25
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	2	0.25
(1,1051)	1:659:A:ASN:H	1:671:A:LEU:HD13	1	0.25
(1,1051)	1:659:A:ASN:H	1:671:A:LEU:HD21	1	0.25
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	3	0.25
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	3	0.25
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	3	0.25
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	19	0.25
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	19	0.25
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	18	0.25
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	16	0.25
(1,469)	1:615:A:LYS:HE2	1:616:A:VAL:H	14	0.25
(1,469)	1:615:A:LYS:HE3	1:616:A:VAL:H	14	0.25
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	14	0.25
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	14	0.25
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	18	0.25
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	18	0.25
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	5	0.25
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	5	0.25
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	2	0.25
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	6	0.25
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	11	0.25
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	16	0.24
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	11	0.24
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	16	0.24
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	16	0.24
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	1	0.24
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	1	0.24
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	1	0.24
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	1	0.24
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	1	0.24
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	5	0.24
(1,496)	1:616:A:VAL:HG13	1:704:A:PRO:HA	17	0.24
(1,496)	1:616:A:VAL:HG21	1:704:A:PRO:HA	17	0.24
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	4	0.24
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	4	0.24
(1,1347)	1:679:A:TYR:HD1	1:685:A:THR:HG21	11	0.23
(1,1347)	1:679:A:TYR:HD2	1:685:A:THR:HG21	11	0.23
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	17	0.23
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	17	0.23
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	4	0.23
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	9	0.23
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	9	0.23
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	12	0.23
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	12	0.23
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	20	0.23
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	20	0.23
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	3	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	3	0.23
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	8	0.23
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	8	0.23
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	14	0.23
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	14	0.23
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	16	0.22
(1,1250)	1:671:A:LEU:HD21	1:693:A:PHE:HZ	6	0.22
(1,1216)	1:670:A:GLN:HE21	1:692:A:THR:HB	12	0.22
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	2	0.22
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	2	0.22
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	14	0.22
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	14	0.22
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE1	11	0.22
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE2	11	0.22
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	16	0.22
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	16	0.22
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	7	0.22
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	7	0.22
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	7	0.22
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	7	0.22
(1,293)	1:608:A:LEU:HD13	1:720:A:THR:HG21	7	0.22
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	5	0.22
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	15	0.21
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	15	0.21
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	18	0.21
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	18	0.21
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	7	0.21
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	7	0.21
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	4	0.21
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	4	0.21
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	15	0.21
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	15	0.21
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	18	0.21
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	18	0.21
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	18	0.21
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	18	0.21
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	1	0.21
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	1	0.21
(1,766)	1:631:A:VAL:HG13	1:641:A:GLY:H	13	0.21
(1,750)	1:630:A:PRO:HB2	1:639:A:ASP:H	2	0.21
(1,750)	1:630:A:PRO:HB3	1:639:A:ASP:H	2	0.21
(1,469)	1:615:A:LYS:HE2	1:616:A:VAL:H	18	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,469)	1:615:A:LYS:HE3	1:616:A:VAL:H	18	0.21
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	6	0.21
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	14	0.21
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	14	0.21
(1,35)	1:587:A:THR:HG21	1:594:A:VAL:HG21	13	0.21
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	3	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	3	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	14	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	14	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	16	0.2
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	16	0.2
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	6	0.2
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	6	0.2
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	7	0.2
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	7	0.2
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	19	0.2
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	19	0.2
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	19	0.2
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	19	0.2
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	19	0.2
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	19	0.2
(1,903)	1:645:A:VAL:HG13	1:652:A:SER:H	18	0.2
(1,903)	1:645:A:VAL:HG21	1:652:A:SER:H	18	0.2
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB2	14	0.2
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB3	14	0.2
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	14	0.2
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	3	0.2
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	3	0.2
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	3	0.2
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	3	0.2
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	5	0.2
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	7	0.19
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	20	0.19
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	15	0.19
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	15	0.19
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	11	0.19
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	11	0.19
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	17	0.19
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	17	0.19
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	11	0.19
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	11	0.19
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	15	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	15	0.19
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	4	0.19
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	4	0.19
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	9	0.19
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	9	0.19
(1,1076)	1:660:A:ALA:H	1:671:A:LEU:HD13	6	0.19
(1,1076)	1:660:A:ALA:H	1:671:A:LEU:HD21	6	0.19
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	7	0.19
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	7	0.19
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	17	0.19
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	17	0.19
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	3	0.19
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	4	0.19
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	17	0.19
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	17	0.19
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	7	0.18
(1,1588)	1:701:A:VAL:HG13	1:718:A:TRP:HZ2	10	0.18
(1,1588)	1:701:A:VAL:HG21	1:718:A:TRP:HZ2	10	0.18
(1,1326)	1:676:A:GLY:HA2	1:687:A:ARG:HB2	9	0.18
(1,1326)	1:676:A:GLY:HA2	1:687:A:ARG:HB3	9	0.18
(1,1326)	1:676:A:GLY:HA3	1:687:A:ARG:HB2	9	0.18
(1,1326)	1:676:A:GLY:HA3	1:687:A:ARG:HB3	9	0.18
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	19	0.18
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	19	0.18
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	4	0.18
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	4	0.18
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	4	0.18
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	4	0.18
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	8	0.18
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	8	0.18
(1,1005)	1:655:A:LEU:HG	1:687:A:ARG:HE	9	0.18
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	16	0.18
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	8	0.18
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	8	0.18
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	19	0.18
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	19	0.18
(1,300)	1:608:A:LEU:HD21	1:718:A:TRP:HZ2	14	0.18
(1,233)	1:605:A:LEU:HG	1:606:A:THR:H	19	0.18
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	4	0.18
(1,203)	1:603:A:PHE:HA	1:669:A:ILE:HD11	9	0.18
(1,172)	1:596:A:ASP:HB3	1:664:A:TYR:HE1	15	0.18
(1,172)	1:596:A:ASP:HB3	1:664:A:TYR:HE2	15	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	16	0.17
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	16	0.17
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	2	0.17
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	18	0.17
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	1	0.17
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	19	0.17
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	19	0.17
(1,1217)	1:670:A:GLN:HE21	1:692:A:THR:HG21	15	0.17
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	16	0.17
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	16	0.17
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	5	0.17
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	5	0.17
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	6	0.17
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	6	0.17
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	6	0.17
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	6	0.17
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB2	4	0.17
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB3	4	0.17
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	20	0.17
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	9	0.17
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	4	0.17
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	4	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	4	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	4	0.17
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	19	0.17
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	19	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	19	0.17
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	19	0.17
(1,280)	1:608:A:LEU:H	1:627:A:VAL:HG13	3	0.17
(1,280)	1:608:A:LEU:H	1:627:A:VAL:HG21	3	0.17
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE1	14	0.17
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE2	14	0.17
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE1	14	0.17
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE2	14	0.17
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	12	0.16
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	15	0.16
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	19	0.16
(1,1560)	1:695:A:CYS:HB2	1:724:A:CYS:HA	3	0.16
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	7	0.16
(1,1353)	1:680:A:ASN:H	1:680:A:ASN:HD21	20	0.16
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB2	14	0.16
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB3	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB2	14	0.16
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB3	14	0.16
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	14	0.16
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	14	0.16
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	13	0.16
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	3	0.16
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	3	0.16
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	10	0.16
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	12	0.16
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	10	0.16
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE1	13	0.16
(1,378)	1:610:A:LYS:HE2	1:614:A:TYR:HE2	13	0.16
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE1	13	0.16
(1,378)	1:610:A:LYS:HE3	1:614:A:TYR:HE2	13	0.16
(1,299)	1:608:A:LEU:HD21	1:718:A:TRP:HE1	14	0.16
(1,287)	1:608:A:LEU:HB3	1:718:A:TRP:HZ2	1	0.16
(1,247)	1:605:A:LEU:HD13	1:693:A:PHE:HB3	11	0.16
(1,247)	1:605:A:LEU:HD21	1:693:A:PHE:HB3	11	0.16
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	14	0.16
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD13	15	0.16
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD21	15	0.16
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	7	0.15
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	7	0.15
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	5	0.15
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	11	0.15
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	14	0.15
(1,1387)	1:685:A:THR:HG21	1:686:A:PRO:HD2	10	0.15
(1,1387)	1:685:A:THR:HG21	1:686:A:PRO:HD3	10	0.15
(1,1298)	1:673:A:TYR:HE1	1:689:A:THR:HG21	4	0.15
(1,1298)	1:673:A:TYR:HE2	1:689:A:THR:HG21	4	0.15
(1,1129)	1:664:A:TYR:HE1	1:669:A:ILE:HB	11	0.15
(1,1129)	1:664:A:TYR:HE2	1:669:A:ILE:HB	11	0.15
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	15	0.15
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	15	0.15
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	15	0.15
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	15	0.15
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB2	12	0.15
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB3	12	0.15
(1,968)	1:653:A:TRP:HA	1:654:A:ASN:HD21	18	0.15
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	13	0.15
(1,766)	1:631:A:VAL:HG13	1:641:A:GLY:H	4	0.15
(1,766)	1:631:A:VAL:HG13	1:641:A:GLY:H	8	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:625:A:ILE:HD11	1:691:A:ILE:HD11	6	0.15
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	3	0.15
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	3	0.15
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	6	0.15
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	11	0.15
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	11	0.15
(1,233)	1:605:A:LEU:HG	1:606:A:THR:H	13	0.15
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	18	0.15
(1,184)	1:598:A:GLN:HE21	1:599:A:ALA:HB1	18	0.15
(1,184)	1:598:A:GLN:HE21	1:599:A:ALA:HB2	18	0.15
(1,184)	1:598:A:GLN:HE21	1:599:A:ALA:HB3	18	0.15
(1,164)	1:596:A:ASP:HB2	1:600:A:GLY:H	4	0.15
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	9	0.15
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	19	0.14
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	19	0.14
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	6	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	5	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	5	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	9	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	9	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	19	0.14
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	19	0.14
(1,1381)	1:684:A:ARG:HG2	1:685:A:THR:H	1	0.14
(1,1381)	1:684:A:ARG:HG3	1:685:A:THR:H	1	0.14
(1,1184)	1:669:A:ILE:HD11	1:724:A:CYS:H	8	0.14
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	9	0.14
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	9	0.14
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	20	0.14
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	20	0.14
(1,1094)	1:662:A:LEU:HA	1:672:A:THR:H	15	0.14
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE1	6	0.14
(1,1004)	1:655:A:LEU:HG	1:679:A:TYR:HE2	6	0.14
(1,937)	1:650:A:ARG:HG2	1:651:A:LYS:H	17	0.14
(1,937)	1:650:A:ARG:HG3	1:651:A:LYS:H	17	0.14
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD2	2	0.14
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD3	2	0.14
(1,718)	1:627:A:VAL:HG21	1:673:A:TYR:HH	2	0.14
(1,718)	1:627:A:VAL:HG21	1:673:A:TYR:HH	17	0.14
(1,715)	1:627:A:VAL:HG13	1:693:A:PHE:HZ	7	0.14
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	19	0.14
(1,664)	1:625:A:ILE:HD11	1:643:A:CYS:H	1	0.14
(1,603)	1:622:A:GLU:HG2	1:624:A:HIS:HD2	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,603)	1:622:A:GLU:HG3	1:624:A:HIS:HD2	4	0.14
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	7	0.14
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	7	0.14
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	9	0.14
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	9	0.14
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD2	7	0.14
(1,449)	1:615:A:LYS:H	1:615:A:LYS:HD3	7	0.14
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	6	0.14
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	6	0.14
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD1	9	0.14
(1,304)	1:608:A:LEU:HD21	1:722:A:TYR:HD2	9	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	4	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	5	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	7	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	8	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	9	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	11	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	12	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	19	0.14
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	20	0.14
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	1	0.14
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	2	0.14
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	3	0.14
(1,133)	1:594:A:VAL:HG21	1:603:A:PHE:HB2	12	0.14
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	15	0.14
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	15	0.14
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	6	0.13
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	6	0.13
(1,1665)	1:707:A:GLN:HE21	1:715:A:ASN:HB2	9	0.13
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	16	0.13
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	16	0.13
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	4	0.13
(1,1585)	1:701:A:VAL:HB	1:702:A:GLY:H	19	0.13
(1,1511)	1:693:A:PHE:HE1	1:718:A:TRP:HH2	11	0.13
(1,1511)	1:693:A:PHE:HE2	1:718:A:TRP:HH2	11	0.13
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG2	10	0.13
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG3	10	0.13
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD1	7	0.13
(1,1346)	1:679:A:TYR:HA	1:679:A:TYR:HD2	7	0.13
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	6	0.13
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	6	0.13
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	13	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	13	0.13
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	8	0.13
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	8	0.13
(1,1069)	1:659:A:ASN:HB2	1:660:A:ALA:H	4	0.13
(1,1069)	1:659:A:ASN:HB3	1:660:A:ALA:H	4	0.13
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD1	3	0.13
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD2	3	0.13
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	1	0.13
(1,903)	1:645:A:VAL:HG13	1:652:A:SER:H	7	0.13
(1,903)	1:645:A:VAL:HG21	1:652:A:SER:H	7	0.13
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	5	0.13
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD1	10	0.13
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD2	10	0.13
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	2	0.13
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	4	0.13
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	5	0.13
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	20	0.13
(1,505)	1:617:A:GLU:H	1:617:A:GLU:HG2	2	0.13
(1,505)	1:617:A:GLU:H	1:617:A:GLU:HG3	2	0.13
(1,419)	1:614:A:TYR:H	1:632:A:SER:H	15	0.13
(1,298)	1:608:A:LEU:HD21	1:701:A:VAL:HA	4	0.13
(1,290)	1:608:A:LEU:HD13	1:701:A:VAL:HA	18	0.13
(1,287)	1:608:A:LEU:HB3	1:718:A:TRP:HZ2	10	0.13
(1,279)	1:608:A:LEU:H	1:627:A:VAL:HB	7	0.13
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	16	0.13
(1,233)	1:605:A:LEU:HG	1:606:A:THR:H	4	0.13
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	20	0.13
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	11	0.13
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	11	0.13
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	20	0.13
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	20	0.13
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD1	14	0.13
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD2	14	0.13
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	8	0.12
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	8	0.12
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	18	0.12
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	18	0.12
(1,1639)	1:706:A:TYR:HA	1:716:A:PHE:HZ	13	0.12
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	2	0.12
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	2	0.12
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	20	0.12
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	13	0.12
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	13	0.12
(1,1592)	1:702:A:GLY:H	1:720:A:THR:HG21	10	0.12
(1,1585)	1:701:A:VAL:HB	1:702:A:GLY:H	2	0.12
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	5	0.12
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	18	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	1	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	1	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	2	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	2	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	7	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	7	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	18	0.12
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	18	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG2	2	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG3	2	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG2	13	0.12
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG3	13	0.12
(1,1380)	1:684:A:ARG:HD2	1:685:A:THR:H	13	0.12
(1,1380)	1:684:A:ARG:HD3	1:685:A:THR:H	13	0.12
(1,1184)	1:669:A:ILE:HD11	1:724:A:CYS:H	9	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	5	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	5	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	12	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	12	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	14	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	14	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	17	0.12
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	17	0.12
(1,1058)	1:659:A:ASN:HB3	1:660:A:ALA:H	4	0.12
(1,973)	1:653:A:TRP:HB2	1:677:A:THR:HG21	10	0.12
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE2	8	0.12
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE3	8	0.12
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	13	0.12
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	13	0.12
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	2	0.12
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	7	0.12
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD1	4	0.12
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD2	4	0.12
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD1	12	0.12
(1,834)	1:641:A:GLY:HA2	1:673:A:TYR:HD2	12	0.12
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	8	0.12
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE1	20	0.12
(1,535)	1:618:A:THR:HG21	1:706:A:TYR:HE2	20	0.12
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	16	0.12
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	16	0.12
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE1	10	0.12
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE2	10	0.12
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD1	5	0.12
(1,297)	1:608:A:LEU:HD21	1:693:A:PHE:HD2	5	0.12
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	1	0.12
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	14	0.12
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	15	0.12
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	15	0.12
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	15	0.12
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	3	0.12
(1,205)	1:603:A:PHE:HB2	1:605:A:LEU:HD13	2	0.12
(1,205)	1:603:A:PHE:HB2	1:605:A:LEU:HD21	2	0.12
(1,164)	1:596:A:ASP:HB2	1:600:A:GLY:H	9	0.12
(1,164)	1:596:A:ASP:HB2	1:600:A:GLY:H	18	0.12
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD13	6	0.12
(1,135)	1:594:A:VAL:HG21	1:662:A:LEU:HD21	6	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	6	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	6	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	8	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	8	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	19	0.12
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	19	0.12
(1,124)	1:594:A:VAL:HG13	1:662:A:LEU:HG	20	0.12
(1,1666)	1:707:A:GLN:HG2	1:715:A:ASN:HA	15	0.11
(1,1666)	1:707:A:GLN:HG3	1:715:A:ASN:HA	15	0.11
(1,1653)	1:706:A:TYR:HE1	1:708:A:GLU:HA	11	0.11
(1,1653)	1:706:A:TYR:HE2	1:708:A:GLU:HA	11	0.11
(1,1631)	1:705:A:GLU:HG2	1:717:A:ARG:H	7	0.11
(1,1631)	1:705:A:GLU:HG3	1:717:A:ARG:H	7	0.11
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	14	0.11
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	14	0.11
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	17	0.11
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	17	0.11
(1,1548)	1:694:A:LEU:HD13	1:717:A:ARG:HD2	19	0.11
(1,1548)	1:694:A:LEU:HD13	1:717:A:ARG:HD3	19	0.11
(1,1548)	1:694:A:LEU:HD21	1:717:A:ARG:HD2	19	0.11
(1,1548)	1:694:A:LEU:HD21	1:717:A:ARG:HD3	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1509)	1:693:A:PHE:HD1	1:723:A:ALA:H	2	0.11
(1,1509)	1:693:A:PHE:HD2	1:723:A:ALA:H	2	0.11
(1,1509)	1:693:A:PHE:HD1	1:723:A:ALA:H	10	0.11
(1,1509)	1:693:A:PHE:HD2	1:723:A:ALA:H	10	0.11
(1,1460)	1:691:A:ILE:HD11	1:718:A:TRP:HE3	13	0.11
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	3	0.11
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	3	0.11
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE1	16	0.11
(1,1454)	1:691:A:ILE:HG12	1:693:A:PHE:HE2	16	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	1	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	2	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	3	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	15	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	17	0.11
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	19	0.11
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG2	5	0.11
(1,1390)	1:687:A:ARG:H	1:687:A:ARG:HG3	5	0.11
(1,1345)	1:679:A:TYR:H	1:687:A:ARG:HB2	9	0.11
(1,1345)	1:679:A:TYR:H	1:687:A:ARG:HB3	9	0.11
(1,1280)	1:673:A:TYR:H	1:690:A:LEU:HA	5	0.11
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	1	0.11
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	1	0.11
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	8	0.11
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	8	0.11
(1,1133)	1:665:A:TYR:H	1:668:A:MET:H	16	0.11
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD1	1	0.11
(1,1062)	1:659:A:ASN:HD21	1:673:A:TYR:HD2	1	0.11
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE1	5	0.11
(1,1012)	1:655:A:LEU:HD13	1:679:A:TYR:HE2	5	0.11
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE1	5	0.11
(1,1012)	1:655:A:LEU:HD21	1:679:A:TYR:HE2	5	0.11
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE2	17	0.11
(1,941)	1:651:A:LYS:H	1:651:A:LYS:HE3	17	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	1	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	1	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	4	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	4	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	5	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	5	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	15	0.11
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	15	0.11
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE1	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE2	1	0.11
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE1	8	0.11
(1,886)	1:644:A:GLN:HE21	1:679:A:TYR:HE2	8	0.11
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	1	0.11
(1,846)	1:642:A:ALA:H	1:673:A:TYR:HE1	19	0.11
(1,846)	1:642:A:ALA:H	1:673:A:TYR:HE2	19	0.11
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB2	4	0.11
(1,833)	1:641:A:GLY:HA2	1:658:A:SER:HB3	4	0.11
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD2	18	0.11
(1,819)	1:640:A:SER:HA	1:657:A:ARG:HD3	18	0.11
(1,724)	1:627:A:VAL:HG13	1:673:A:TYR:HH	11	0.11
(1,724)	1:627:A:VAL:HG21	1:673:A:TYR:HH	11	0.11
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	1	0.11
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	12	0.11
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	12	0.11
(1,419)	1:614:A:TYR:H	1:632:A:SER:H	10	0.11
(1,298)	1:608:A:LEU:HD21	1:701:A:VAL:HA	15	0.11
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD1	15	0.11
(1,289)	1:608:A:LEU:HD13	1:693:A:PHE:HD2	15	0.11
(1,287)	1:608:A:LEU:HB3	1:718:A:TRP:HZ2	3	0.11
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	2	0.11
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	10	0.11
(1,259)	1:606:A:THR:H	1:606:A:THR:HG21	18	0.11
(1,201)	1:603:A:PHE:H	1:669:A:ILE:HD11	16	0.11
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE1	8	0.11
(1,177)	1:596:A:ASP:HB2	1:664:A:TYR:HE2	8	0.11
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE1	8	0.11
(1,177)	1:596:A:ASP:HB3	1:664:A:TYR:HE2	8	0.11
(1,17)	1:586:A:ARG:HG3	1:664:A:TYR:HB3	5	0.11
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD1	8	0.11
(1,10)	1:586:A:ARG:HA	1:664:A:TYR:HD2	8	0.11
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	9	0.1
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	9	0.1
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	11	0.1
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	11	0.1
(1,1629)	1:705:A:GLU:HB2	1:718:A:TRP:H	15	0.1
(1,1629)	1:705:A:GLU:HB3	1:718:A:TRP:H	15	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	9	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	9	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	12	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	12	0.1
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG2	19	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1607)	1:703:A:PHE:HZ	1:705:A:GLU:HG3	19	0.1
(1,1568)	1:696:A:ASP:H	1:720:A:THR:H	20	0.1
(1,1562)	1:695:A:CYS:HB3	1:724:A:CYS:HA	11	0.1
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	6	0.1
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	7	0.1
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	9	0.1
(1,1423)	1:690:A:LEU:H	1:690:A:LEU:HG	12	0.1
(1,1381)	1:684:A:ARG:HG2	1:685:A:THR:H	8	0.1
(1,1381)	1:684:A:ARG:HG3	1:685:A:THR:H	8	0.1
(1,1381)	1:684:A:ARG:HG2	1:685:A:THR:H	13	0.1
(1,1381)	1:684:A:ARG:HG3	1:685:A:THR:H	13	0.1
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB2	3	0.1
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB3	3	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB2	3	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB3	3	0.1
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB2	19	0.1
(1,1349)	1:679:A:TYR:HD1	1:712:A:SER:HB3	19	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB2	19	0.1
(1,1349)	1:679:A:TYR:HD2	1:712:A:SER:HB3	19	0.1
(1,1218)	1:670:A:GLN:HG2	1:671:A:LEU:H	7	0.1
(1,1218)	1:670:A:GLN:HG3	1:671:A:LEU:H	7	0.1
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD1	2	0.1
(1,1180)	1:669:A:ILE:HG12	1:693:A:PHE:HD2	2	0.1
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD2	19	0.1
(1,1080)	1:661:A:LYS:H	1:661:A:LYS:HD3	19	0.1
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD1	15	0.1
(1,1007)	1:655:A:LEU:HD13	1:714:A:TYR:HD2	15	0.1
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB2	20	0.1
(1,982)	1:653:A:TRP:HE1	1:679:A:TYR:HB3	20	0.1
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	11	0.1
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	11	0.1
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD2	18	0.1
(1,932)	1:650:A:ARG:H	1:650:A:ARG:HD3	18	0.1
(1,858)	1:643:A:CYS:HA	1:655:A:LEU:HG	17	0.1
(1,724)	1:627:A:VAL:HG13	1:673:A:TYR:HH	13	0.1
(1,724)	1:627:A:VAL:HG21	1:673:A:TYR:HH	13	0.1
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	6	0.1
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	15	0.1
(1,695)	1:626:A:ASN:HD21	1:632:A:SER:H	18	0.1
(1,556)	1:620:A:LYS:HE2	1:621:A:TYR:H	17	0.1
(1,556)	1:620:A:LYS:HE3	1:621:A:TYR:H	17	0.1
(1,473)	1:615:A:LYS:HG2	1:703:A:PHE:HZ	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,473)	1:615:A:LYS:HG3	1:703:A:PHE:HZ	5	0.1
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE1	14	0.1
(1,415)	1:614:A:TYR:H	1:614:A:TYR:HE2	14	0.1
(1,257)	1:605:A:LEU:HD13	1:724:A:CYS:H	10	0.1
(1,257)	1:605:A:LEU:HD21	1:724:A:CYS:H	10	0.1
(1,215)	1:604:A:ASP:H	1:669:A:ILE:HD11	7	0.1
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD1	5	0.1
(1,131)	1:594:A:VAL:HG21	1:601:A:PHE:HD2	5	0.1
(1,19)	1:586:A:ARG:HB2	1:663:A:SER:HB2	16	0.1
(1,19)	1:586:A:ARG:HB2	1:663:A:SER:HB3	16	0.1
(1,19)	1:586:A:ARG:HB3	1:663:A:SER:HB2	16	0.1
(1,19)	1:586:A:ARG:HB3	1:663:A:SER:HB3	16	0.1

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

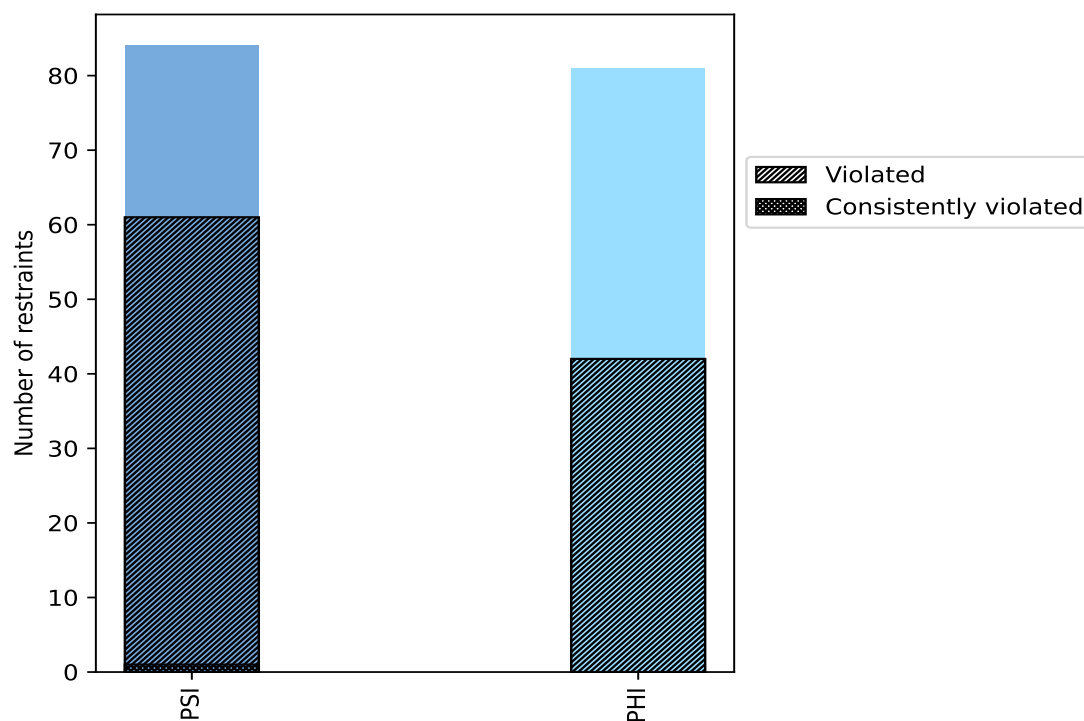
10.1 Summary of dihedral-angle violations [i](#)

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	84	50.9	61	72.6	37.0	1	1.2	0.6
PHI	81	49.1	42	51.9	25.5	0	0.0	0.0
Total	165	100.0	103	62.4	62.4	1	0.6	0.6

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](#)



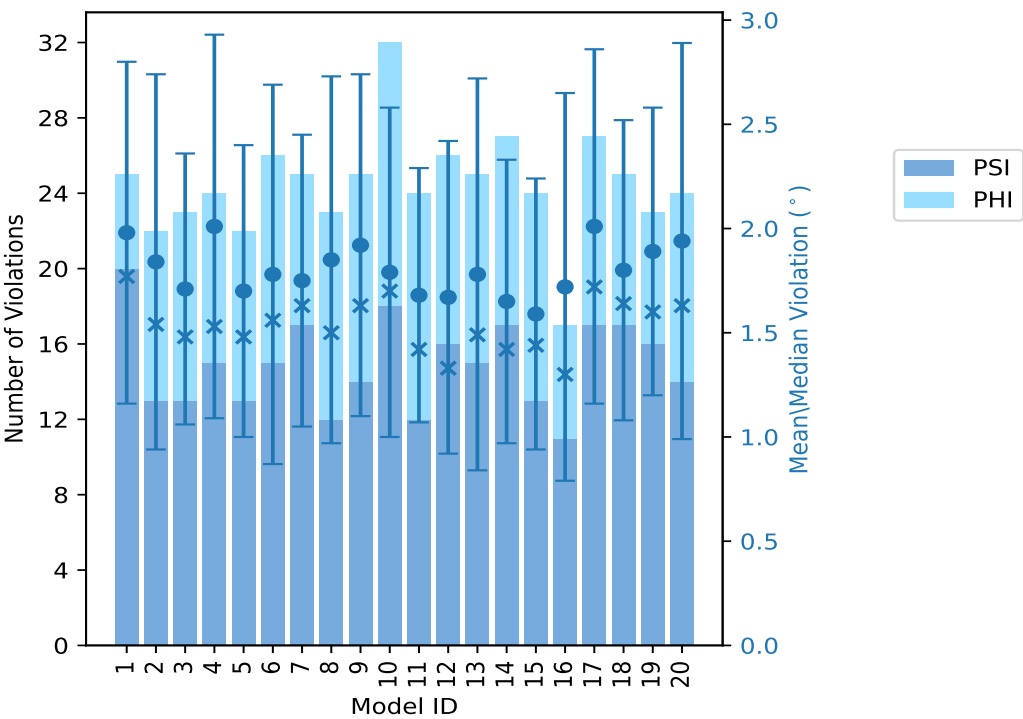
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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	20	5	25	1.98	4.46	0.82	1.77
2	13	9	22	1.84	4.47	0.9	1.54
3	13	10	23	1.71	3.58	0.65	1.48
4	15	9	24	2.01	3.91	0.92	1.53
5	13	9	22	1.7	3.89	0.7	1.48
6	15	11	26	1.78	5.63	0.91	1.56
7	17	8	25	1.75	3.96	0.7	1.63
8	12	11	23	1.85	4.76	0.88	1.5
9	14	11	25	1.92	4.04	0.82	1.63
10	18	14	32	1.79	4.84	0.79	1.7
11	12	12	24	1.68	3.61	0.61	1.42
12	16	10	26	1.67	4.48	0.75	1.33
13	15	10	25	1.78	4.75	0.94	1.49
14	17	10	27	1.65	3.87	0.68	1.42
15	13	11	24	1.59	3.67	0.65	1.44
16	11	6	17	1.72	4.31	0.93	1.3
17	17	10	27	2.01	4.65	0.85	1.72
18	17	8	25	1.8	3.97	0.72	1.64
19	16	7	23	1.89	3.33	0.69	1.6
20	14	10	24	1.94	4.81	0.95	1.63

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	%
17	9	26	1	5.0
10	7	17	2	10.0
9	7	16	3	15.0
2	5	7	4	20.0
3	3	6	5	25.0
2	1	3	6	30.0
3	2	5	7	35.0
3	2	5	8	40.0
3	0	3	9	45.0
1	3	4	10	50.0
1	0	1	11	55.0

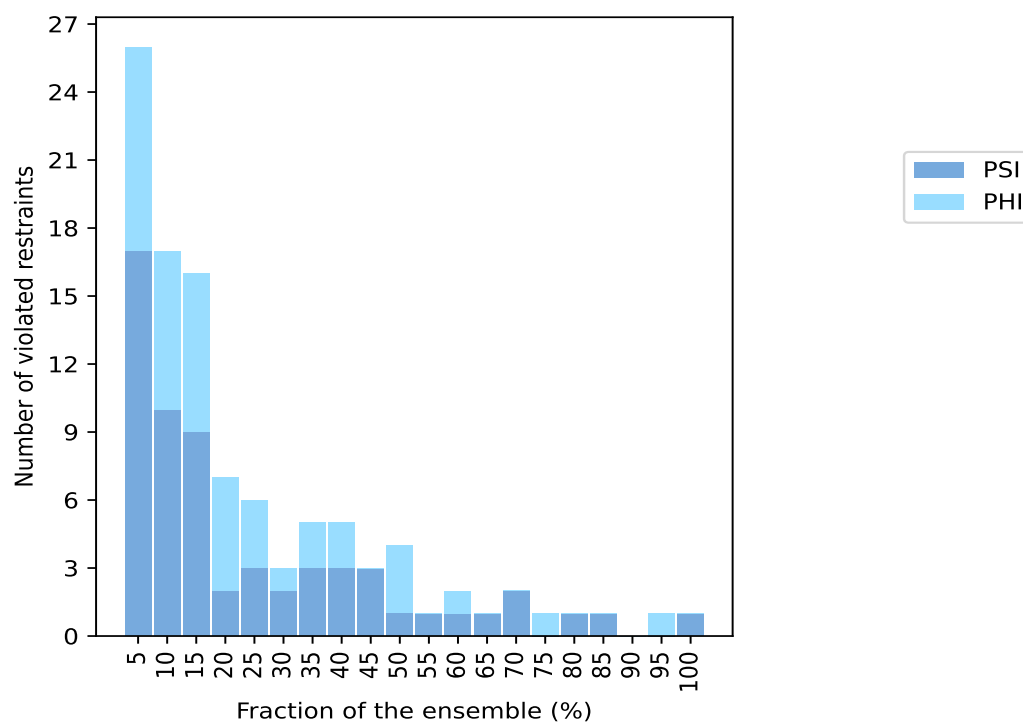
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
1	1	2	12	60.0
1	0	1	13	65.0
2	0	2	14	70.0
0	1	1	15	75.0
1	0	1	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	1	1	19	95.0
1	0	1	20	100.0

¹ Number of models with violations

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

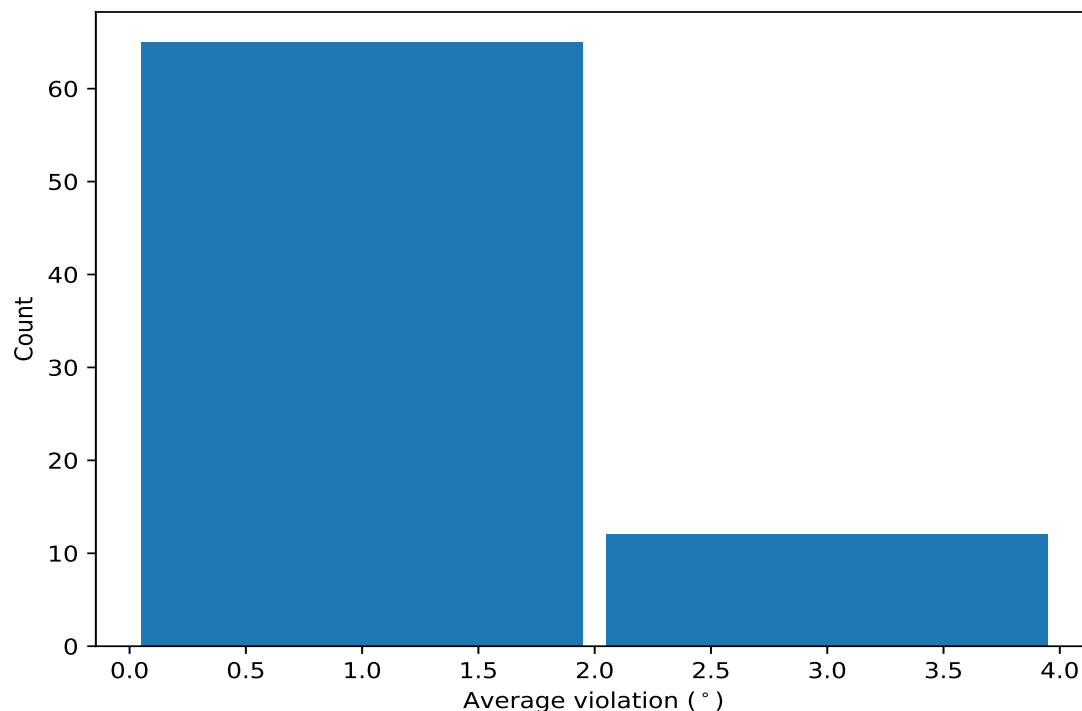


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	20	3.8	0.76	3.77
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	19	2.15	0.59	2.11
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	17	1.76	0.62	1.45
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	16	1.72	0.4	1.74
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	15	1.75	0.43	1.69
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	14	3.33	1.1	3.4
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	14	1.53	0.36	1.44
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	13	1.59	0.38	1.47
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	12	1.86	0.69	1.77
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	12	1.5	0.38	1.47
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	11	2.69	1.21	2.57
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	10	2.45	0.95	2.24
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	10	1.54	0.52	1.4
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	10	1.39	0.34	1.25
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	10	1.36	0.22	1.35
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	9	1.84	0.66	1.52
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	9	1.61	0.35	1.62
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	9	1.6	0.31	1.58
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	8	2.09	0.71	2.13
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	8	1.96	0.76	1.96

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	8	1.87	0.47	1.84
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	8	1.46	0.33	1.46
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	8	1.38	0.25	1.29
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	7	2.15	0.56	2.16
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	7	2.11	1.29	1.4
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	7	1.55	0.36	1.41
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	7	1.4	0.24	1.36
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	7	1.39	0.32	1.22
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	6	1.81	0.21	1.78
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	6	1.53	0.35	1.53
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	6	1.44	0.47	1.28
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	5	1.85	0.76	1.76
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	5	1.67	0.6	1.56
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	5	1.47	0.28	1.63
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	5	1.42	0.23	1.53
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	5	1.39	0.27	1.35
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	5	1.23	0.15	1.23
(1,24)	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1:603:A:PHE:N	4	2.0	0.14	2.07
(1,103)	1:663:A:SER:C	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	4	1.82	0.57	1.76
(1,19)	1:598:A:GLN:C	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	4	1.81	0.49	1.7
(1,164)	1:723:A:ALA:C	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	4	1.76	0.48	1.65
(1,137)	1:695:A:CYS:C	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	4	1.67	0.65	1.5
(1,106)	1:669:A:ILE:N	1:669:A:ILE:CA	1:669:A:ILE:C	1:670:A:GLN:N	4	1.59	0.4	1.4
(1,32)	1:608:A:LEU:C	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	4	1.19	0.01	1.19
(1,157)	1:719:A:TYR:N	1:719:A:TYR:CA	1:719:A:TYR:C	1:720:A:THR:N	3	1.96	0.21	1.84
(1,165)	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	1:725:A:PRO:N	3	1.76	0.46	1.84
(1,104)	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	1:665:A:TYR:N	3	1.75	0.33	1.72
(1,150)	1:712:A:SER:C	1:713:A:THR:N	1:713:A:THR:CA	1:713:A:THR:C	3	1.72	0.6	1.7
(1,86)	1:648:A:SER:C	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	3	1.68	0.46	1.98
(1,121)	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	1:686:A:PRO:N	3	1.62	0.56	1.37
(1,1)	1:585:A:SER:C	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	3	1.46	0.55	1.09
(1,148)	1:710:A:ASP:C	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	3	1.38	0.03	1.38
(1,101)	1:662:A:LEU:N	1:662:A:LEU:CA	1:662:A:LEU:C	1:663:A:SER:N	3	1.36	0.23	1.38
(1,52)	1:622:A:GLU:C	1:623:A:PHE:N	1:623:A:PHE:CA	1:623:A:PHE:C	3	1.33	0.16	1.34
(1,51)	1:622:A:GLU:N	1:622:A:GLU:CA	1:622:A:GLU:C	1:623:A:PHE:N	3	1.23	0.3	1.03
(1,132)	1:692:A:THR:C	1:693:A:PHE:N	1:693:A:PHE:CA	1:693:A:PHE:C	3	1.19	0.2	1.08
(1,91)	1:652:A:SER:N	1:652:A:SER:CA	1:652:A:SER:C	1:653:A:TRP:N	3	1.18	0.08	1.15
(1,95)	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	1:655:A:LEU:N	3	1.16	0.07	1.11
(1,163)	1:722:A:TYR:N	1:722:A:TYR:CA	1:722:A:TYR:C	1:723:A:ALA:N	3	1.16	0.05	1.13
(1,153)	1:716:A:PHE:C	1:717:A:ARG:N	1:717:A:ARG:CA	1:717:A:ARG:C	3	1.12	0.11	1.05
(1,135)	1:694:A:LEU:N	1:694:A:LEU:CA	1:694:A:LEU:C	1:695:A:CYS:N	2	2.74	0.08	2.74
(1,41)	1:615:A:LYS:N	1:615:A:LYS:CA	1:615:A:LYS:C	1:616:A:VAL:N	2	2.3	0.51	2.3
(1,13)	1:595:A:PHE:C	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	2	2.24	1.0	2.24
(1,26)	1:603:A:PHE:N	1:603:A:PHE:CA	1:603:A:PHE:C	1:604:A:ASP:N	2	1.85	0.26	1.85
(1,112)	1:674:A:ARG:N	1:674:A:ARG:CA	1:674:A:ARG:C	1:675:A:ASP:N	2	1.7	0.68	1.7
(1,43)	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	1:617:A:GLU:N	2	1.66	0.07	1.66
(1,42)	1:615:A:LYS:C	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	2	1.56	0.39	1.56
(1,120)	1:684:A:ARG:C	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	2	1.5	0.06	1.5
(1,12)	1:595:A:PHE:N	1:595:A:PHE:CA	1:595:A:PHE:C	1:596:A:ASP:N	2	1.5	0.12	1.5
(1,21)	1:600:A:GLY:C	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	2	1.44	0.21	1.44
(1,122)	1:686:A:PRO:N	1:686:A:PRO:CA	1:686:A:PRO:C	1:687:A:ARG:N	2	1.37	0.26	1.37

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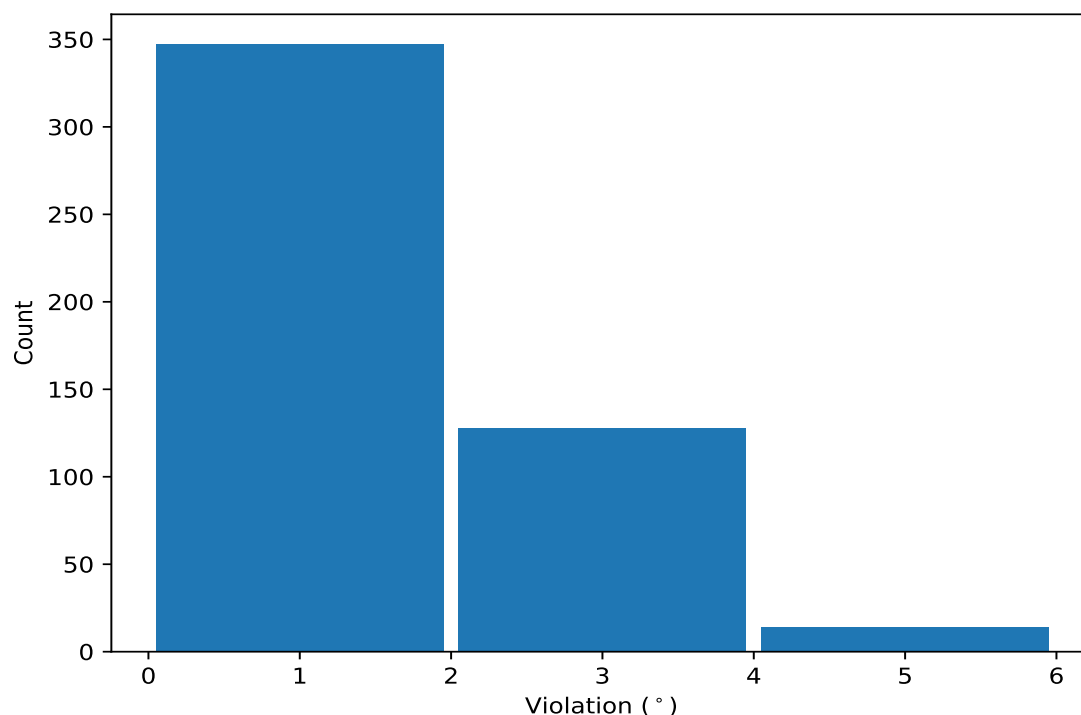
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,50)	1:619:A:ASP:C	1:620:A:LYS:N	1:620:A:LYS:CA	1:620:A:LYS:C	2	1.26	0.05	1.26
(1,94)	1:653:A:TRP:C	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	2	1.25	0.14	1.25
(1,49)	1:619:A:ASP:N	1:619:A:ASP:CA	1:619:A:ASP:C	1:620:A:LYS:N	2	1.22	0.1	1.22
(1,45)	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	1:618:A:THR:N	2	1.16	0.01	1.16
(1,44)	1:616:A:VAL:C	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	2	1.12	0.09	1.12
(1,129)	1:691:A:ILE:N	1:691:A:ILE:CA	1:691:A:ILE:C	1:692:A:THR:N	2	1.09	0.01	1.09

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 (°)
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	6	5.63

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	10	4.84
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	20	4.81
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	8	4.76
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	13	4.75
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	20	4.68
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	17	4.65
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	12	4.48
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	2	4.47
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	1	4.46
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	13	4.39
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	16	4.31
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	9	4.04
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	9	4.03
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	18	3.97
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	2	3.96
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	7	3.96
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	4	3.91
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	5	3.89
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	10	3.87
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	14	3.87
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	4	3.84
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	9	3.67
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	15	3.67
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	11	3.61
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	3	3.58
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	4	3.56
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1	3.51
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	17	3.48
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	16	3.48
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	8	3.39
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	15	3.39
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	19	3.33
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	4	3.33
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	4	3.24
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	19	3.24
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	18	3.24
(1,13)	1:595:A:PHE:C	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	14	3.24
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	1	3.22
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	17	3.18
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	7	3.11
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	5	3.11
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1	3.11
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	20	3.05
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	2	3.05
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	3	2.94
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	17	2.94
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	17	2.9
(1,135)	1:694:A:LEU:N	1:694:A:LEU:CA	1:694:A:LEU:C	1:695:A:CYS:N	13	2.83
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	6	2.82
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	9	2.82
(1,41)	1:615:A:LYS:N	1:615:A:LYS:CA	1:615:A:LYS:C	1:616:A:VAL:N	14	2.82

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	17	2.78
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	16	2.78
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	5	2.76
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	19	2.76
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	8	2.76
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	12	2.73
(1,137)	1:695:A:CYS:C	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	18	2.69
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	17	2.68
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	4	2.67
(1,135)	1:694:A:LEU:N	1:694:A:LEU:CA	1:694:A:LEU:C	1:695:A:CYS:N	4	2.66
(1,103)	1:663:A:SER:C	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	7	2.66
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	3	2.59
(1,19)	1:598:A:GLN:C	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	6	2.59
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	19	2.57
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	11	2.56
(1,65)	1:632:A:SER:N	1:632:A:SER:CA	1:632:A:SER:C	1:633:A:VAL:N	18	2.54
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	18	2.53
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	6	2.53
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	19	2.5
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	19	2.5
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1	2.48
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	18	2.48
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	7	2.47
(1,164)	1:723:A:ALA:C	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	12	2.46
(1,150)	1:712:A:SER:C	1:713:A:THR:N	1:713:A:THR:CA	1:713:A:THR:C	10	2.46
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	4	2.46
(1,121)	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	1:686:A:PRO:N	11	2.39
(1,112)	1:674:A:ARG:N	1:674:A:ARG:CA	1:674:A:ARG:C	1:675:A:ASP:N	19	2.39
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	14	2.39
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	6	2.37
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	8	2.36
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	7	2.34
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	12	2.33
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	8	2.33
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	19	2.33
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	2	2.31
(1,165)	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	1:725:A:PRO:N	12	2.28
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	10	2.27
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	17	2.27
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	17	2.27
(1,106)	1:669:A:ILE:N	1:669:A:ILE:CA	1:669:A:ILE:C	1:670:A:GLN:N	10	2.26
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	3	2.26
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	13	2.25
(1,157)	1:719:A:TYR:N	1:719:A:TYR:CA	1:719:A:TYR:C	1:720:A:THR:N	10	2.25
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	11	2.25
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	9	2.24
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	15	2.24
(1,1)	1:585:A:SER:C	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	8	2.24
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	2	2.22
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	11	2.21
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	20	2.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	3	2.2
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	16	2.2
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	11	2.19
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	8	2.18
(1,104)	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	1:665:A:TYR:N	4	2.17
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	2	2.17
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	8	2.16
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	1	2.16
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	1	2.16
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	9	2.15
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	12	2.14
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	7	2.14
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	11	2.13
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	3	2.13
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	18	2.13
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	20	2.13
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	20	2.12
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	1	2.11
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	14	2.11
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	17	2.11
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	1	2.1
(1,26)	1:603:A:PHE:N	1:603:A:PHE:CA	1:603:A:PHE:C	1:604:A:ASP:N	13	2.1
(1,24)	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1:603:A:PHE:N	12	2.1
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	10	2.08
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	20	2.08
(1,24)	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1:603:A:PHE:N	1	2.08
(1,108)	1:672:A:THR:N	1:672:A:THR:CA	1:672:A:THR:C	1:673:A:TYR:N	5	2.07
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	19	2.06
(1,24)	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1:603:A:PHE:N	10	2.06
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	8	2.03
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	2	2.02
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	16	2.02
(1,86)	1:648:A:SER:C	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	3	2.02
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	19	2.02
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	19	2.02
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	12	2.02
(1,125)	1:688:A:ALA:C	1:689:A:THR:N	1:689:A:THR:CA	1:689:A:THR:C	11	2.01
(1,103)	1:663:A:SER:C	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	10	2.0
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	20	2.0
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	17	1.99
(1,86)	1:648:A:SER:C	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	17	1.98
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	10	1.98
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	7	1.98
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	13	1.97
(1,42)	1:615:A:LYS:C	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	15	1.95
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	13	1.95
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	3	1.94
(1,164)	1:723:A:ALA:C	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	9	1.93
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	8	1.93
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	13	1.89
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	13	1.89

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	7	1.89
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	20	1.88
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	6	1.88
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	1	1.88
(1,154)	1:717:A:ARG:C	1:718:A:TRP:N	1:718:A:TRP:CA	1:718:A:TRP:C	10	1.87
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	9	1.87
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	9	1.86
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	7	1.85
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	1	1.85
(1,165)	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	1:725:A:PRO:N	9	1.84
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	14	1.84
(1,157)	1:719:A:TYR:N	1:719:A:TYR:CA	1:719:A:TYR:C	1:720:A:THR:N	5	1.84
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	12	1.84
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	5	1.83
(1,93)	1:653:A:TRP:N	1:653:A:TRP:CA	1:653:A:TRP:C	1:654:A:ASN:N	6	1.83
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	20	1.83
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	2	1.82
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	6	1.81
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	3	1.81
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	10	1.81
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	10	1.8
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	9	1.8
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	5	1.79
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	18	1.79
(1,41)	1:615:A:LYS:N	1:615:A:LYS:CA	1:615:A:LYS:C	1:616:A:VAL:N	18	1.79
(1,157)	1:719:A:TYR:N	1:719:A:TYR:CA	1:719:A:TYR:C	1:720:A:THR:N	7	1.78
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	9	1.78
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	1	1.77
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	18	1.77
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	10	1.77
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	20	1.77
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	1	1.76
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	11	1.76
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	10	1.76
(1,137)	1:695:A:CYS:C	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	13	1.75
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	1	1.75
(1,24)	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	1:603:A:PHE:N	6	1.75
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	6	1.74
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	7	1.74
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	3	1.74
(1,19)	1:598:A:GLN:C	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	8	1.74
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	14	1.73
(1,43)	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	1:617:A:GLU:N	18	1.73
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	4	1.73
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	5	1.72
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	17	1.72
(1,104)	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	1:665:A:TYR:N	17	1.72
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	2	1.71
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	10	1.71
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	15	1.71
(1,150)	1:712:A:SER:C	1:713:A:THR:N	1:713:A:THR:CA	1:713:A:THR:C	13	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	18	1.7
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	14	1.7
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	10	1.69
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	6	1.69
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	17	1.69
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	7	1.68
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	6	1.68
(1,19)	1:598:A:GLN:C	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	17	1.67
(1,51)	1:622:A:GLU:N	1:622:A:GLU:CA	1:622:A:GLU:C	1:623:A:PHE:N	14	1.66
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	5	1.66
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	20	1.65
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	4	1.65
(1,21)	1:600:A:GLY:C	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	10	1.65
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	18	1.64
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	11	1.63
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	7	1.63
(1,122)	1:686:A:PRO:N	1:686:A:PRO:CA	1:686:A:PRO:C	1:687:A:ARG:N	9	1.63
(1,101)	1:662:A:LEU:N	1:662:A:LEU:CA	1:662:A:LEU:C	1:663:A:SER:N	14	1.63
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	2	1.63
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	13	1.63
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	15	1.62
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	12	1.62
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	1	1.62
(1,12)	1:595:A:PHE:N	1:595:A:PHE:CA	1:595:A:PHE:C	1:596:A:ASP:N	14	1.62
(1,17)	1:597:A:SER:C	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	20	1.61
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	19	1.6
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	17	1.6
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	6	1.59
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	16	1.59
(1,43)	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	1:617:A:GLU:N	4	1.59
(1,26)	1:603:A:PHE:N	1:603:A:PHE:CA	1:603:A:PHE:C	1:604:A:ASP:N	20	1.59
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	3	1.58
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	12	1.58
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	9	1.57
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	2	1.57
(1,120)	1:684:A:ARG:C	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	9	1.56
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	5	1.56
(1,146)	1:705:A:GLU:C	1:706:A:TYR:N	1:706:A:TYR:CA	1:706:A:TYR:C	15	1.55
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	1	1.55
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	20	1.54
(1,33)	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	1:610:A:LYS:N	1	1.54
(1,59)	1:626:A:ASN:N	1:626:A:ASN:CA	1:626:A:ASN:C	1:627:A:VAL:N	14	1.53
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	15	1.53
(1,106)	1:669:A:ILE:N	1:669:A:ILE:CA	1:669:A:ILE:C	1:670:A:GLN:N	20	1.52
(1,103)	1:663:A:SER:C	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	6	1.52
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	5	1.52
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	20	1.52
(1,52)	1:622:A:GLU:C	1:623:A:PHE:N	1:623:A:PHE:CA	1:623:A:PHE:C	11	1.52
(1,140)	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	1:699:A:ALA:N	2	1.51
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	10	1.51
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	18	1.51

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	2	1.51
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	10	1.5
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	15	1.5
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	17	1.5
(1,11)	1:594:A:VAL:C	1:595:A:PHE:N	1:595:A:PHE:CA	1:595:A:PHE:C	8	1.5
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	13	1.49
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	15	1.48
(1,132)	1:692:A:THR:C	1:693:A:PHE:N	1:693:A:PHE:CA	1:693:A:PHE:C	15	1.48
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	19	1.48
(1,47)	1:618:A:THR:N	1:618:A:THR:CA	1:618:A:THR:C	1:619:A:ASP:N	3	1.48
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	4	1.47
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	14	1.47
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	9	1.47
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	19	1.47
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	19	1.46
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	4	1.46
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	12	1.45
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	7	1.45
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	3	1.45
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	9	1.45
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	18	1.44
(1,120)	1:684:A:ARG:C	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	4	1.44
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	15	1.44
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	4	1.43
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	5	1.43
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	11	1.43
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	15	1.43
(1,124)	1:688:A:ALA:N	1:688:A:ALA:CA	1:688:A:ALA:C	1:689:A:THR:N	6	1.42
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	14	1.42
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	15	1.41
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	14	1.41
(1,148)	1:710:A:ASP:C	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	11	1.41
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	1	1.41
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	17	1.41
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	20	1.4
(1,99)	1:661:A:LYS:N	1:661:A:LYS:CA	1:661:A:LYS:C	1:662:A:LEU:N	8	1.4
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	6	1.4
(1,94)	1:653:A:TRP:C	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	9	1.39
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	4	1.39
(1,164)	1:723:A:ALA:C	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	6	1.38
(1,148)	1:710:A:ASP:C	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	17	1.38
(1,101)	1:662:A:LEU:N	1:662:A:LEU:CA	1:662:A:LEU:C	1:663:A:SER:N	15	1.38
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	10	1.38
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	9	1.37
(1,121)	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	1:686:A:PRO:N	12	1.37
(1,104)	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	1:665:A:TYR:N	5	1.37
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	4	1.37
(1,12)	1:595:A:PHE:N	1:595:A:PHE:CA	1:595:A:PHE:C	1:596:A:ASP:N	5	1.37
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	17	1.36
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	1	1.36
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	17	1.36

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	14	1.36
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	6	1.36
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	3	1.36
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	4	1.35
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	14	1.35
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	11	1.35
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	9	1.35
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	7	1.35
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	5	1.35
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	8	1.35
(1,148)	1:710:A:ASP:C	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	19	1.34
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	11	1.34
(1,52)	1:622:A:GLU:C	1:623:A:PHE:N	1:623:A:PHE:CA	1:623:A:PHE:C	9	1.34
(1,18)	1:598:A:GLN:N	1:598:A:GLN:CA	1:598:A:GLN:C	1:599:A:ALA:N	18	1.34
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	20	1.33
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	9	1.33
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	10	1.33
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	15	1.33
(1,49)	1:619:A:ASP:N	1:619:A:ASP:CA	1:619:A:ASP:C	1:620:A:LYS:N	16	1.32
(1,48)	1:618:A:THR:C	1:619:A:ASP:N	1:619:A:ASP:CA	1:619:A:ASP:C	13	1.32
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	13	1.31
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	18	1.31
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	2	1.31
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	8	1.31
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	15	1.31
(1,50)	1:619:A:ASP:C	1:620:A:LYS:N	1:620:A:LYS:CA	1:620:A:LYS:C	10	1.31
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	4	1.31
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	16	1.3
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	16	1.3
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	18	1.3
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	20	1.3
(1,4)	1:587:A:THR:N	1:587:A:THR:CA	1:587:A:THR:C	1:588:A:GLU:N	6	1.3
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	12	1.29
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	7	1.29
(1,106)	1:669:A:ILE:N	1:669:A:ILE:CA	1:669:A:ILE:C	1:670:A:GLN:N	8	1.29
(1,91)	1:652:A:SER:N	1:652:A:SER:CA	1:652:A:SER:C	1:653:A:TRP:N	17	1.29
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	5	1.29
(1,61)	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	1:629:A:GLY:N	7	1.29
(1,153)	1:716:A:PHE:C	1:717:A:ARG:N	1:717:A:ARG:CA	1:717:A:ARG:C	12	1.28
(1,106)	1:669:A:ILE:N	1:669:A:ILE:CA	1:669:A:ILE:C	1:670:A:GLN:N	13	1.28
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	19	1.28
(1,164)	1:723:A:ALA:C	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	14	1.27
(1,74)	1:642:A:ALA:N	1:642:A:ALA:CA	1:642:A:ALA:C	1:643:A:CYS:N	12	1.27
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	2	1.27
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	19	1.26
(1,95)	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	1:655:A:LEU:N	15	1.26
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	2	1.26
(1,8)	1:593:A:THR:N	1:593:A:THR:CA	1:593:A:THR:C	1:594:A:VAL:N	18	1.26
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	3	1.25
(1,137)	1:695:A:CYS:C	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	7	1.25
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	13	1.25

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	6	1.25
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	5	1.25
(1,13)	1:595:A:PHE:C	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	11	1.25
(1,113)	1:676:A:GLY:C	1:677:A:THR:N	1:677:A:THR:CA	1:677:A:THR:C	11	1.24
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	11	1.24
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	2	1.24
(1,19)	1:598:A:GLN:C	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	11	1.24
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	19	1.24
(1,163)	1:722:A:TYR:N	1:722:A:TYR:CA	1:722:A:TYR:C	1:723:A:ALA:N	7	1.23
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	18	1.23
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	9	1.23
(1,23)	1:601:A:PHE:C	1:602:A:SER:N	1:602:A:SER:CA	1:602:A:SER:C	14	1.23
(1,21)	1:600:A:GLY:C	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	12	1.23
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	1	1.23
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	12	1.23
(1,15)	1:596:A:ASP:C	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	10	1.23
(1,105)	1:664:A:TYR:C	1:665:A:TYR:N	1:665:A:TYR:CA	1:665:A:TYR:C	2	1.22
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	8	1.22
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	19	1.22
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	6	1.22
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	16	1.22
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	12	1.22
(1,44)	1:616:A:VAL:C	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	1	1.22
(1,50)	1:619:A:ASP:C	1:620:A:LYS:N	1:620:A:LYS:CA	1:620:A:LYS:C	20	1.21
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	19	1.21
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	11	1.21
(1,6)	1:588:A:GLU:N	1:588:A:GLU:CA	1:588:A:GLU:C	1:589:A:GLY:N	7	1.21
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	9	1.2
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	20	1.2
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	5	1.2
(1,32)	1:608:A:LEU:C	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	14	1.2
(1,32)	1:608:A:LEU:C	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	17	1.2
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	10	1.19
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	13	1.19
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	15	1.19
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	8	1.18
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	14	1.18
(1,32)	1:608:A:LEU:C	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	8	1.18
(1,165)	1:724:A:CYS:N	1:724:A:CYS:CA	1:724:A:CYS:C	1:725:A:PRO:N	10	1.17
(1,149)	1:711:A:ASN:N	1:711:A:ASN:CA	1:711:A:ASN:C	1:712:A:SER:N	6	1.17
(1,115)	1:678:A:PRO:N	1:678:A:PRO:CA	1:678:A:PRO:C	1:679:A:TYR:N	1	1.17
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	11	1.17
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	16	1.17
(1,45)	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	1:618:A:THR:N	18	1.17
(1,42)	1:615:A:LYS:C	1:616:A:VAL:N	1:616:A:VAL:CA	1:616:A:VAL:C	3	1.17
(1,32)	1:608:A:LEU:C	1:609:A:THR:N	1:609:A:THR:CA	1:609:A:THR:C	5	1.17
(1,128)	1:690:A:LEU:N	1:690:A:LEU:CA	1:690:A:LEU:C	1:691:A:ILE:N	18	1.16
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	3	1.16
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	3	1.16
(1,29)	1:607:A:PRO:N	1:607:A:PRO:CA	1:607:A:PRO:C	1:608:A:LEU:N	3	1.16
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	16	1.16

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	10	1.15
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	20	1.15
(1,91)	1:652:A:SER:N	1:652:A:SER:CA	1:652:A:SER:C	1:653:A:TRP:N	7	1.15
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	14	1.15
(1,45)	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	1:618:A:THR:N	17	1.15
(1,25)	1:602:A:SER:C	1:603:A:PHE:N	1:603:A:PHE:CA	1:603:A:PHE:C	13	1.15
(1,2)	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	1:587:A:THR:N	9	1.15
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	3	1.14
(1,89)	1:650:A:ARG:N	1:650:A:ARG:CA	1:650:A:ARG:C	1:651:A:LYS:N	13	1.14
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	12	1.14
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	15	1.14
(1,52)	1:622:A:GLU:C	1:623:A:PHE:N	1:623:A:PHE:CA	1:623:A:PHE:C	7	1.14
(1,163)	1:722:A:TYR:N	1:722:A:TYR:CA	1:722:A:TYR:C	1:723:A:ALA:N	12	1.13
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	11	1.13
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	16	1.13
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	6	1.13
(1,158)	1:719:A:TYR:C	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	12	1.12
(1,103)	1:663:A:SER:C	1:664:A:TYR:N	1:664:A:TYR:CA	1:664:A:TYR:C	18	1.12
(1,49)	1:619:A:ASP:N	1:619:A:ASP:CA	1:619:A:ASP:C	1:620:A:LYS:N	10	1.12
(1,20)	1:599:A:ALA:N	1:599:A:ALA:CA	1:599:A:ALA:C	1:600:A:GLY:N	14	1.12
(1,163)	1:722:A:TYR:N	1:722:A:TYR:CA	1:722:A:TYR:C	1:723:A:ALA:N	14	1.11
(1,161)	1:721:A:SER:N	1:721:A:SER:CA	1:721:A:SER:C	1:722:A:TYR:N	15	1.11
(1,122)	1:686:A:PRO:N	1:686:A:PRO:CA	1:686:A:PRO:C	1:687:A:ARG:N	11	1.11
(1,95)	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	1:655:A:LEU:N	4	1.11
(1,60)	1:627:A:VAL:C	1:628:A:CYS:N	1:628:A:CYS:CA	1:628:A:CYS:C	18	1.11
(1,129)	1:691:A:ILE:N	1:691:A:ILE:CA	1:691:A:ILE:C	1:692:A:THR:N	7	1.1
(1,121)	1:685:A:THR:N	1:685:A:THR:CA	1:685:A:THR:C	1:686:A:PRO:N	10	1.1
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	12	1.1
(1,95)	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	1:655:A:LEU:N	3	1.1
(1,94)	1:653:A:TRP:C	1:654:A:ASN:N	1:654:A:ASN:CA	1:654:A:ASN:C	3	1.1
(1,62)	1:630:A:PRO:C	1:631:A:VAL:N	1:631:A:VAL:CA	1:631:A:VAL:C	13	1.1
(1,55)	1:624:A:HIS:N	1:624:A:HIS:CA	1:624:A:HIS:C	1:625:A:ILE:N	7	1.1
(1,145)	1:704:A:PRO:N	1:704:A:PRO:CA	1:704:A:PRO:C	1:705:A:GLU:N	10	1.09
(1,91)	1:652:A:SER:N	1:652:A:SER:CA	1:652:A:SER:C	1:653:A:TRP:N	16	1.09
(1,66)	1:632:A:SER:C	1:633:A:VAL:N	1:633:A:VAL:CA	1:633:A:VAL:C	4	1.09
(1,1)	1:585:A:SER:C	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	6	1.09
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	2	1.08
(1,132)	1:692:A:THR:C	1:693:A:PHE:N	1:693:A:PHE:CA	1:693:A:PHE:C	5	1.08
(1,129)	1:691:A:ILE:N	1:691:A:ILE:CA	1:691:A:ILE:C	1:692:A:THR:N	16	1.08
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	13	1.08
(1,101)	1:662:A:LEU:N	1:662:A:LEU:CA	1:662:A:LEU:C	1:663:A:SER:N	19	1.07
(1,98)	1:659:A:ASN:C	1:660:A:ALA:N	1:660:A:ALA:CA	1:660:A:ALA:C	17	1.07
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	8	1.07
(1,87)	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	1:650:A:ARG:N	20	1.06
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	14	1.06
(1,53)	1:623:A:PHE:N	1:623:A:PHE:CA	1:623:A:PHE:C	1:624:A:HIS:N	4	1.06
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	5	1.06
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	4	1.06
(1,1)	1:585:A:SER:C	1:586:A:ARG:N	1:586:A:ARG:CA	1:586:A:ARG:C	16	1.06
(1,155)	1:718:A:TRP:N	1:718:A:TRP:CA	1:718:A:TRP:C	1:719:A:TYR:N	15	1.05
(1,153)	1:716:A:PHE:C	1:717:A:ARG:N	1:717:A:ARG:CA	1:717:A:ARG:C	14	1.05

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,138)	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	1:697:A:ARG:N	15	1.05
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	2	1.05
(1,153)	1:716:A:PHE:C	1:717:A:ARG:N	1:717:A:ARG:CA	1:717:A:ARG:C	8	1.04
(1,143)	1:702:A:GLY:C	1:703:A:PHE:N	1:703:A:PHE:CA	1:703:A:PHE:C	3	1.04
(1,139)	1:697:A:ARG:C	1:698:A:ASP:N	1:698:A:ASP:CA	1:698:A:ASP:C	15	1.04
(1,136)	1:694:A:LEU:C	1:695:A:CYS:N	1:695:A:CYS:CA	1:695:A:CYS:C	10	1.04
(1,85)	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	1:649:A:ASP:N	5	1.04
(1,75)	1:642:A:ALA:C	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	8	1.04
(1,34)	1:610:A:LYS:C	1:611:A:LYS:N	1:611:A:LYS:CA	1:611:A:LYS:C	6	1.04
(1,14)	1:596:A:ASP:N	1:596:A:ASP:CA	1:596:A:ASP:C	1:597:A:SER:N	11	1.04
(1,159)	1:720:A:THR:N	1:720:A:THR:CA	1:720:A:THR:C	1:721:A:SER:N	1	1.03
(1,86)	1:648:A:SER:C	1:649:A:ASP:N	1:649:A:ASP:CA	1:649:A:ASP:C	18	1.03
(1,51)	1:622:A:GLU:N	1:622:A:GLU:CA	1:622:A:GLU:C	1:623:A:PHE:N	13	1.03
(1,44)	1:616:A:VAL:C	1:617:A:GLU:N	1:617:A:GLU:CA	1:617:A:GLU:C	6	1.03
(1,132)	1:692:A:THR:C	1:693:A:PHE:N	1:693:A:PHE:CA	1:693:A:PHE:C	16	1.02
(1,112)	1:674:A:ARG:N	1:674:A:ARG:CA	1:674:A:ARG:C	1:675:A:ASP:N	12	1.02
(1,39)	1:614:A:TYR:N	1:614:A:TYR:CA	1:614:A:TYR:C	1:615:A:LYS:N	13	1.02
(1,133)	1:693:A:PHE:N	1:693:A:PHE:CA	1:693:A:PHE:C	1:694:A:LEU:N	10	1.01
(1,97)	1:657:A:ARG:N	1:657:A:ARG:CA	1:657:A:ARG:C	1:658:A:SER:N	7	1.01
(1,84)	1:647:A:ARG:C	1:648:A:SER:N	1:648:A:SER:CA	1:648:A:SER:C	14	1.01
(1,82)	1:646:A:SER:N	1:646:A:SER:CA	1:646:A:SER:C	1:647:A:ARG:N	2	1.01
(1,51)	1:622:A:GLU:N	1:622:A:GLU:CA	1:622:A:GLU:C	1:623:A:PHE:N	19	1.01
(1,28)	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	1:605:A:LEU:N	17	1.01
(1,27)	1:603:A:PHE:C	1:604:A:ASP:N	1:604:A:ASP:CA	1:604:A:ASP:C	8	1.01
(1,22)	1:601:A:PHE:N	1:601:A:PHE:CA	1:601:A:PHE:C	1:602:A:SER:N	12	1.01
(1,16)	1:597:A:SER:N	1:597:A:SER:CA	1:597:A:SER:C	1:598:A:GLN:N	13	1.01
(1,150)	1:712:A:SER:C	1:713:A:THR:N	1:713:A:THR:CA	1:713:A:THR:C	2	1.0
(1,137)	1:695:A:CYS:C	1:696:A:ASP:N	1:696:A:ASP:CA	1:696:A:ASP:C	12	1.0
(1,76)	1:643:A:CYS:N	1:643:A:CYS:CA	1:643:A:CYS:C	1:644:A:GLN:N	1	1.0