



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 07:36 PM UTC

PDB ID : 2L8Y / pdb_00002l8y
BMRB ID : 17431
Title : Solution structure of the E. coli outer membrane protein RcsF (periplasmatic domain)
Authors : Rogov, V.V.; Rogova, N.Y.; Bernhard, F.; Lohr, F.; Doetsch, V.
Deposited on : 2011-01-27

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

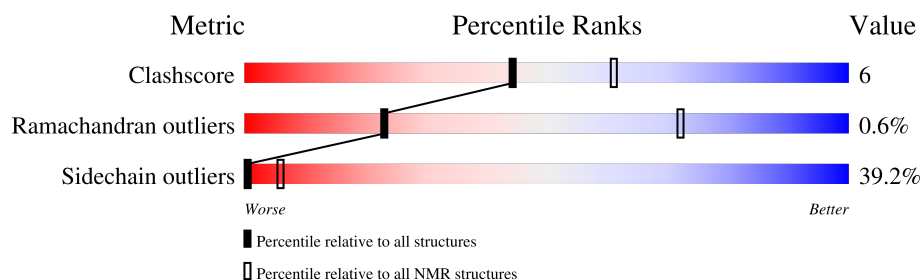
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	105	

2 Ensemble composition and analysis

This entry contains 25 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:47-A:134 (88)	0.74	1

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 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 5, 9, 10, 13, 18, 20
2	4, 6, 8, 12, 16, 17, 21
3	11, 15, 19, 22, 24
4	3, 7, 23, 25
Single-model clusters	14

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1564 atoms, of which 790 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein rcsF.

Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1564	476	790	143	148	7	

There is a discrepancy between the modelled and reference sequences:

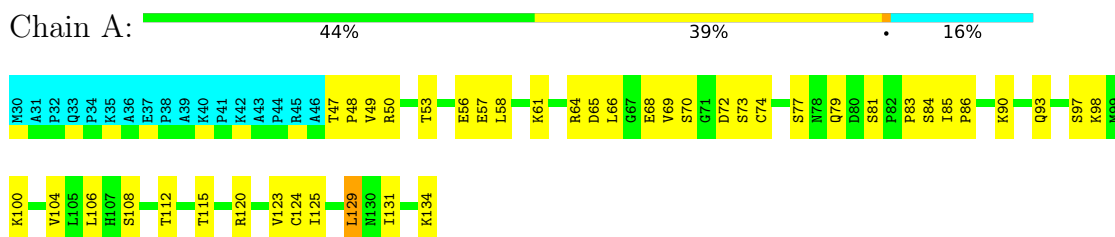
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P69411

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: Protein rcsF

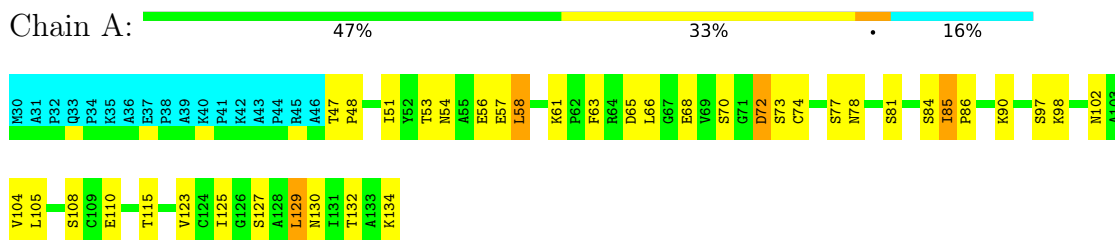


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

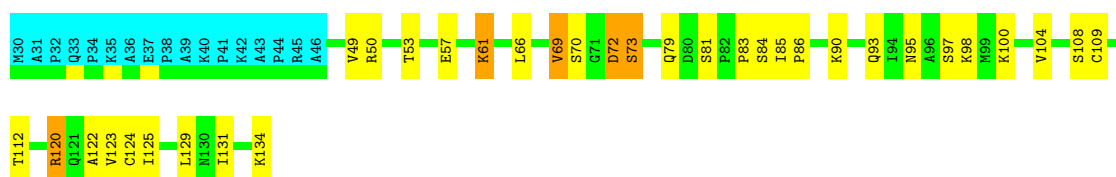
- Molecule 1: Protein rcsF



4.2.2 Score per residue for model 2

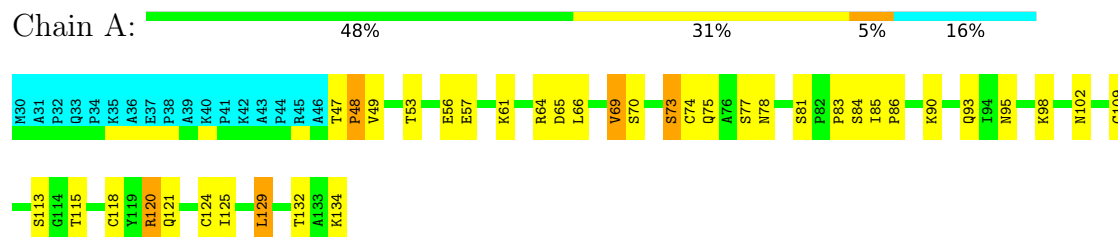
- Molecule 1: Protein rcsF





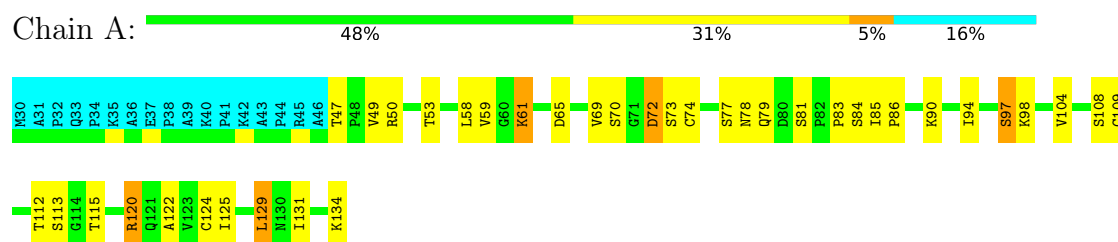
4.2.3 Score per residue for model 3

- Molecule 1: Protein rcsF



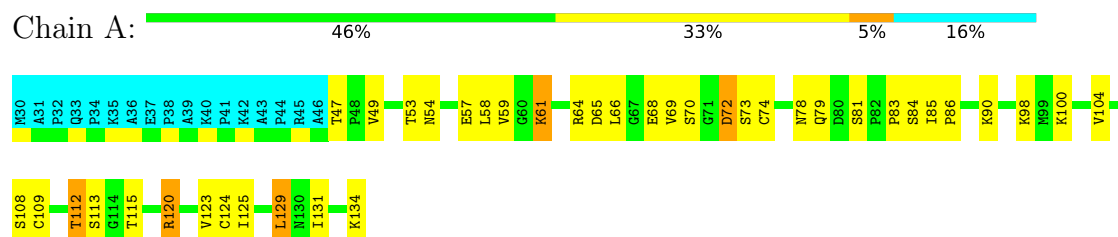
4.2.4 Score per residue for model 4

- Molecule 1: Protein rcsF



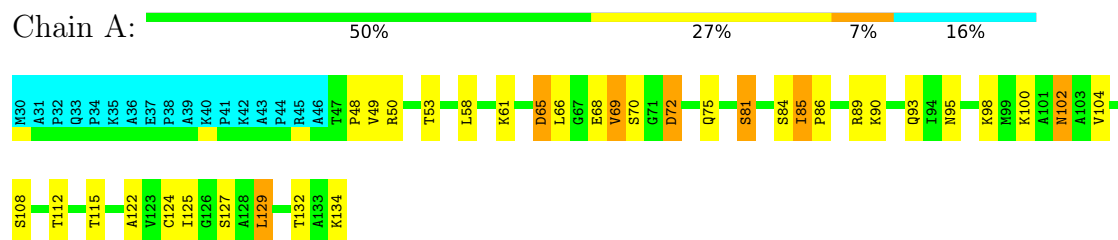
4.2.5 Score per residue for model 5

- Molecule 1: Protein rcsF



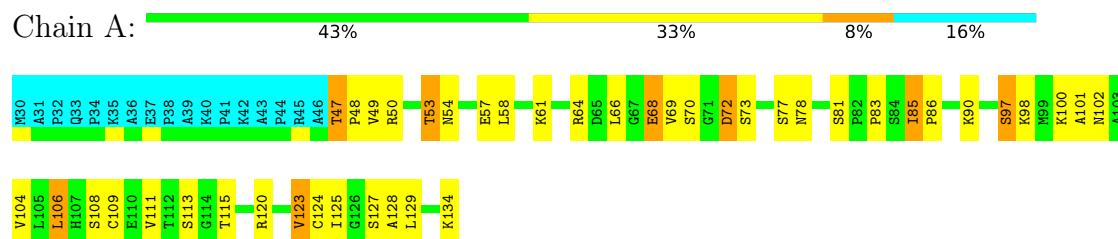
4.2.6 Score per residue for model 6

- Molecule 1: Protein rcsF



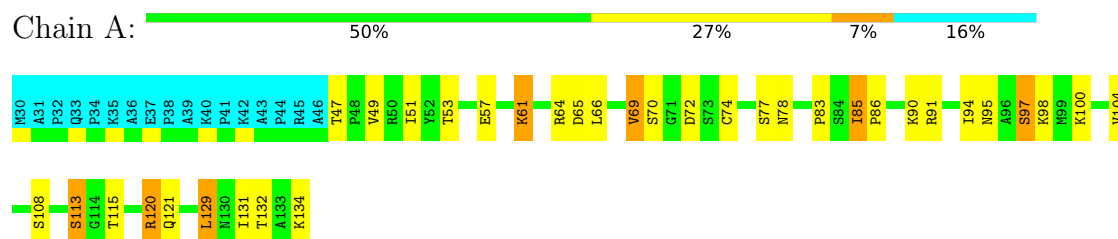
4.2.7 Score per residue for model 7

- Molecule 1: Protein rcsF



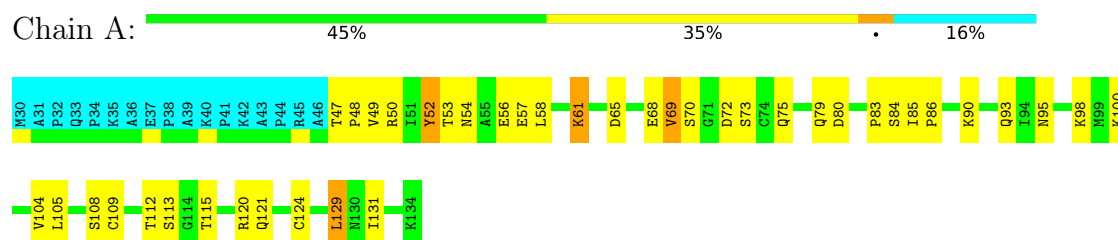
4.2.8 Score per residue for model 8

- Molecule 1: Protein rcsF



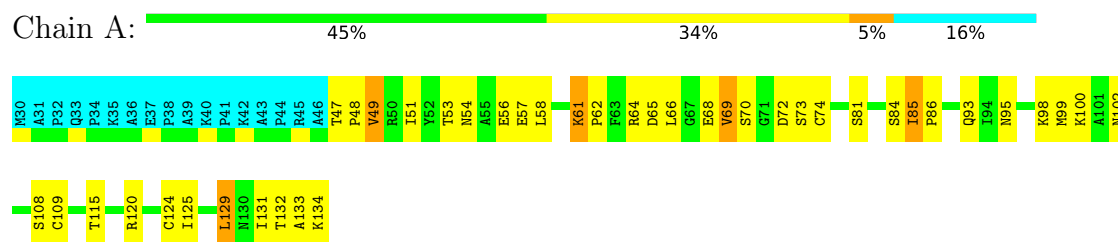
4.2.9 Score per residue for model 9

- Molecule 1: Protein rcsF



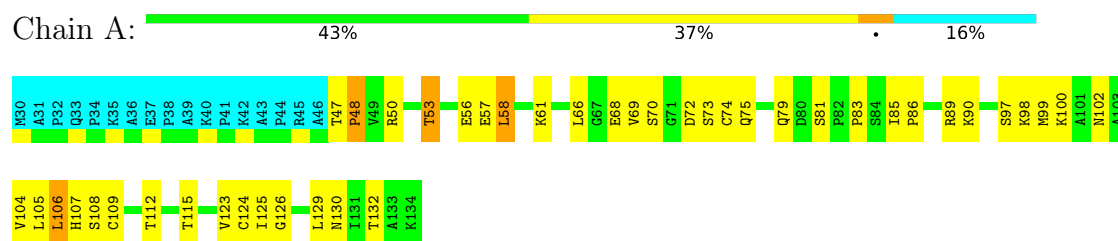
4.2.10 Score per residue for model 10

- Molecule 1: Protein rcsF



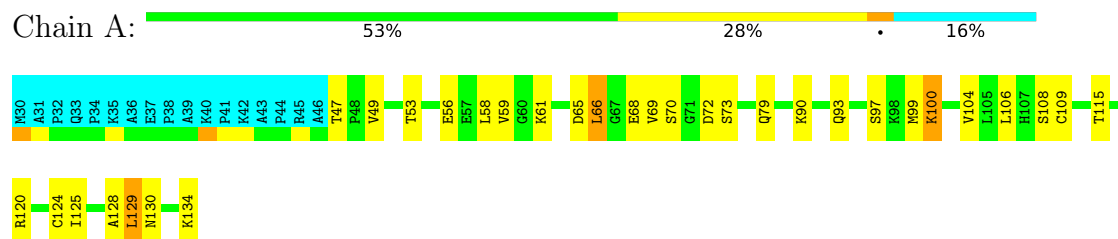
4.2.11 Score per residue for model 11

- Molecule 1: Protein rcsF



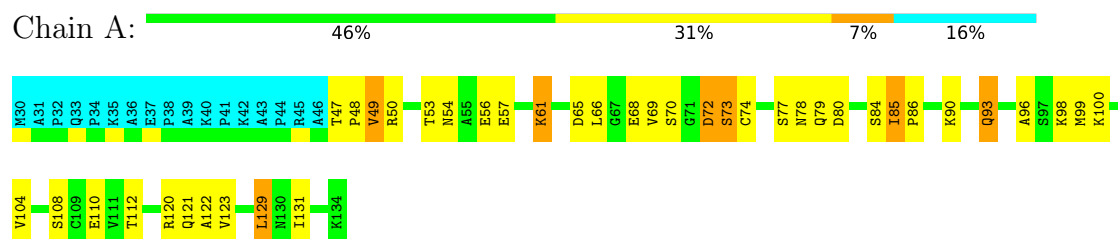
4.2.12 Score per residue for model 12

- Molecule 1: Protein rcsF



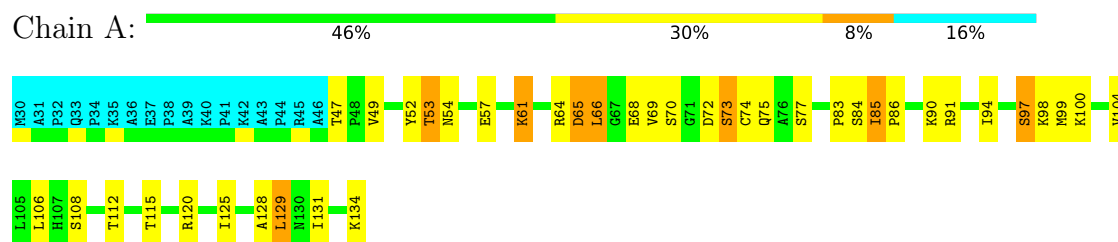
4.2.13 Score per residue for model 13

- Molecule 1: Protein rcsF



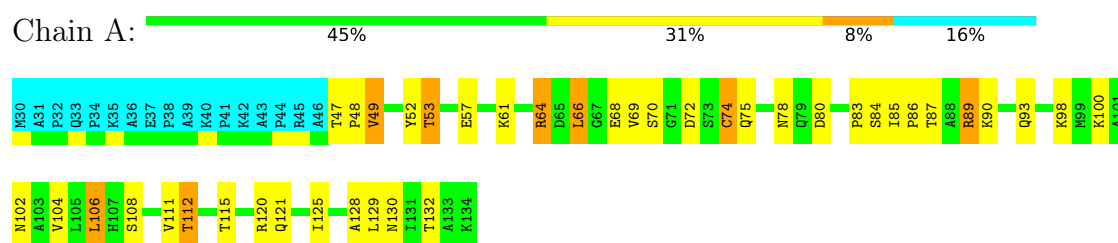
4.2.14 Score per residue for model 14

- Molecule 1: Protein rcsF



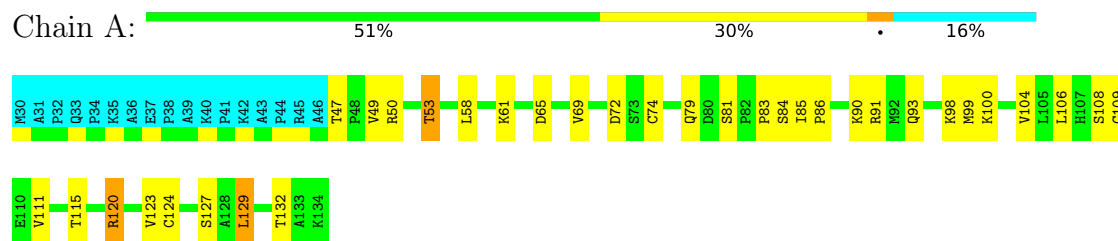
4.2.15 Score per residue for model 15

- Molecule 1: Protein rcsF



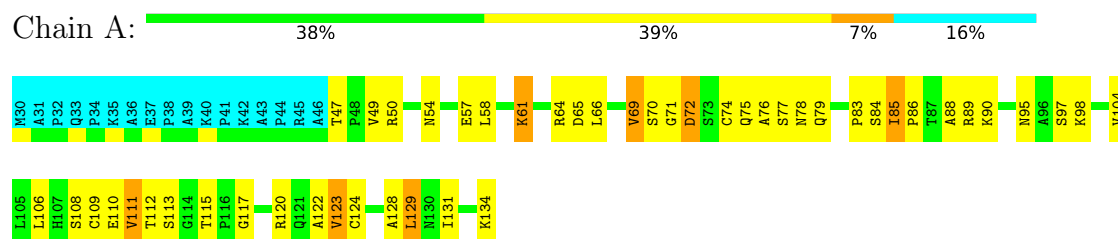
4.2.16 Score per residue for model 16

- Molecule 1: Protein rcsF



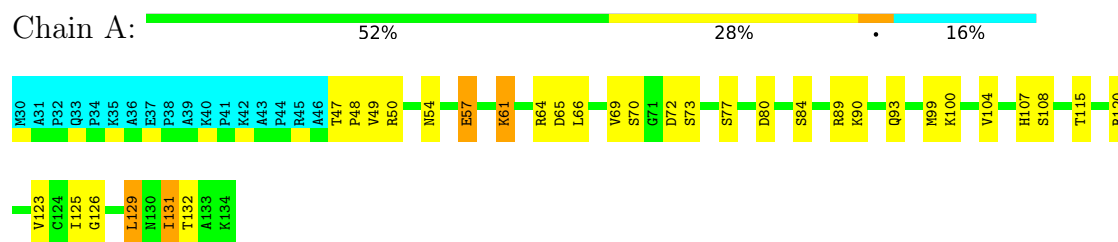
4.2.17 Score per residue for model 17

- Molecule 1: Protein rcsF



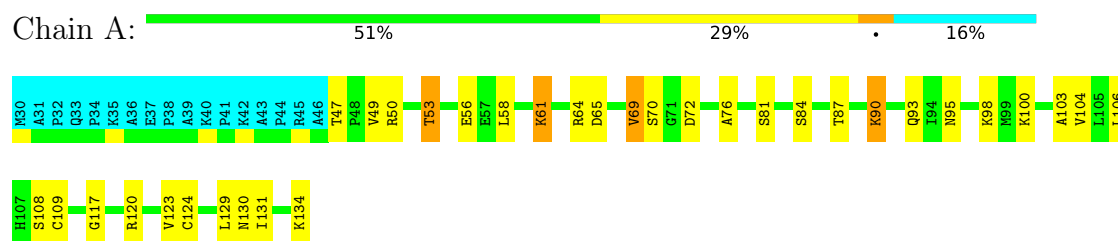
4.2.18 Score per residue for model 18

- Molecule 1: Protein rcsF



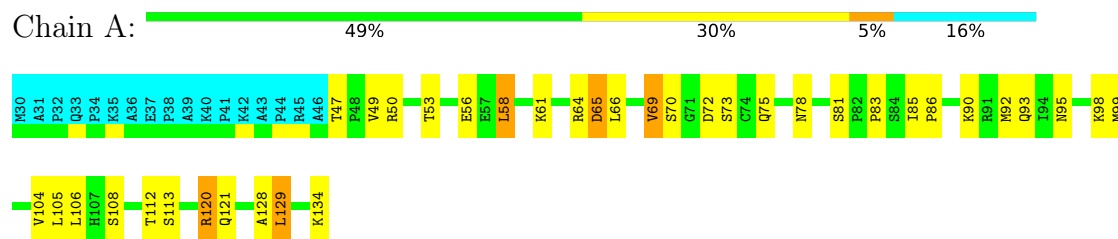
4.2.19 Score per residue for model 19

- Molecule 1: Protein rcsF



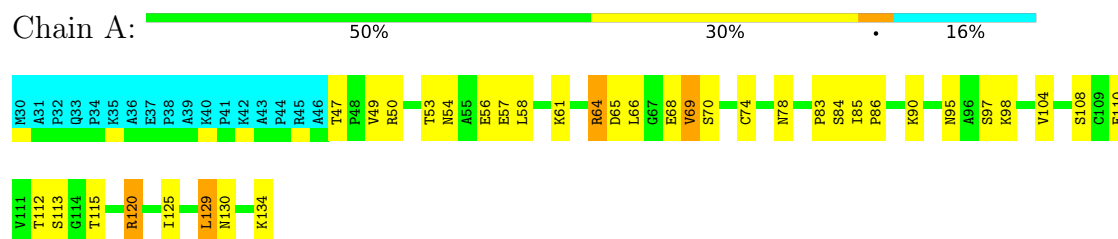
4.2.20 Score per residue for model 20

- Molecule 1: Protein rcsF



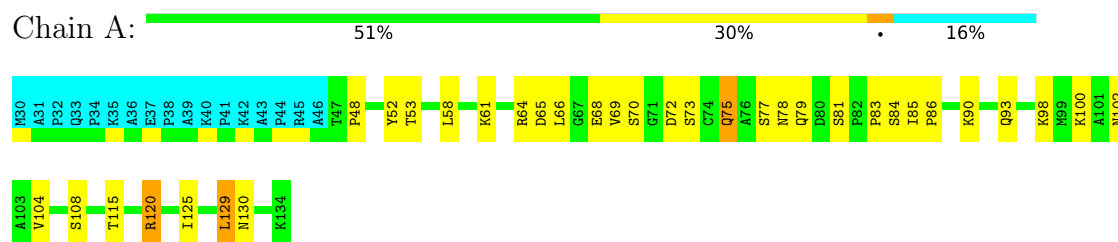
4.2.21 Score per residue for model 21

- Molecule 1: Protein rcsF



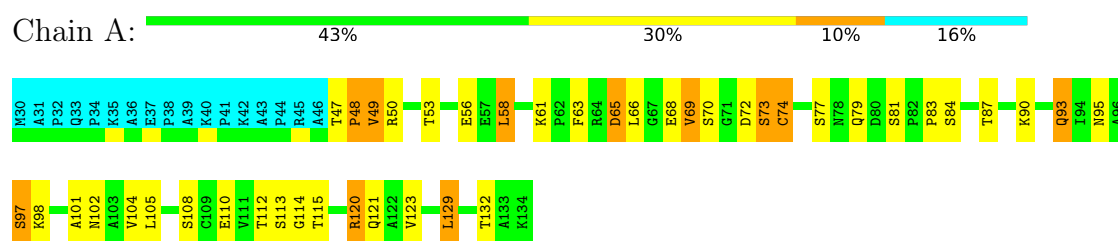
4.2.22 Score per residue for model 22

- Molecule 1: Protein rcsF



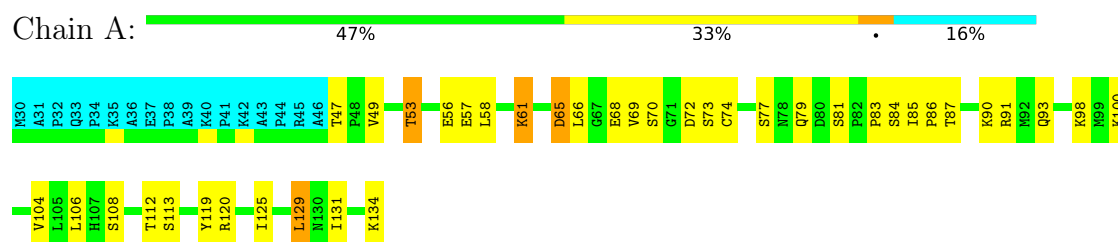
4.2.23 Score per residue for model 23

- Molecule 1: Protein rcsF



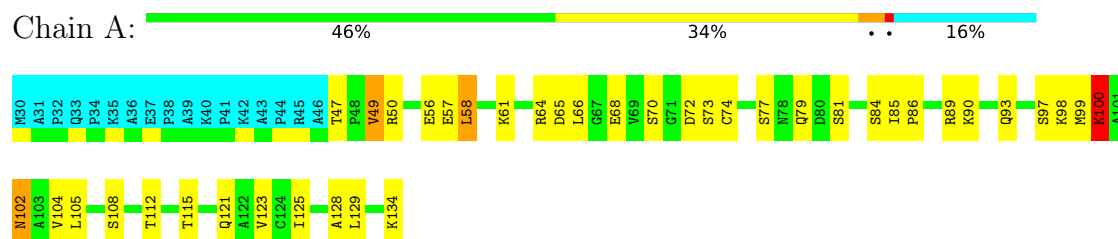
4.2.24 Score per residue for model 24

- Molecule 1: Protein rcsF



4.2.25 Score per residue for model 25

- Molecule 1: Protein rcsF



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 25 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	structure solution	1.0.5
ARIA	refinement	1

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	1101
Number of shifts mapped to atoms	1101
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	650	653	652	8±2
All	All	16250	16325	16300	208

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

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:PRO:HG3	1:A:120:ARG:HB3	0.90	1.44	3	12
1:A:109:CYS:HA	1:A:124:CYS:HA	0.79	1.54	3	5
1:A:113:SER:HB3	1:A:120:ARG:HD3	0.77	1.56	8	1
1:A:65:ASP:HA	1:A:129:LEU:HD12	0.75	1.59	13	19
1:A:73:SER:HB3	1:A:83:PRO:HA	0.74	1.59	14	2
1:A:68:GLU:HA	1:A:127:SER:HA	0.73	1.57	6	2
1:A:113:SER:HA	1:A:120:ARG:HD2	0.72	1.60	23	1
1:A:61:LYS:HD2	1:A:131:ILE:HD12	0.66	1.68	8	11
1:A:69:VAL:HG21	1:A:95:ASN:HB3	0.63	1.70	17	10
1:A:74:CYS:HB2	1:A:121:GLN:HG3	0.61	1.70	23	2
1:A:113:SER:HB3	1:A:120:ARG:CD	0.60	2.27	8	1
1:A:54:ASN:HB3	1:A:57:GLU:HG3	0.59	1.74	10	7
1:A:72:ASP:HB2	1:A:123:VAL:HG22	0.58	1.74	5	3
1:A:53:THR:HG23	1:A:106:LEU:HB3	0.58	1.76	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ARG:HB3	1:A:130:ASN:HB3	0.57	1.75	19	3
1:A:107:HIS:CD2	1:A:126:GLY:HA2	0.56	2.35	18	2
1:A:111:VAL:HA	1:A:122:ALA:HA	0.55	1.77	17	1
1:A:48:PRO:O	1:A:102:ASN:HB2	0.54	2.03	10	8
1:A:75:GLN:HG3	1:A:83:PRO:HD3	0.53	1.79	11	3
1:A:63:PHE:HD2	1:A:129:LEU:HG	0.53	1.64	23	1
1:A:58:LEU:HD23	1:A:105:LEU:HD13	0.52	1.82	25	5
1:A:83:PRO:HG3	1:A:120:ARG:CB	0.51	2.35	21	2
1:A:84:SER:HB2	1:A:87:THR:OG1	0.51	2.06	15	4
1:A:63:PHE:CD2	1:A:129:LEU:HG	0.51	2.41	23	1
1:A:61:LYS:HD2	1:A:131:ILE:HG13	0.50	1.83	18	1
1:A:68:GLU:CA	1:A:127:SER:HA	0.50	2.35	6	1
1:A:112:THR:O	1:A:120:ARG:HA	0.50	2.06	15	1
1:A:99:MET:O	1:A:100:LYS:HB2	0.50	2.04	25	1
1:A:72:ASP:HB2	1:A:123:VAL:HG12	0.50	1.83	17	1
1:A:83:PRO:CG	1:A:120:ARG:HB3	0.49	2.30	3	3
1:A:49:VAL:HB	1:A:102:ASN:HA	0.49	1.83	15	1
1:A:72:ASP:HA	1:A:122:ALA:O	0.49	2.07	13	4
1:A:83:PRO:HG2	1:A:120:ARG:HG3	0.49	1.83	14	2
1:A:85:ILE:N	1:A:86:PRO:HD2	0.49	2.23	4	19
1:A:66:LEU:HD11	1:A:130:ASN:HB2	0.48	1.85	22	3
1:A:85:ILE:HB	1:A:86:PRO:HD3	0.48	1.84	9	2
1:A:66:LEU:HB3	1:A:128:ALA:O	0.47	2.09	17	1
1:A:95:ASN:O	1:A:98:LYS:HG3	0.47	2.10	17	1
1:A:112:THR:O	1:A:120:ARG:HD3	0.47	2.09	5	1
1:A:49:VAL:HA	1:A:102:ASN:O	0.47	2.10	25	2
1:A:49:VAL:HG13	1:A:93:GLN:HG2	0.47	1.86	25	1
1:A:66:LEU:HB2	1:A:128:ALA:O	0.46	2.10	12	6
1:A:118:CYS:HB3	1:A:121:GLN:HB2	0.46	1.88	3	1
1:A:49:VAL:HG21	1:A:93:GLN:HG2	0.46	1.86	13	1
1:A:85:ILE:HG22	1:A:89:ARG:HD2	0.46	1.87	15	1
1:A:72:ASP:HB2	1:A:123:VAL:HG13	0.45	1.89	7	1
1:A:69:VAL:HG11	1:A:96:ALA:HB2	0.45	1.88	13	1
1:A:50:ARG:O	1:A:103:ALA:HA	0.45	2.11	19	1
1:A:73:SER:HB2	1:A:83:PRO:HA	0.45	1.88	3	1
1:A:75:GLN:NE2	1:A:80:ASP:HB3	0.44	2.28	9	1
1:A:76:ALA:HA	1:A:117:GLY:O	0.44	2.12	17	2
1:A:97:SER:HA	1:A:101:ALA:O	0.44	2.13	7	2
1:A:71:GLY:O	1:A:88:ALA:HB1	0.44	2.13	17	1
1:A:75:GLN:HE22	1:A:80:ASP:HB3	0.44	1.72	15	1
1:A:75:GLN:HB3	1:A:81:SER:O	0.43	2.13	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:89:ARG:HG3	1:A:124:CYS:SG	0.43	2.53	6	1
1:A:63:PHE:CE2	1:A:129:LEU:HG	0.43	2.49	1	1
1:A:102:ASN:OD1	1:A:130:ASN:HA	0.43	2.13	22	2
1:A:83:PRO:HG2	1:A:120:ARG:HG2	0.43	1.90	24	1
1:A:94:ILE:HA	1:A:97:SER:OG	0.42	2.14	8	3
1:A:83:PRO:CG	1:A:120:ARG:HG3	0.42	2.44	7	2
1:A:72:ASP:HA	1:A:123:VAL:HA	0.42	1.91	19	1
1:A:73:SER:O	1:A:83:PRO:HB3	0.42	2.14	23	1
1:A:54:ASN:HB3	1:A:57:GLU:HB2	0.42	1.91	18	1
1:A:83:PRO:HG2	1:A:120:ARG:CG	0.42	2.44	14	1
1:A:69:VAL:CG2	1:A:95:ASN:HB3	0.42	2.44	8	3
1:A:90:LYS:HE3	1:A:93:GLN:NE2	0.42	2.29	19	1
1:A:54:ASN:OD1	1:A:56:GLU:HB3	0.42	2.14	9	1
1:A:49:VAL:CG1	1:A:93:GLN:HG2	0.42	2.45	23	2
1:A:121:GLN:HG2	1:A:123:VAL:HG23	0.42	1.91	25	1
1:A:52:TYR:O	1:A:105:LEU:HA	0.41	2.15	9	1
1:A:113:SER:OG	1:A:120:ARG:HD2	0.41	2.15	3	1
1:A:62:PRO:HB2	1:A:133:ALA:HA	0.41	1.92	10	1
1:A:66:LEU:CD1	1:A:130:ASN:HB2	0.41	2.45	12	1
1:A:73:SER:O	1:A:121:GLN:HA	0.41	2.16	13	1
1:A:92:MET:HE2	1:A:92:MET:HB3	0.40	1.84	20	1
1:A:113:SER:CB	1:A:120:ARG:HD3	0.40	2.37	8	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	87/105 (83%)	79±2 (91±3%)	8±2 (9±2%)	1±1 (1±1%)	23	72
All	All	2175/2625 (83%)	1972 (91%)	189 (9%)	14 (1%)	23	72

All 4 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	48	PRO	7
1	A	47	THR	4
1	A	100	LYS	2
1	A	114	GLY	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	73/85 (86%)	44±3 (61±4%)	29±3 (39±4%)	0 6
All	All	1825/2125 (86%)	1109 (61%)	716 (39%)	0 6

All 58 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	61	LYS	25
1	A	129	LEU	25
1	A	70	SER	24
1	A	90	LYS	24
1	A	108	SER	24
1	A	104	VAL	23
1	A	53	THR	22
1	A	72	ASP	22
1	A	98	LYS	22
1	A	49	VAL	22
1	A	69	VAL	22
1	A	115	THR	20
1	A	47	THR	19
1	A	58	LEU	18
1	A	73	SER	18
1	A	100	LYS	18
1	A	125	ILE	17
1	A	134	LYS	17
1	A	74	CYS	16
1	A	81	SER	16
1	A	84	SER	16
1	A	66	LEU	15

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Mol	Chain	Res	Type	Models (Total)
1	A	68	GLU	15
1	A	112	THR	15
1	A	120	ARG	15
1	A	50	ARG	14
1	A	93	GLN	14
1	A	77	SER	13
1	A	79	GLN	13
1	A	64	ARG	13
1	A	56	GLU	12
1	A	78	ASN	12
1	A	97	SER	12
1	A	57	GLU	10
1	A	132	THR	10
1	A	113	SER	9
1	A	85	ILE	8
1	A	99	MET	8
1	A	109	CYS	7
1	A	124	CYS	7
1	A	65	ASP	7
1	A	123	VAL	7
1	A	106	LEU	6
1	A	110	GLU	5
1	A	89	ARG	5
1	A	75	GLN	4
1	A	111	VAL	4
1	A	91	ARG	4
1	A	52	TYR	4
1	A	51	ILE	3
1	A	59	VAL	3
1	A	121	GLN	3
1	A	127	SER	2
1	A	102	ASN	2
1	A	80	ASP	2
1	A	54	ASN	1
1	A	131	ILE	1
1	A	119	TYR	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 81% 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	1101
Number of shifts mapped to atoms	1101
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	99	-0.03 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	93	0.11 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	95	0.09 ± 0.19	None needed (< 0.5 ppm)
^{15}N	83	-0.40 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 1012 atoms were assigned a chemical shift out of a possible 1127. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	424/434 (98%)	173/176 (98%)	173/176 (98%)	78/82 (95%)
Sidechain	558/657 (85%)	383/428 (89%)	172/200 (86%)	3/29 (10%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	30/36 (83%)	15/17 (88%)	15/17 (88%)	0/2 (0%)
Overall	1012/1127 (90%)	571/621 (92%)	360/393 (92%)	81/113 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1100 atoms were assigned a chemical shift out of a possible 1351. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	462/509 (91%)	185/205 (90%)	194/210 (92%)	83/94 (88%)
Sidechain	608/806 (75%)	411/525 (78%)	194/245 (79%)	3/36 (8%)
Aromatic	30/36 (83%)	15/17 (88%)	15/17 (88%)	0/2 (0%)
Overall	1100/1351 (81%)	611/747 (82%)	403/472 (85%)	86/132 (65%)

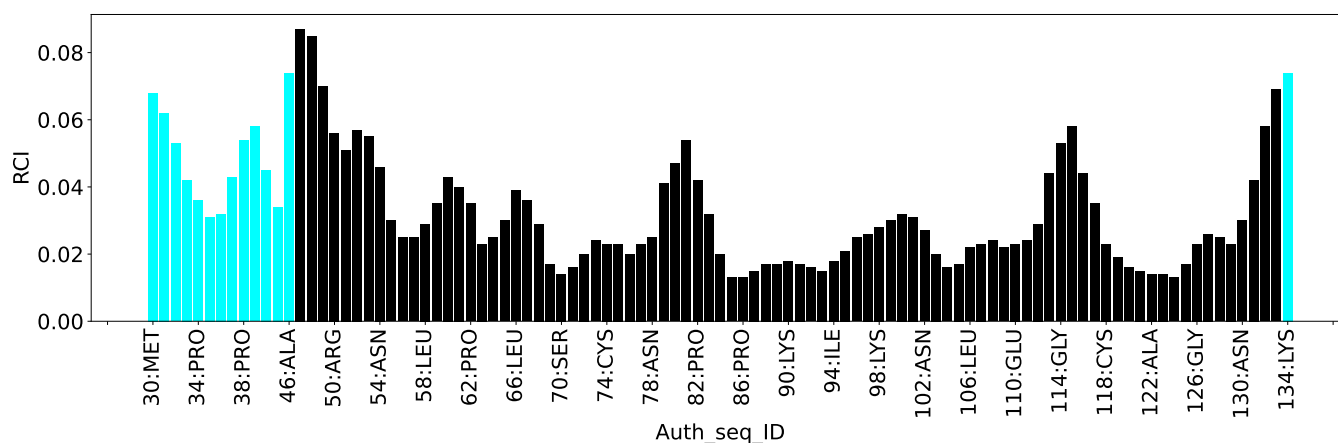
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	1135
Intra-residue ($ i-j =0$)	147
Sequential ($ i-j =1$)	251
Medium range ($ i-j >1$ and $ i-j <5$)	194
Long range ($ i-j \geq 5$)	533
Inter-chain	0
Hydrogen bond restraints	6
Disulfide bond restraints	4
Total dihedral-angle restraints	129
Number of unmapped restraints	0
Number of restraints per residue	12.0
Number of long range restraints per residue ¹	5.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	26.6	0.2
0.2-0.5 (Medium)	30.7	0.39
>0.5 (Large)	1.0	1.39

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)	12.8	9.96
10.0-20.0 (Medium)	5.7	19.97
>20.0 (Large)	4.2	55.28

9 Distance violation analysis

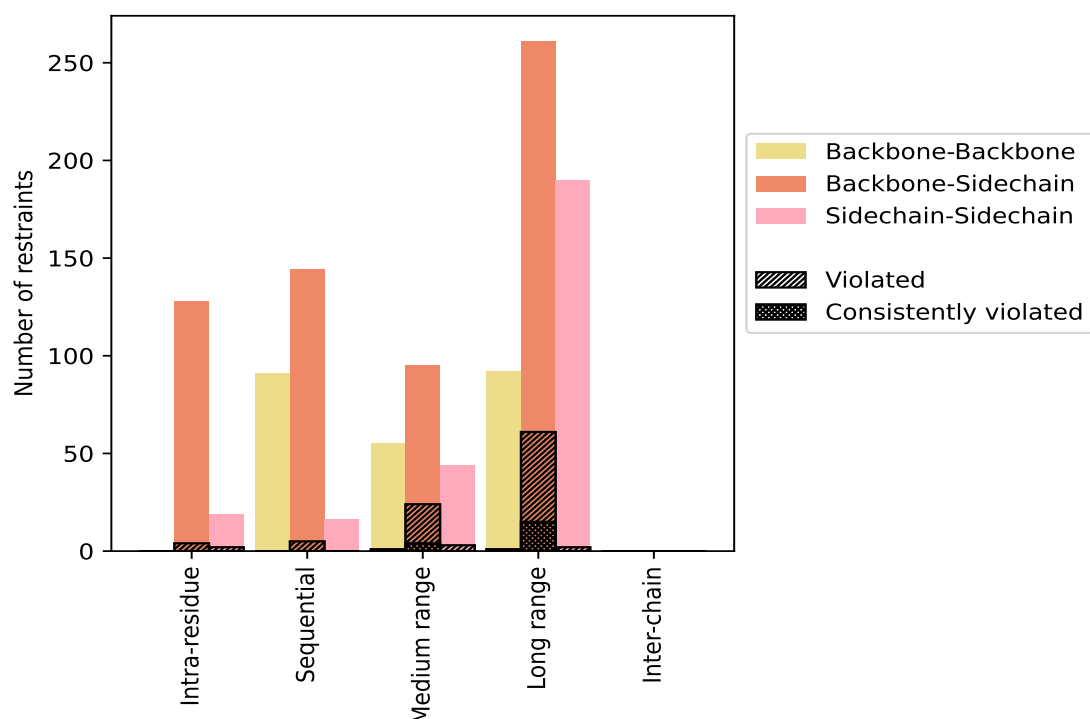
9.1 Summary of distance violations

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$)	147	13.0	6	4.1	0.5	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	128	11.3	4	3.1	0.4	0	0.0	0.0
Sidechain-Sidechain	19	1.7	2	10.5	0.2	0	0.0	0.0
Sequential ($ i-j =1$)	251	22.1	5	2.0	0.4	0	0.0	0.0
Backbone-Backbone	91	8.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	144	12.7	5	3.5	0.4	0	0.0	0.0
Sidechain-Sidechain	16	1.4	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	194	17.1	28	14.4	2.5	4	2.1	0.4
Backbone-Backbone	55	4.8	1	1.8	0.1	0	0.0	0.0
Backbone-Sidechain	95	8.4	24	25.3	2.1	4	4.2	0.4
Sidechain-Sidechain	44	3.9	3	6.8	0.3	0	0.0	0.0
Long range ($ i-j \geq 5$)	533	47.0	59	11.1	5.2	15	2.8	1.3
Backbone-Backbone	92	8.1	1	1.1	0.1	0	0.0	0.0
Backbone-Sidechain	255	22.5	56	22.0	4.9	15	5.9	1.3
Sidechain-Sidechain	186	16.4	2	1.1	0.2	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	6	0.5	5	83.3	0.4	0	0.0	0.0
Disulfide bond	4	0.4	0	0.0	0.0	0	0.0	0.0
Total	1135	100.0	103	9.1	9.1	19	1.7	1.7
Backbone-Backbone	238	21.0	2	0.8	0.2	0	0.0	0.0
Backbone-Sidechain	628	55.3	94	15.0	8.3	19	3.0	1.7
Sidechain-Sidechain	269	23.7	7	2.6	0.6	0	0.0	0.0

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	1	1	21	41	0	64	0.22	0.72	0.1	0.21
2	0	1	19	41	0	61	0.22	1.05	0.12	0.21
3	0	1	19	38	0	58	0.21	0.95	0.11	0.21
4	1	1	17	35	0	54	0.21	0.7	0.08	0.2
5	0	1	17	44	0	62	0.21	0.66	0.08	0.22
6	0	2	19	39	0	60	0.23	1.13	0.13	0.22
7	1	1	19	40	0	61	0.23	1.39	0.16	0.21
8	0	1	16	38	0	55	0.21	0.3	0.05	0.21
9	0	0	15	42	0	57	0.22	1.15	0.14	0.2
10	0	1	20	39	0	60	0.21	0.84	0.1	0.2

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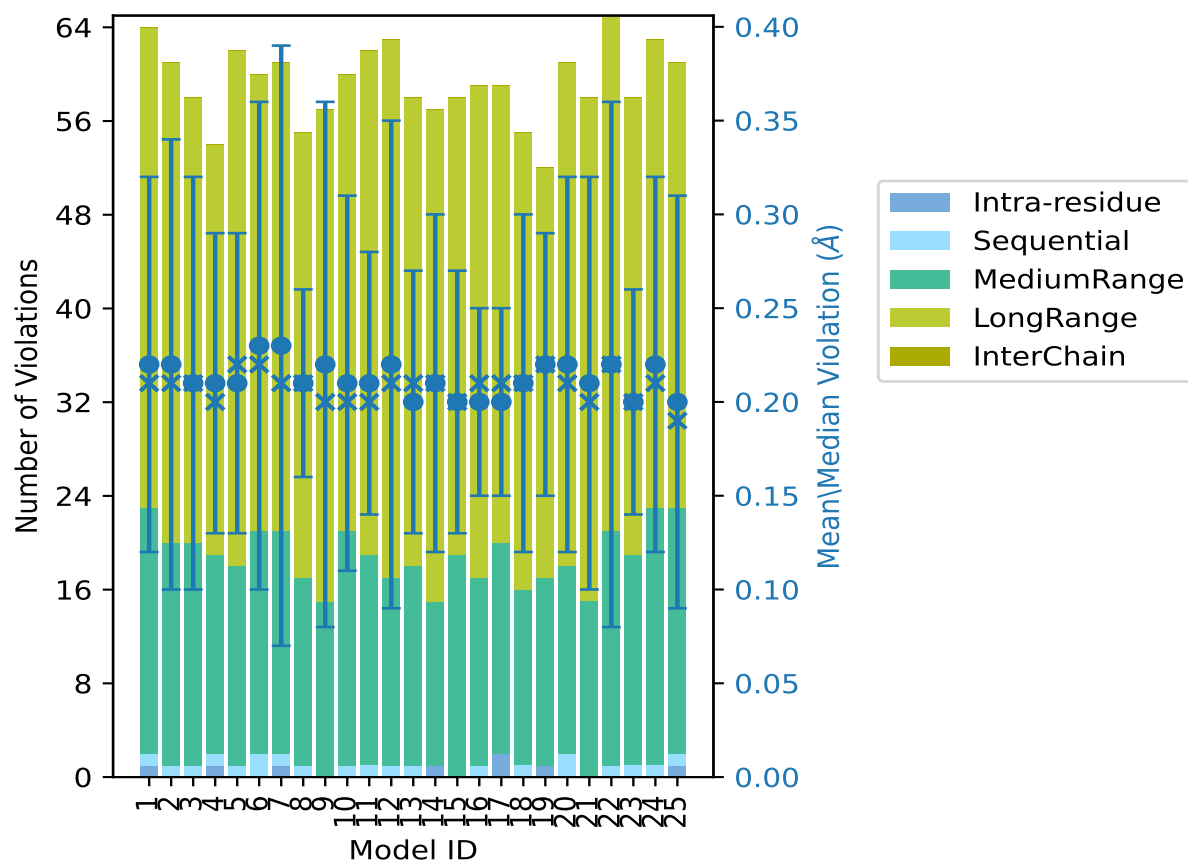
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	0	1	18	43	0	62	0.21	0.62	0.07	0.2
12	0	1	16	46	0	63	0.22	1.19	0.13	0.21
13	0	1	17	40	0	58	0.2	0.6	0.07	0.21
14	1	0	14	42	0	57	0.21	0.79	0.09	0.21
15	0	0	19	39	0	58	0.2	0.52	0.07	0.2
16	0	1	16	42	0	59	0.2	0.32	0.05	0.21
17	2	0	18	39	0	59	0.2	0.31	0.05	0.21
18	0	1	15	39	0	55	0.21	0.8	0.09	0.21
19	1	0	16	35	0	52	0.22	0.54	0.07	0.22
20	0	2	16	43	0	61	0.22	0.82	0.1	0.21
21	0	0	15	43	0	58	0.21	0.94	0.11	0.2
22	0	1	20	44	0	65	0.22	1.27	0.14	0.22
23	0	1	18	39	0	58	0.2	0.39	0.06	0.2
24	0	1	22	40	0	63	0.22	0.93	0.1	0.21
25	1	1	21	38	0	61	0.2	0.95	0.11	0.19

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

⁵Inter-chain restraints, ⁶Standard deviation

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



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

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

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1027(IR:141, SQ:246, MR:166, LR:474, 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	%
4	1	3	5	0	13	1	4.0
2	1	1	4	0	8	2	8.0
0	2	0	1	0	3	3	12.0
0	0	0	1	0	1	4	16.0
0	0	0	2	0	2	5	20.0
0	0	1	0	0	1	6	24.0

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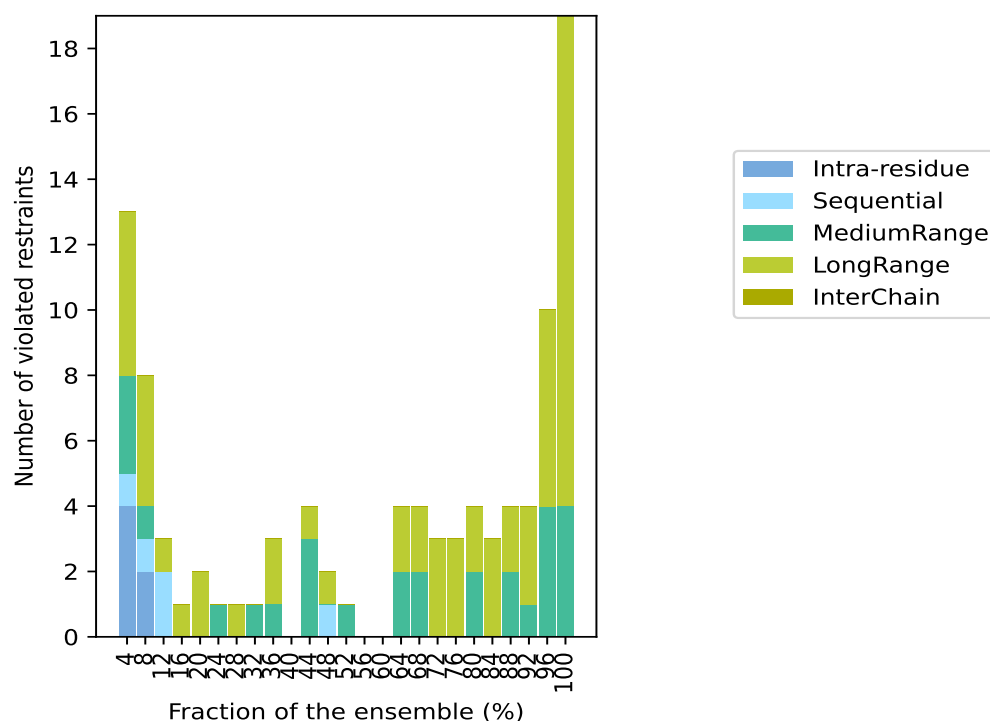
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Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	1	0	1	7	28.0
0	0	1	0	0	1	8	32.0
0	0	1	2	0	3	9	36.0
0	0	0	0	0	0	10	40.0
0	0	3	1	0	4	11	44.0
0	1	0	1	0	2	12	48.0
0	0	1	0	0	1	13	52.0
0	0	0	0	0	0	14	56.0
0	0	0	0	0	0	15	60.0
0	0	2	2	0	4	16	64.0
0	0	2	2	0	4	17	68.0
0	0	0	3	0	3	18	72.0
0	0	0	3	0	3	19	76.0
0	0	2	2	0	4	20	80.0
0	0	0	3	0	3	21	84.0
0	0	2	2	0	4	22	88.0
0	0	1	3	0	4	23	92.0
0	0	4	6	0	10	24	96.0
0	0	4	15	0	19	25	100.0

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

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

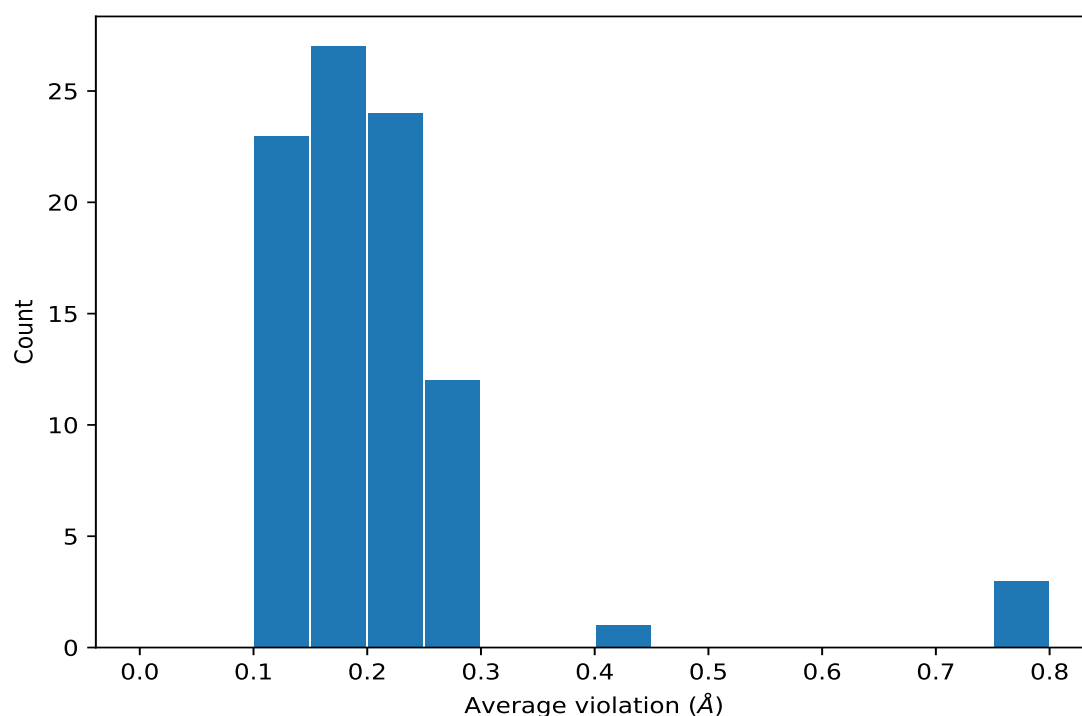
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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)
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	25	0.75	0.33	0.7
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	25	0.75	0.33	0.7
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	25	0.75	0.33	0.7
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	25	0.3	0.04	0.3
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	25	0.27	0.02	0.27
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	25	0.26	0.03	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	25	0.26	0.03	0.26
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	25	0.26	0.03	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	25	0.26	0.02	0.26
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	25	0.25	0.02	0.26
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	25	0.25	0.02	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	25	0.25	0.02	0.25
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	25	0.25	0.02	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	25	0.25	0.02	0.25
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	25	0.24	0.03	0.25
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	25	0.24	0.04	0.24

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	25	0.22	0.03	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	25	0.21	0.02	0.22
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	25	0.21	0.04	0.21
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	25	0.2	0.03	0.21
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	25	0.18	0.02	0.18
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	24	0.25	0.03	0.25
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	24	0.22	0.04	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	24	0.22	0.03	0.22
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	24	0.21	0.04	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	24	0.21	0.03	0.22
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	24	0.2	0.05	0.21
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	24	0.19	0.05	0.19
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	24	0.19	0.04	0.2
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	24	0.18	0.04	0.18
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	24	0.16	0.02	0.16
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	23	0.22	0.05	0.23
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	23	0.21	0.02	0.21
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	23	0.21	0.04	0.22
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	23	0.18	0.04	0.19
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	22	0.23	0.04	0.23
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	22	0.2	0.03	0.21
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	22	0.2	0.04	0.2
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	22	0.13	0.02	0.13
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	21	0.2	0.03	0.22
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	21	0.2	0.03	0.2
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	21	0.18	0.04	0.18
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	20	0.22	0.03	0.23
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	20	0.21	0.05	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	20	0.19	0.04	0.2
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	20	0.16	0.03	0.16
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	19	0.22	0.05	0.24
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	19	0.17	0.03	0.18
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	19	0.17	0.02	0.17
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	18	0.19	0.02	0.2
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	18	0.19	0.02	0.19
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	18	0.17	0.03	0.16
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	17	0.2	0.04	0.22
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	17	0.19	0.04	0.2
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	17	0.17	0.03	0.17
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	17	0.14	0.02	0.14
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	16	0.19	0.04	0.2
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	16	0.15	0.03	0.15

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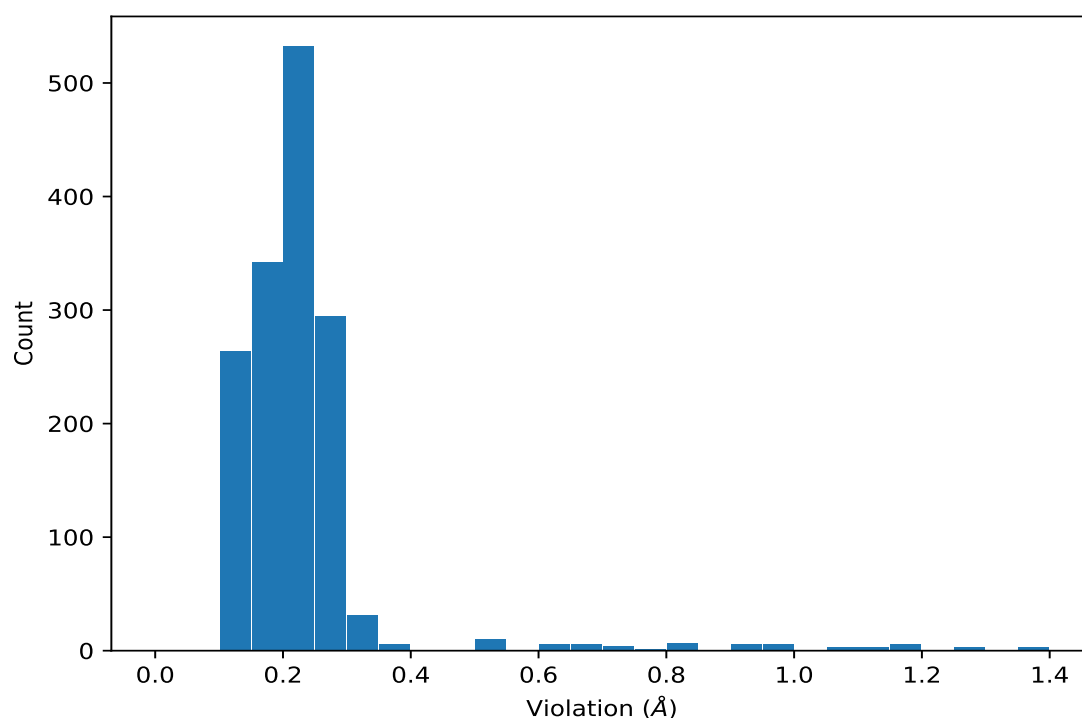
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	16	0.14	0.02	0.15
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	16	0.14	0.02	0.14
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	13	0.17	0.04	0.17
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	12	0.16	0.04	0.15
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	12	0.15	0.02	0.15
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	11	0.4	0.25	0.27
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	11	0.16	0.03	0.16
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	11	0.14	0.02	0.13
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	11	0.13	0.02	0.13
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	9	0.19	0.04	0.19
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	9	0.17	0.05	0.17
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	9	0.15	0.02	0.15
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	9	0.14	0.04	0.13
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	8	0.16	0.04	0.16
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	7	0.14	0.03	0.12
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	6	0.12	0.01	0.12
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	5	0.17	0.03	0.18
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	5	0.16	0.03	0.17
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	5	0.14	0.05	0.12
(3,18)	1:62:A:PRO:O	1:132:A:THR:H	4	0.14	0.02	0.14
(4,6)	1:114:A:GLY:H	1:119:A:TYR:O	3	0.16	0.04	0.15
(3,76)	1:110:A:GLU:H	1:123:A:VAL:O	3	0.15	0.01	0.15
(1,259)	1:66:A:LEU:HG	1:67:A:GLY:H	3	0.11	0.02	0.1
(1,653)	1:95:A:ASN:HB2	1:96:A:ALA:HA	3	0.11	0.0	0.11
(3,23)	1:67:A:GLY:N	1:128:A:ALA:O	2	0.2	0.04	0.2
(1,587)	1:90:A:LYS:HE3	1:93:A:GLN:HG3	2	0.16	0.05	0.16
(1,455)	1:78:A:ASN:HA	1:78:A:ASN:HD22	2	0.15	0.02	0.15
(1,54)	1:50:A:ARG:HB3	1:50:A:ARG:HD2	2	0.14	0.03	0.14
(1,233)	1:64:A:ARG:HB2	1:132:A:THR:HB	2	0.13	0.03	0.13
(3,68)	1:105:A:LEU:O	1:127:A:SER:H	2	0.12	0.02	0.12
(1,260)	1:66:A:LEU:HG	1:129:A:LEU:HA	2	0.12	0.01	0.12
(1,530)	1:86:A:PRO:HD3	1:87:A:THR:H	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)
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	7	1.39
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	7	1.39
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	7	1.39
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	22	1.27
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	22	1.27
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	22	1.27
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	12	1.19
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	12	1.19
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	12	1.19
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	9	1.15
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	9	1.15
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	9	1.15
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	6	1.13
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	6	1.13
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	6	1.13
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	2	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	2	1.05
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	2	1.05
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	3	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	3	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	3	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	25	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	25	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	25	0.95
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	21	0.94
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	21	0.94
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	21	0.94
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	24	0.93
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	24	0.93
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	24	0.93
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	10	0.84
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	10	0.84
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	10	0.84
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	20	0.82
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	18	0.8
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	18	0.8
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	18	0.8
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	14	0.79
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	1	0.72
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	4	0.7
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	4	0.7
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	4	0.7
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	5	0.66
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	5	0.66
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	5	0.66
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	1	0.65
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	1	0.65
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	1	0.65
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	11	0.62
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	11	0.62
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	11	0.62
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	13	0.6
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	13	0.6
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	13	0.6
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	9	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	19	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	19	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	19	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	20	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	20	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	20	0.54
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	15	0.52
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	15	0.52
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	15	0.52
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	23	0.39
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	23	0.39
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	23	0.39
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	7	0.37
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	14	0.35
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	21	0.35
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	10	0.34
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	15	0.34
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	3	0.33
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	4	0.33
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	9	0.32
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	19	0.32
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	25	0.32
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	10	0.32
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	16	0.32
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	16	0.32
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	16	0.32
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	14	0.31
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	17	0.31
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	11	0.31
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	11	0.31
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	3	0.31
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	1	0.31
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	9	0.31
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	23	0.31
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	20	0.31
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	6	0.3
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	1	0.3
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	2	0.3
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	7	0.3
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	20	0.3
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	24	0.3
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	13	0.3
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	8	0.3
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	17	0.3
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	18	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	24	0.3
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	5	0.29
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	21	0.29
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	23	0.29
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	12	0.29
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	19	0.29
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	1	0.29
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	16	0.29
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	24	0.29
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	15	0.29
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	17	0.29
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	2	0.29
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	16	0.29
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	23	0.29
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	22	0.29
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	7	0.29
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	11	0.29
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	20	0.29
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	2	0.29
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	24	0.29
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	6	0.29
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	3	0.28
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	22	0.28
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	11	0.28
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	25	0.28
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	22	0.28
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	24	0.28
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	25	0.28
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	5	0.28
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	16	0.28
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	4	0.28
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	21	0.28
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	24	0.28
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	17	0.28
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	5	0.28
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	8	0.28
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	15	0.28
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	9	0.28
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	12	0.28
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	12	0.28
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	20	0.28
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	5	0.28

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	10	0.28
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	24	0.28
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	17	0.28
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	12	0.28
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	16	0.28
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	19	0.28
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	22	0.28
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	16	0.28
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	1	0.28
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	24	0.28
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	15	0.28
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	6	0.28
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	16	0.28
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	22	0.28
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	8	0.28
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	8	0.28
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	8	0.28
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	8	0.28
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	19	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	1	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	2	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	11	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	13	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	20	0.27
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	23	0.27
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	5	0.27
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	8	0.27
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	15	0.27
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	19	0.27
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	21	0.27
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	2	0.27
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	13	0.27
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	6	0.27
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	8	0.27
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	9	0.27
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	23	0.27
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	3	0.27
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	7	0.27
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	6	0.27
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	1	0.27
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	2	0.27
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	17	0.27
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	22	0.27
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	12	0.27
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	11	0.27
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	19	0.27
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	21	0.27
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	22	0.27
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	6	0.27
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	22	0.27
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	12	0.27
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	14	0.27
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	18	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	6	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	7	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	10	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	11	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	15	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	18	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	24	0.27
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	25	0.27
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	13	0.27
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	11	0.27
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	13	0.27
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	10	0.27
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	12	0.27
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	18	0.27
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	6	0.27
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	16	0.27
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	23	0.27
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	24	0.27
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	7	0.27
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	8	0.27
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	9	0.27
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	11	0.27
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	11	0.27
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	12	0.27
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	15	0.26
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	18	0.26
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	8	0.26
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	16	0.26
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	17	0.26
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	18	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	4	0.26
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	6	0.26
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	13	0.26
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	20	0.26
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	24	0.26
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	7	0.26
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	17	0.26
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	9	0.26
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	12	0.26
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	19	0.26
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	21	0.26
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	24	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	1	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	5	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	6	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	10	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	18	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	19	0.26
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	22	0.26
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	5	0.26
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	2	0.26
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	7	0.26
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	10	0.26
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	12	0.26
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	23	0.26
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	25	0.26
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	17	0.26
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	2	0.26
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	4	0.26
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	8	0.26
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	12	0.26
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	3	0.26
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	13	0.26
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	25	0.26
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	9	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	3	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	19	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	20	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	21	0.26
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	23	0.26
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	19	0.26
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	8	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	13	0.26
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	20	0.26
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	21	0.26
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	23	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	3	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	5	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	7	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	9	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	15	0.26
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	25	0.26
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	10	0.26
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	19	0.26
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	3	0.26
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	12	0.26
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	22	0.26
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	13	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	1	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	7	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	11	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	14	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	15	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	21	0.26
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	25	0.26
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	1	0.26
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	12	0.26
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	14	0.26
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	16	0.26
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	19	0.26
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	19	0.25
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	1	0.25
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	2	0.25
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	24	0.25
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	3	0.25
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	6	0.25
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	22	0.25
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	9	0.25
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	12	0.25
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	19	0.25
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	11	0.25
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	1	0.25
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	2	0.25
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	3	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	7	0.25
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	10	0.25
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	10	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	1	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	3	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	8	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	14	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	17	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	18	0.25
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	21	0.25
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	20	0.25
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	4	0.25
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	24	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	2	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	9	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	11	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	13	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	14	0.25
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	23	0.25
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	17	0.25
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	19	0.25
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	9	0.25
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	13	0.25
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	23	0.25
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	24	0.25
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	14	0.25
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	1	0.25
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	6	0.25
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	13	0.25
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	18	0.25
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	20	0.25
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	25	0.25
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	11	0.25
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	14	0.25
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	15	0.25
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	22	0.25
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	5	0.25
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	7	0.25
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	15	0.25
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	2	0.25
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	18	0.25
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	23	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	6	0.25
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	19	0.25
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	24	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	7	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	8	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	9	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	15	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	22	0.25
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	25	0.25
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	20	0.25
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	2	0.25
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	20	0.25
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	1	0.25
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	4	0.25
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	5	0.25
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	9	0.25
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	14	0.25
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	12	0.25
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	12	0.25
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	20	0.25
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	22	0.25
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	24	0.25
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	11	0.25
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	24	0.25
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	5	0.25
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	6	0.25
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	23	0.25
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	1	0.25
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	25	0.25
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	5	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	3	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	9	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	10	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	11	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	14	0.25
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	16	0.25
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	3	0.25
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	5	0.25
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	10	0.25
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	17	0.25
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	4	0.25
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	6	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	1	0.25
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	24	0.25
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	7	0.24
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	12	0.24
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	8	0.24
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	4	0.24
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	7	0.24
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	10	0.24
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	8	0.24
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	12	0.24
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	18	0.24
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	2	0.24
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	9	0.24
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	18	0.24
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	2	0.24
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	24	0.24
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	4	0.24
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	5	0.24
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	6	0.24
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	15	0.24
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	19	0.24
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	11	0.24
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	22	0.24
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	23	0.24
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	14	0.24
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	18	0.24
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	22	0.24
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	25	0.24
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	5	0.24
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	12	0.24
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	16	0.24
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	25	0.24
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	6	0.24
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	15	0.24
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	1	0.24
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	11	0.24
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	10	0.24
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	16	0.24
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	14	0.24
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	5	0.24
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	9	0.24
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	10	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	14	0.24
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	17	0.24
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	18	0.24
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	23	0.24
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	25	0.24
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	7	0.24
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	10	0.24
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	1	0.24
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	21	0.24
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	4	0.24
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	6	0.24
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	9	0.24
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	12	0.24
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	22	0.24
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	7	0.24
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	10	0.24
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	24	0.24
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	5	0.24
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	6	0.24
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	7	0.24
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	13	0.24
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	22	0.24
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	2	0.24
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	4	0.24
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	11	0.24
(3,23)	1:67:A:GLY:N	1:128:A:ALA:O	17	0.24
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	10	0.24
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	22	0.24
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	21	0.24
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	6	0.24
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	2	0.24
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	13	0.24
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	1	0.24
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	5	0.24
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	25	0.24
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	23	0.24
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	4	0.24
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	9	0.24
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	18	0.24
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	19	0.24
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	20	0.24
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	12	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	18	0.24
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	22	0.24
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	16	0.24
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	15	0.24
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	17	0.24
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	18	0.24
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	22	0.24
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	23	0.24
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	13	0.23
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	1	0.23
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	6	0.23
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	11	0.23
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	13	0.23
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	14	0.23
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	25	0.23
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	18	0.23
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	5	0.23
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	21	0.23
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	25	0.23
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	6	0.23
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	13	0.23
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	15	0.23
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	19	0.23
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	25	0.23
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	9	0.23
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	14	0.23
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	16	0.23
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	22	0.23
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	4	0.23
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	5	0.23
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	19	0.23
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	5	0.23
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	8	0.23
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	12	0.23
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	14	0.23
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	15	0.23
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	23	0.23
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	15	0.23
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	16	0.23
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	18	0.23
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	15	0.23
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	7	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	12	0.23
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	17	0.23
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	3	0.23
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	9	0.23
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	10	0.23
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	11	0.23
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	22	0.23
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	15	0.23
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	17	0.23
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	19	0.23
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	23	0.23
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	10	0.23
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	19	0.23
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	22	0.23
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	25	0.23
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	18	0.23
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	21	0.23
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	17	0.23
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	5	0.23
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	20	0.23
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	4	0.23
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	7	0.23
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	10	0.23
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	13	0.23
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	3	0.23
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	2	0.23
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	3	0.23
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	20	0.23
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	3	0.23
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	13	0.23
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	5	0.23
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	14	0.23
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	15	0.23
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	5	0.23
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	18	0.23
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	8	0.23
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	11	0.23
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	21	0.23
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	1	0.23
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	16	0.23
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	17	0.23
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	21	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	24	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	1	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	5	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	8	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	13	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	15	0.23
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	18	0.23
(3,31)	1:71:A:GLY:N	1:124:A:CYS:O	17	0.23
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	1	0.23
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	11	0.23
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	20	0.23
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	21	0.23
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	8	0.23
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	18	0.23
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	19	0.23
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	13	0.23
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	19	0.23
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	2	0.23
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	9	0.23
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	19	0.23
(3,19)	1:64:A:ARG:N	1:130:A:ASN:O	14	0.23
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	5	0.23
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	22	0.23
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	6	0.23
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	7	0.23
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	21	0.23
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	23	0.23
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	6	0.23
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	10	0.23
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	21	0.23
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	2	0.23
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	12	0.23
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	13	0.23
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	7	0.23
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	17	0.23
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	7	0.23
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	8	0.23
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	4	0.23
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	20	0.23
(1,281)	1:67:A:GLY:HA3	1:68:A:GLU:HB2	6	0.23
(1,281)	1:67:A:GLY:HA3	1:68:A:GLU:HB3	6	0.23
(4,6)	1:114:A:GLY:H	1:119:A:TYR:O	22	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	18	0.22
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	7	0.22
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	8	0.22
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	17	0.22
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	20	0.22
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	2	0.22
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	15	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	7	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	12	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	20	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	21	0.22
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	22	0.22
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	3	0.22
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	14	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	1	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	3	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	4	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	6	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	21	0.22
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	25	0.22
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	10	0.22
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	20	0.22
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	2	0.22
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	7	0.22
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	12	0.22
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	13	0.22
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	20	0.22
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	12	0.22
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	16	0.22
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	13	0.22
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	15	0.22
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	1	0.22
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	2	0.22
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	14	0.22
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	21	0.22
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	23	0.22
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	25	0.22
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	3	0.22
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	5	0.22
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	2	0.22
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	10	0.22
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	14	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	15	0.22
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	7	0.22
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	6	0.22
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	8	0.22
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	16	0.22
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	3	0.22
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	23	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	3	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	4	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	5	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	9	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	16	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	18	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	21	0.22
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	24	0.22
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	20	0.22
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	4	0.22
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	6	0.22
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	10	0.22
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	22	0.22
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	24	0.22
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	2	0.22
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	3	0.22
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	6	0.22
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	7	0.22
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	18	0.22
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	23	0.22
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	16	0.22
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	2	0.22
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	7	0.22
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	6	0.22
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	22	0.22
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	2	0.22
(3,35)	1:73:A:SER:N	1:122:A:ALA:O	13	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	1	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	5	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	6	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	8	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	14	0.22
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	15	0.22
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	4	0.22
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	6	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	16	0.22
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	22	0.22
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	25	0.22
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	16	0.22
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	14	0.22
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	10	0.22
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	5	0.22
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	6	0.22
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	23	0.22
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	15	0.22
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	17	0.22
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	4	0.22
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	16	0.22
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	25	0.22
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	5	0.22
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	22	0.22
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	24	0.22
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	1	0.22
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	2	0.22
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	3	0.22
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	9	0.22
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	10	0.22
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	17	0.22
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	24	0.22
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	5	0.22
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	13	0.22
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	22	0.22
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	2	0.21
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	8	0.21
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	2	0.21
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	8	0.21
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	18	0.21
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	24	0.21
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	20	0.21
(3,79)	1:112:A:THR:N	1:121:A:GLN:O	24	0.21
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	1	0.21
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	3	0.21
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	5	0.21
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	9	0.21
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	23	0.21
(3,77)	1:110:A:GLU:O	1:123:A:VAL:N	17	0.21
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	16	0.21
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	13	0.21
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	17	0.21
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	7	0.21
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	16	0.21
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	9	0.21
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	17	0.21
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	21	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	1	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	5	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	6	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	8	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	19	0.21
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	21	0.21
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	11	0.21
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	3	0.21
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	13	0.21
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	18	0.21
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	19	0.21
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	20	0.21
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	3	0.21
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	6	0.21
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	9	0.21
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	10	0.21
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	24	0.21
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	1	0.21
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	20	0.21
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	24	0.21
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	23	0.21
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	4	0.21
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	7	0.21
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	16	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	4	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	8	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	12	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	22	0.21
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	24	0.21
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	20	0.21
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	11	0.21
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	19	0.21
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	21	0.21
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	1	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	2	0.21
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	14	0.21
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	7	0.21
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	7	0.21
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	8	0.21
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	13	0.21
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	20	0.21
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	16	0.21
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	19	0.21
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	24	0.21
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	13	0.21
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	2	0.21
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	5	0.21
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	4	0.21
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	20	0.21
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	24	0.21
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	4	0.21
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	25	0.21
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	7	0.21
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	8	0.21
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	25	0.21
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	12	0.21
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	21	0.21
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	11	0.21
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	16	0.21
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	19	0.21
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	23	0.21
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	11	0.21
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	12	0.21
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	14	0.21
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	7	0.21
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	11	0.21
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	12	0.21
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	18	0.21
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	24	0.21
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	6	0.21
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	14	0.21
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	17	0.21
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	8	0.21
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	21	0.21
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	3	0.21
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	14	0.21
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	6	0.21
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	8	0.21
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	17	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	1	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	3	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	7	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	11	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	12	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	14	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	16	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	17	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	18	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	19	0.21
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	25	0.21
(3,5)	1:52:A:TYR:N	1:104:A:VAL:O	8	0.21
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	14	0.21
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	16	0.21
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	19	0.21
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	20	0.21
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	12	0.21
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	14	0.21
(1,587)	1:90:A:LYS:HE3	1:93:A:GLN:HG3	16	0.21
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	17	0.21
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	17	0.21
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	17	0.21
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	3	0.21
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	5	0.2
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	19	0.2
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	20	0.2
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	4	0.2
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	9	0.2
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	11	0.2
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	17	0.2
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	2	0.2
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	24	0.2
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	6	0.2
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	13	0.2
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	21	0.2
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	22	0.2
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	10	0.2
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	19	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	20	0.2
(3,73)	1:108:A:SER:O	1:125:A:ILE:N	11	0.2
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	5	0.2
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	5	0.2
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	23	0.2
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	7	0.2
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	12	0.2
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	16	0.2
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	17	0.2
(3,63)	1:103:A:ALA:O	1:129:A:LEU:N	8	0.2
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	1	0.2
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	2	0.2
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	9	0.2
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	16	0.2
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	23	0.2
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	8	0.2
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	12	0.2
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	17	0.2
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	2	0.2
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	17	0.2
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	1	0.2
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	14	0.2
(3,51)	1:89:A:ARG:O	1:93:A:GLN:N	21	0.2
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	12	0.2
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	17	0.2
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	20	0.2
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	23	0.2
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	11	0.2
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	21	0.2
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	11	0.2
(3,43)	1:85:A:ILE:O	1:89:A:ARG:N	6	0.2
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	10	0.2
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	15	0.2
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	8	0.2
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	3	0.2
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	8	0.2
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	12	0.2
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	3	0.2
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	12	0.2
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	20	0.2
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	22	0.2
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	24	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	4	0.2
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	10	0.2
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	16	0.2
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	16	0.2
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	2	0.2
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	25	0.2
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	2	0.2
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	21	0.2
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	8	0.2
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	11	0.2
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	17	0.2
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	11	0.2
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	18	0.2
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	21	0.2
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	24	0.2
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	15	0.2
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	9	0.2
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	24	0.2
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	8	0.2
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	13	0.2
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	4	0.2
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	11	0.2
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	19	0.2
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	2	0.2
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	3	0.2
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	25	0.2
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	7	0.2
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE1	14	0.2
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE2	14	0.2
(1,285)	1:67:A:GLY:HA2	1:99:A:MET:HE3	14	0.2
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	12	0.19
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	11	0.19
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	12	0.19
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	14	0.19
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	7	0.19
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	14	0.19
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	23	0.19
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	14	0.19
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	16	0.19
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	17	0.19
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	7	0.19
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	9	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	16	0.19
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	23	0.19
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	23	0.19
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	1	0.19
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	7	0.19
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	23	0.19
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	2	0.19
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	24	0.19
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	25	0.19
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	4	0.19
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	20	0.19
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	17	0.19
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	22	0.19
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	13	0.19
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	18	0.19
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	22	0.19
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	9	0.19
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	25	0.19
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	15	0.19
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	8	0.19
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	3	0.19
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	12	0.19
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	24	0.19
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	22	0.19
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	25	0.19
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	8	0.19
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	20	0.19
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	1	0.19
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	4	0.19
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	5	0.19
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	22	0.19
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	20	0.19
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	25	0.19
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	20	0.19
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	1	0.19
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	5	0.19
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	6	0.19
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	8	0.19
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	11	0.19
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	5	0.19
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	6	0.19
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	21	0.19
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	9	0.19
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	15	0.19
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	12	0.19
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	16	0.19
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	24	0.19
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	11	0.19
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	21	0.19
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	6	0.19
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	22	0.19
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	14	0.19
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	16	0.19
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	8	0.19
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	15	0.19
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	20	0.19
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	10	0.19
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	18	0.19
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	6	0.19
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	11	0.19
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	23	0.19
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	21	0.19
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	1	0.19
(1,48)	1:50:A:ARG:HA	1:50:A:ARG:HD3	4	0.19
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	7	0.18
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	9	0.18
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	17	0.18
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	21	0.18
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	25	0.18
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	3	0.18
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	10	0.18
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	11	0.18
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	10	0.18
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	24	0.18
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	25	0.18
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	14	0.18
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	9	0.18
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	22	0.18
(3,65)	1:105:A:LEU:N	1:127:A:SER:O	10	0.18
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	25	0.18
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	4	0.18
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	7	0.18
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	13	0.18
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	18	0.18
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	23	0.18
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	11	0.18
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	14	0.18
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	17	0.18
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	4	0.18
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	14	0.18
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	15	0.18
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	23	0.18
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	19	0.18
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	6	0.18
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	1	0.18
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	23	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	7	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	8	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	12	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	17	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	18	0.18
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	21	0.18
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	14	0.18
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	24	0.18
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	6	0.18
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	1	0.18
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	4	0.18
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	9	0.18
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	9	0.18
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	14	0.18
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	15	0.18
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	16	0.18
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	17	0.18
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	21	0.18
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	21	0.18
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	24	0.18
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	20	0.18
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	24	0.18
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	10	0.18
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	15	0.18
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	9	0.18
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	24	0.18
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	20	0.18
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	25	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	2	0.18
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	10	0.18
(3,7)	1:52:A:TYR:O	1:106:A:LEU:N	4	0.18
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	13	0.18
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	2	0.18
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	3	0.18
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	4	0.18
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	5	0.18
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	15	0.18
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	25	0.18
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	7	0.18
(1,54)	1:50:A:ARG:HB3	1:50:A:ARG:HD2	7	0.18
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	1	0.17
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	16	0.17
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	24	0.17
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	24	0.17
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	18	0.17
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	22	0.17
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	25	0.17
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	13	0.17
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	6	0.17
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	23	0.17
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	5	0.17
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	3	0.17
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	10	0.17
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	14	0.17
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	11	0.17
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	2	0.17
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	5	0.17
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	21	0.17
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	4	0.17
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	10	0.17
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	15	0.17
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	20	0.17
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	22	0.17
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	24	0.17
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	3	0.17
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	7	0.17
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	2	0.17
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	13	0.17
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	19	0.17
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	23	0.17
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	16	0.17
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	1	0.17
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	9	0.17
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	11	0.17
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	19	0.17
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	22	0.17
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	9	0.17
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	6	0.17
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	4	0.17
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	23	0.17
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	1	0.17
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	4	0.17
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	8	0.17
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	12	0.17
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	22	0.17
(3,18)	1:62:A:PRO:O	1:132:A:THR:H	22	0.17
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	1	0.17
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	8	0.17
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	17	0.17
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	22	0.17
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	24	0.17
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	23	0.17
(3,6)	1:52:A:TYR:H	1:104:A:VAL:O	4	0.17
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	7	0.17
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	12	0.17
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	17	0.17
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	24	0.17
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	15	0.17
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	21	0.17
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	1	0.17
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	20	0.17
(1,455)	1:78:A:ASN:HA	1:78:A:ASN:HD22	19	0.17
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	15	0.17
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	9	0.16
(3,76)	1:110:A:GLU:H	1:123:A:VAL:O	4	0.16
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	12	0.16
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	12	0.16
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	15	0.16
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	18	0.16
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	20	0.16
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	22	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	14	0.16
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	4	0.16
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	9	0.16
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	18	0.16
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	20	0.16
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	5	0.16
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	21	0.16
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	10	0.16
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	19	0.16
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	19	0.16
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	2	0.16
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	24	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	1	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	2	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	7	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	9	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	10	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	13	0.16
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	18	0.16
(3,49)	1:88:A:ALA:O	1:92:A:MET:N	6	0.16
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	10	0.16
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	14	0.16
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	8	0.16
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	25	0.16
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	17	0.16
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	23	0.16
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	5	0.16
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	23	0.16
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	21	0.16
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	24	0.16
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	18	0.16
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	4	0.16
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	11	0.16
(3,23)	1:67:A:GLY:N	1:128:A:ALA:O	20	0.16
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	12	0.16
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	2	0.16
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	23	0.16
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	11	0.16
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	15	0.16
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	5	0.16
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	6	0.16
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	20	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	13	0.16
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	14	0.16
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	20	0.16
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	22	0.16
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	9	0.16
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	18	0.16
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	20	0.16
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	16	0.16
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	4	0.16
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	6	0.16
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	13	0.16
(1,233)	1:64:A:ARG:HB2	1:132:A:THR:HB	2	0.16
(4,6)	1:114:A:GLY:H	1:119:A:TYR:O	19	0.15
(4,5)	1:114:A:GLY:N	1:119:A:TYR:O	22	0.15
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	3	0.15
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	6	0.15
(3,82)	1:112:A:THR:O	1:121:A:GLN:H	15	0.15
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	23	0.15
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	12	0.15
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	19	0.15
(3,76)	1:110:A:GLU:H	1:123:A:VAL:O	7	0.15
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	2	0.15
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	11	0.15
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	19	0.15
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	10	0.15
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	13	0.15
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	18	0.15
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	8	0.15
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	6	0.15
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	19	0.15
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	15	0.15
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	19	0.15
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	20	0.15
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	1	0.15
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	11	0.15
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	24	0.15
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	15	0.15
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	21	0.15
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	3	0.15
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	12	0.15
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	16	0.15
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	7	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	10	0.15
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	11	0.15
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	12	0.15
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	8	0.15
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	23	0.15
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	4	0.15
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	15	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	3	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	6	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	13	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	15	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	20	0.15
(3,44)	1:85:A:ILE:O	1:89:A:ARG:H	25	0.15
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	9	0.15
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	25	0.15
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	24	0.15
(3,34)	1:71:A:GLY:O	1:124:A:CYS:H	10	0.15
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	1	0.15
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	13	0.15
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	16	0.15
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	23	0.15
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	9	0.15
(3,18)	1:62:A:PRO:O	1:132:A:THR:H	16	0.15
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	11	0.15
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	25	0.15
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	1	0.15
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	16	0.15
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	22	0.15
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	8	0.15
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	9	0.15
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	5	0.15
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	6	0.15
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	7	0.15
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	19	0.15
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	5	0.15
(1,247)	1:66:A:LEU:H	1:66:A:LEU:HG	17	0.15
(3,80)	1:112:A:THR:H	1:121:A:GLN:O	21	0.14
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	4	0.14
(3,76)	1:110:A:GLU:H	1:123:A:VAL:O	18	0.14
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	15	0.14
(3,74)	1:108:A:SER:O	1:125:A:ILE:H	22	0.14
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	7	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	9	0.14
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	16	0.14
(3,68)	1:105:A:LEU:O	1:127:A:SER:H	15	0.14
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	3	0.14
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	10	0.14
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	3	0.14
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	17	0.14
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	1	0.14
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	18	0.14
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	22	0.14
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	24	0.14
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	1	0.14
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	16	0.14
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	10	0.14
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	24	0.14
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	18	0.14
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	22	0.14
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	25	0.14
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	8	0.14
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	3	0.14
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	11	0.14
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	16	0.14
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	9	0.14
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	18	0.14
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	22	0.14
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	10	0.14
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	14	0.14
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	12	0.14
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	13	0.14
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	23	0.14
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	2	0.14
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	13	0.14
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	3	0.14
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	4	0.14
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	10	0.14
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	13	0.14
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	5	0.14
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	1	0.14
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	18	0.14
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	15	0.14
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	24	0.14
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	6	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	16	0.14
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	25	0.14
(1,589)	1:91:A:ARG:H	1:91:A:ARG:HD2	14	0.14
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	2	0.14
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	4	0.14
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	13	0.14
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	18	0.14
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	3	0.14
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	12	0.14
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	17	0.14
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	20	0.14
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	25	0.14
(1,259)	1:66:A:LEU:HG	1:67:A:GLY:H	23	0.14
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	5	0.13
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	25	0.13
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	1	0.13
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	25	0.13
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	17	0.13
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	25	0.13
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	4	0.13
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	6	0.13
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	1	0.13
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	9	0.13
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	23	0.13
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	24	0.13
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	21	0.13
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	3	0.13
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	13	0.13
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	17	0.13
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	22	0.13
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	4	0.13
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	2	0.13
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	15	0.13
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	2	0.13
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	13	0.13
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	25	0.13
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	14	0.13
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	1	0.13
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	18	0.13
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	5	0.13
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	17	0.13
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	21	0.13
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	1	0.13
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	11	0.13
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	19	0.13
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	18	0.13
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	2	0.13
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	7	0.13
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	11	0.13
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	14	0.13
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	15	0.13
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	22	0.13
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	2	0.13
(3,24)	1:67:A:GLY:H	1:128:A:ALA:O	20	0.13
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	14	0.13
(3,21)	1:64:A:ARG:O	1:130:A:ASN:N	16	0.13
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	20	0.13
(3,18)	1:62:A:PRO:O	1:132:A:THR:H	5	0.13
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	1	0.13
(3,12)	1:55:A:ALA:O	1:59:A:VAL:H	16	0.13
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	3	0.13
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	13	0.13
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	2	0.13
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	21	0.13
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	5	0.13
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	18	0.13
(1,455)	1:78:A:ASN:HA	1:78:A:ASN:HD22	25	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	2	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	5	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	8	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	11	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	14	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	16	0.13
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	23	0.13
(1,368)	1:71:A:GLY:HA3	1:91:A:ARG:HD3	3	0.13
(1,260)	1:66:A:LEU:HG	1:129:A:LEU:HA	17	0.13
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	21	0.13
(4,6)	1:114:A:GLY:H	1:119:A:TYR:O	14	0.12
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	3	0.12
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	19	0.12
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	8	0.12
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	13	0.12
(3,69)	1:107:A:HIS:N	1:125:A:ILE:O	21	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	3	0.12
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	16	0.12
(3,66)	1:105:A:LEU:H	1:127:A:SER:O	11	0.12
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	7	0.12
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	12	0.12
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	10	0.12
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	16	0.12
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	7	0.12
(3,59)	1:93:A:GLN:O	1:97:A:SER:N	25	0.12
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	3	0.12
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	7	0.12
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	4	0.12
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	17	0.12
(3,55)	1:91:A:ARG:O	1:95:A:ASN:N	3	0.12
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	4	0.12
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	7	0.12
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	23	0.12
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	6	0.12
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	7	0.12
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	9	0.12
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	15	0.12
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	6	0.12
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	13	0.12
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	12	0.12
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	25	0.12
(3,39)	1:75:A:GLN:O	1:119:A:TYR:N	16	0.12
(3,38)	1:73:A:SER:O	1:122:A:ALA:H	9	0.12
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	17	0.12
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	25	0.12
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	9	0.12
(3,32)	1:71:A:GLY:H	1:124:A:CYS:O	23	0.12
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	11	0.12
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	14	0.12
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	12	0.12
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	2	0.12
(3,27)	1:69:A:VAL:N	1:126:A:GLY:O	17	0.12
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	8	0.12
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	1	0.12
(3,22)	1:64:A:ARG:O	1:130:A:ASN:H	18	0.12
(3,20)	1:64:A:ARG:H	1:130:A:ASN:O	5	0.12
(3,4)	1:50:A:ARG:O	1:104:A:VAL:H	19	0.12
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	3	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	22	0.12
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	11	0.12
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	1	0.12
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	21	0.12
(1,201)	1:63:A:PHE:HA	1:131:A:ILE:HB	10	0.12
(4,4)	1:102:A:ASN:H	1:129:A:LEU:O	23	0.11
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	3	0.11
(4,2)	1:75:A:GLN:H	1:120:A:ARG:O	15	0.11
(3,81)	1:112:A:THR:O	1:121:A:GLN:N	10	0.11
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	20	0.11
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	5	0.11
(3,70)	1:107:A:HIS:H	1:125:A:ILE:O	17	0.11
(3,68)	1:105:A:LEU:O	1:127:A:SER:H	23	0.11
(3,67)	1:105:A:LEU:O	1:127:A:SER:N	13	0.11
(3,64)	1:103:A:ALA:O	1:129:A:LEU:H	15	0.11
(3,61)	1:94:A:ILE:O	1:98:A:LYS:N	2	0.11
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	24	0.11
(3,58)	1:92:A:MET:O	1:96:A:ALA:H	12	0.11
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	6	0.11
(3,57)	1:92:A:MET:O	1:96:A:ALA:N	21	0.11
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	8	0.11
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	12	0.11
(3,56)	1:91:A:ARG:O	1:95:A:ASN:H	22	0.11
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	22	0.11
(3,54)	1:90:A:LYS:O	1:94:A:ILE:H	25	0.11
(3,53)	1:90:A:LYS:O	1:94:A:ILE:N	13	0.11
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	5	0.11
(3,47)	1:87:A:THR:O	1:91:A:ARG:N	1	0.11
(3,45)	1:86:A:PRO:O	1:90:A:LYS:N	25	0.11
(3,42)	1:84:A:SER:O	1:88:A:ALA:H	4	0.11
(3,41)	1:84:A:SER:O	1:88:A:ALA:N	21	0.11
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	21	0.11
(3,36)	1:73:A:SER:H	1:122:A:ALA:O	16	0.11
(3,33)	1:71:A:GLY:O	1:124:A:CYS:N	18	0.11
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	7	0.11
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	15	0.11
(3,28)	1:69:A:VAL:H	1:126:A:GLY:O	25	0.11
(3,25)	1:67:A:GLY:O	1:128:A:ALA:N	21	0.11
(3,18)	1:62:A:PRO:O	1:132:A:THR:H	20	0.11
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	10	0.11
(3,15)	1:58:A:LEU:O	1:61:A:LYS:N	24	0.11
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,11)	1:55:A:ALA:O	1:59:A:VAL:N	20	0.11
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	12	0.11
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	13	0.11
(3,2)	1:50:A:ARG:H	1:102:A:ASN:O	25	0.11
(1,653)	1:95:A:ASN:HB2	1:96:A:ALA:HA	10	0.11
(1,653)	1:95:A:ASN:HB2	1:96:A:ALA:HA	11	0.11
(1,587)	1:90:A:LYS:HE3	1:93:A:GLN:HG3	5	0.11
(1,565)	1:89:A:ARG:HB2	1:89:A:ARG:HD3	17	0.11
(1,530)	1:86:A:PRO:HD3	1:87:A:THR:H	24	0.11
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	4	0.11
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	10	0.11
(1,500)	1:84:A:SER:HB3	1:87:A:THR:HB	15	0.11
(1,473)	1:83:A:PRO:HA	1:84:A:SER:HB3	5	0.11
(1,379)	1:72:A:ASP:H	1:88:A:ALA:HA	22	0.11
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	9	0.11
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	15	0.11
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	18	0.11
(1,376)	1:71:A:GLY:HA2	1:92:A:MET:HB3	22	0.11
(1,351)	1:70:A:SER:HB3	1:123:A:VAL:HG11	17	0.11
(1,351)	1:70:A:SER:HB3	1:123:A:VAL:HG12	17	0.11
(1,351)	1:70:A:SER:HB3	1:123:A:VAL:HG13	17	0.11
(1,260)	1:66:A:LEU:HG	1:129:A:LEU:HA	14	0.11
(1,191)	1:61:A:LYS:HD3	1:63:A:PHE:HB3	11	0.11
(1,54)	1:50:A:ARG:HB3	1:50:A:ARG:HD2	1	0.11
(4,1)	1:75:A:GLN:N	1:120:A:ARG:O	5	0.1
(3,78)	1:110:A:GLU:O	1:123:A:VAL:H	10	0.1
(3,75)	1:110:A:GLU:N	1:123:A:VAL:O	11	0.1
(3,62)	1:94:A:ILE:O	1:98:A:LYS:H	10	0.1
(3,60)	1:93:A:GLN:O	1:97:A:SER:H	21	0.1
(3,52)	1:89:A:ARG:O	1:93:A:GLN:H	25	0.1
(3,50)	1:88:A:ALA:O	1:92:A:MET:H	20	0.1
(3,48)	1:87:A:THR:O	1:91:A:ARG:H	2	0.1
(3,40)	1:75:A:GLN:O	1:119:A:TYR:H	13	0.1
(3,37)	1:73:A:SER:O	1:122:A:ALA:N	3	0.1
(3,30)	1:69:A:VAL:O	1:126:A:GLY:H	12	0.1
(3,29)	1:69:A:VAL:O	1:126:A:GLY:N	25	0.1
(3,26)	1:67:A:GLY:O	1:128:A:ALA:H	10	0.1
(3,17)	1:62:A:PRO:O	1:132:A:THR:N	2	0.1
(3,8)	1:52:A:TYR:O	1:106:A:LEU:H	9	0.1
(3,3)	1:50:A:ARG:O	1:104:A:VAL:N	23	0.1
(3,1)	1:50:A:ARG:N	1:102:A:ASN:O	10	0.1
(1,685)	1:98:A:LYS:HA	1:100:A:LYS:H	25	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,653)	1:95:A:ASN:HB2	1:96:A:ALA:HA	12	0.1
(1,530)	1:86:A:PRO:HD3	1:87:A:THR:H	22	0.1
(1,438)	1:75:A:GLN:HG3	1:120:A:ARG:H	22	0.1
(1,259)	1:66:A:LEU:HG	1:67:A:GLY:H	3	0.1
(1,259)	1:66:A:LEU:HG	1:67:A:GLY:H	20	0.1
(1,233)	1:64:A:ARG:HB2	1:132:A:THR:HB	13	0.1

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

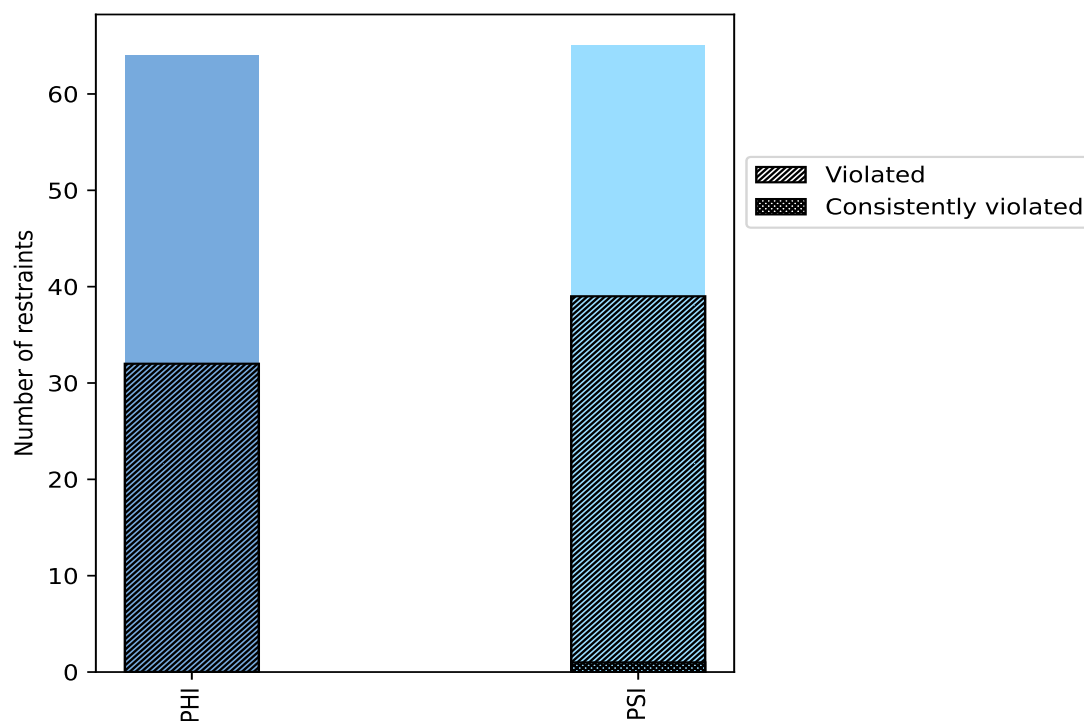
10.1 Summary of dihedral-angle violations [i](#)

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
PHI	64	49.6	32	50.0	24.8	0	0.0	0.0
PSI	65	50.4	39	60.0	30.2	1	1.5	0.8
Total	129	100.0	71	55.0	55.0	1	0.8	0.8

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](#)



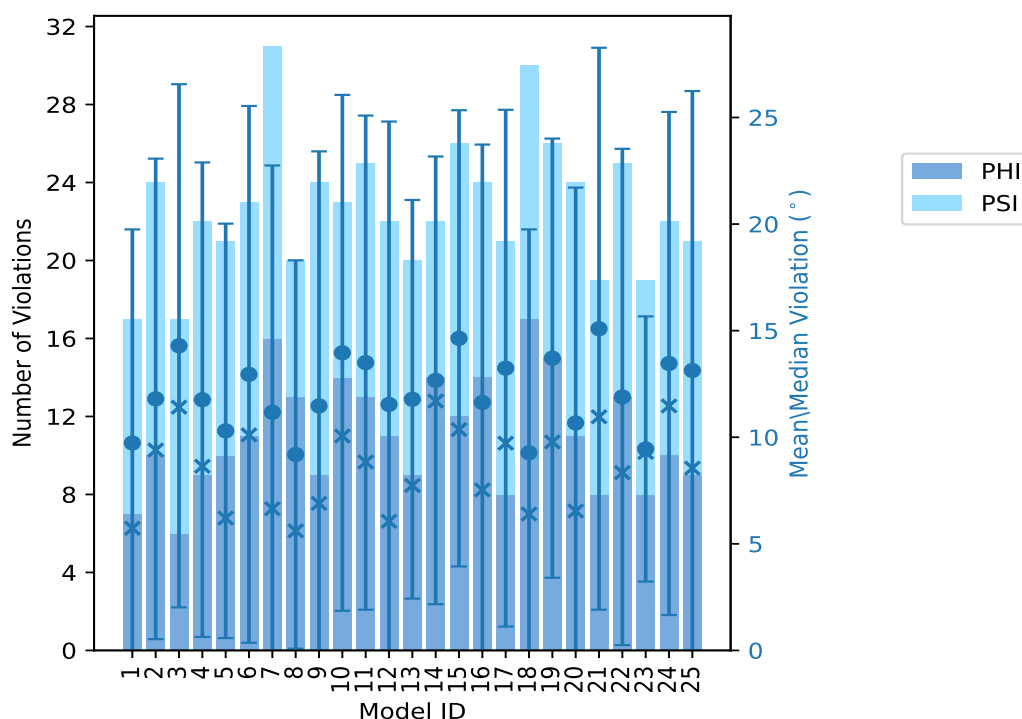
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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 (°)
	PHI	PSI	Total				
1	7	10	17	9.73	39.7	10.02	5.73
2	10	14	24	11.8	54.42	11.27	9.4
3	6	11	17	14.29	41.15	12.27	11.41
4	9	13	22	11.76	43.51	11.13	8.64
5	10	11	21	10.3	34.35	9.72	6.21
6	11	12	23	12.95	55.28	12.59	10.11
7	16	15	31	11.17	54.47	11.58	6.65
8	13	7	20	9.19	33.08	9.11	5.61
9	9	15	24	11.47	54.07	11.94	6.9
10	14	9	23	13.96	54.69	12.1	10.06
11	13	12	25	13.5	48.67	11.59	8.84
12	11	11	22	11.54	51.49	13.27	6.06
13	9	11	20	11.78	37.65	9.35	7.74
14	14	8	22	12.67	40.48	10.5	11.7
15	12	14	26	14.64	36.73	10.7	10.36
16	14	10	24	11.63	43.84	12.1	7.53
17	8	13	21	13.24	54.58	12.12	9.72
18	17	13	30	9.27	53.2	10.48	6.4
19	15	11	26	13.71	40.44	10.3	9.78
20	11	13	24	10.67	44.4	11.04	6.54
21	8	11	19	15.09	53.84	13.18	10.96
22	13	12	25	11.89	50.38	11.64	8.34
23	8	11	19	9.45	24.44	6.22	9.29
24	10	12	22	13.46	54.65	11.8	11.47
25	9	12	21	13.13	53.96	13.11	8.55

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
3	6	9	1	4.0
4	6	10	2	8.0
0	7	7	3	12.0
5	2	7	4	16.0
4	2	6	5	20.0
4	2	6	6	24.0
0	0	0	7	28.0
2	1	3	8	32.0
0	1	1	9	36.0
0	0	0	10	40.0
0	0	0	11	44.0

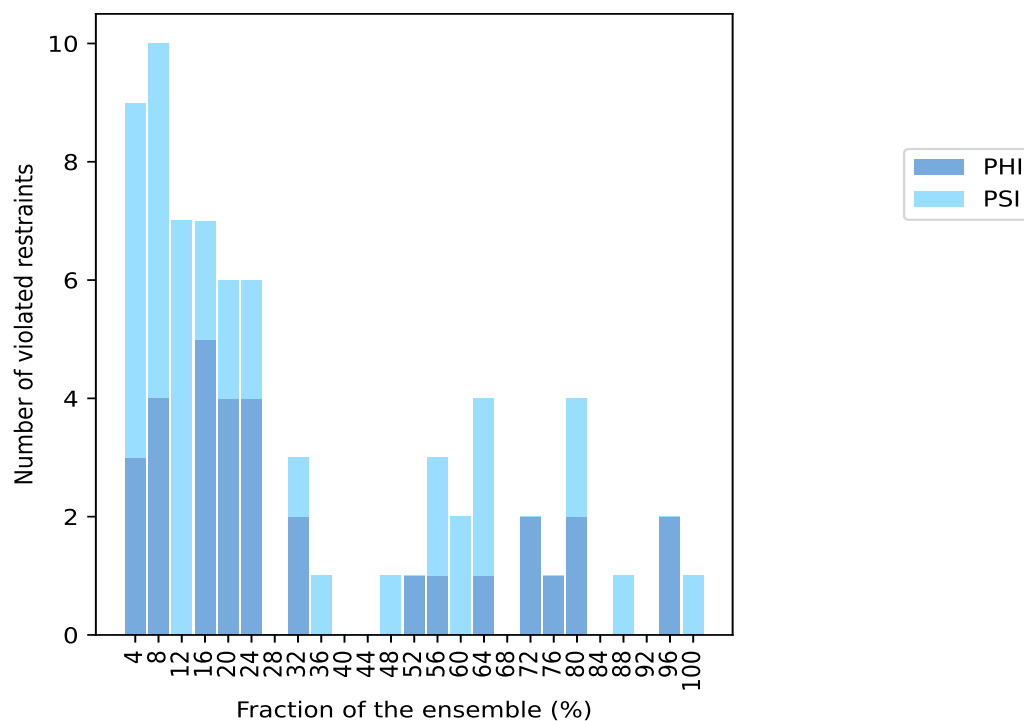
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	1	1	12	48.0
1	0	1	13	52.0
1	2	3	14	56.0
0	2	2	15	60.0
1	3	4	16	64.0
0	0	0	17	68.0
2	0	2	18	72.0
1	0	1	19	76.0
2	2	4	20	80.0
0	0	0	21	84.0
0	1	1	22	88.0
0	0	0	23	92.0
2	0	2	24	96.0
0	1	1	25	100.0

¹ Number of models with violations

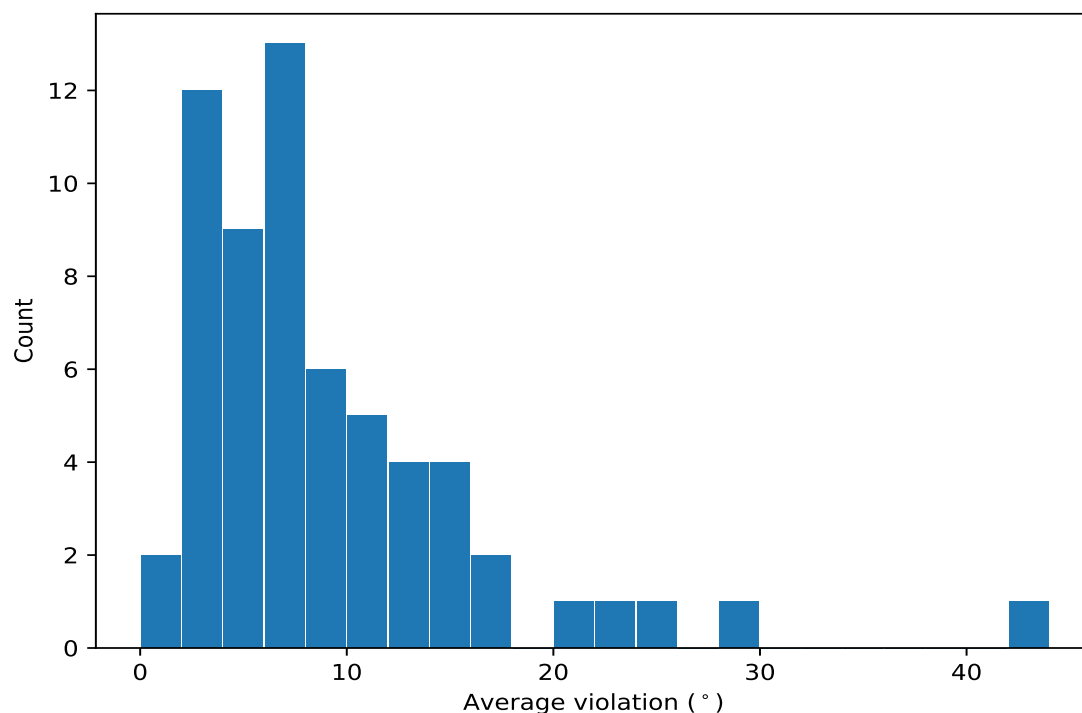
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble [i](#)



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
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	25	42.81	13.13	48.67
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	24	21.78	8.81	22.17
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	24	15.2	7.16	18.24
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	22	9.91	6.11	10.38
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	20	29.84	5.12	31.37
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	20	14.59	9.41	11.83
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	20	12.97	6.41	13.73
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	20	7.41	4.25	7.46
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	19	6.72	4.52	6.12
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	18	10.99	6.43	11.24
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	18	8.02	4.61	6.9
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	16	11.41	4.21	10.54
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	16	9.57	5.03	10.52

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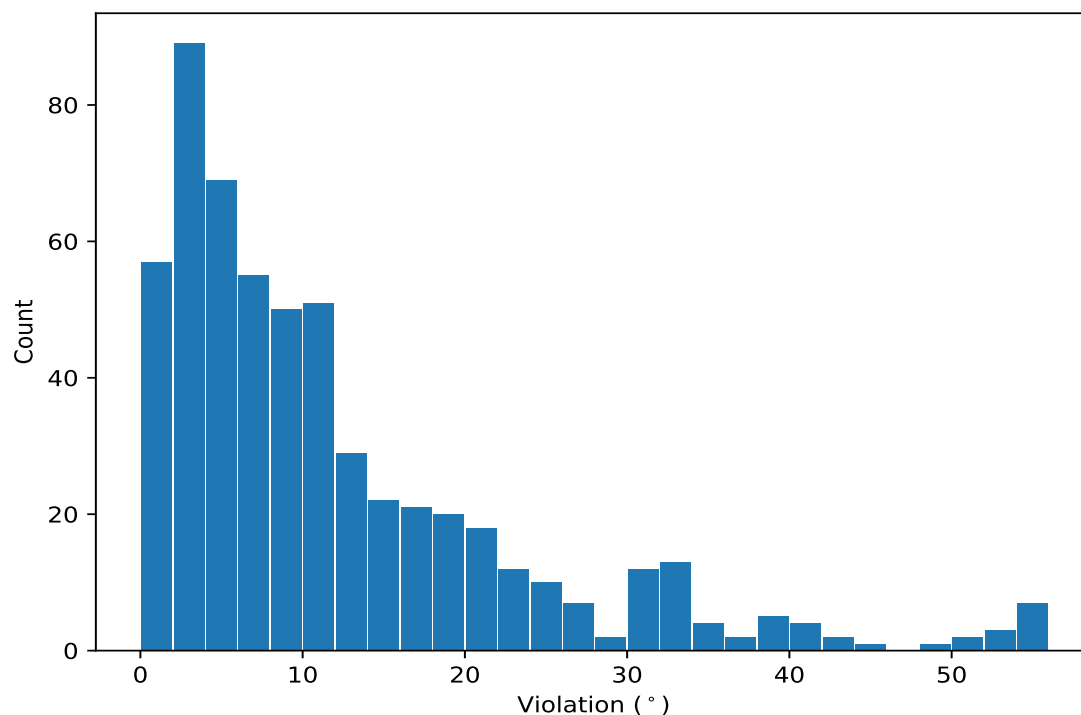
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	16	4.28	2.11	3.46
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	16	3.1	2.0	2.34
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	15	10.2	7.68	6.89
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	15	5.04	2.52	4.72
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	14	24.22	9.74	24.26
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	14	23.41	13.7	21.2
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	14	12.27	6.1	13.88
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	13	7.57	2.37	7.68
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	12	3.97	2.99	2.88
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	9	8.04	5.35	8.34
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	8	9.91	6.9	8.88
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	8	6.36	3.85	5.8
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	8	3.94	2.59	2.51
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	6	16.77	15.75	10.4
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	6	6.51	4.73	4.72
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	6	6.35	4.88	4.11
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	6	6.25	2.85	6.92
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	6	5.18	1.97	4.43
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	6	4.47	3.0	4.1
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	5	15.99	13.22	8.14
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	5	11.32	3.76	11.54
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	5	10.47	5.29	9.06
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	5	7.14	2.65	6.6
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	5	5.1	3.14	4.85
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	5	2.47	1.03	2.59
(1,96)	1:110:A:GLU:C	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	4	16.61	9.62	15.69
(1,45)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:SER:N	4	12.55	3.3	12.6
(1,10)	1:52:A:TYR:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	4	9.3	2.62	9.88
(1,108)	1:122:A:ALA:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	4	6.9	2.97	7.39
(1,24)	1:63:A:PHE:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	4	5.44	1.83	4.56
(1,77)	1:95:A:ASN:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	4	3.23	1.8	2.52
(1,35)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLY:N	4	2.94	1.77	2.55
(1,43)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:ALA:N	3	13.19	6.33	8.97
(1,25)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:ASP:N	3	6.05	2.58	5.72
(1,41)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	3	4.85	4.47	2.0
(1,105)	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	1:122:A:ALA:N	3	4.27	1.88	5.23
(1,76)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:96:A:ALA:N	3	2.72	1.63	2.09
(1,37)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	3	2.71	1.08	2.63
(1,64)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LYS:N	3	1.45	0.2	1.56
(1,101)	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	1:114:A:GLY:N	2	14.68	5.56	14.68
(1,123)	1:130:A:ASN:N	1:130:A:ASN:CA	1:130:A:ASN:C	1:131:A:ILE:N	2	7.74	5.79	7.74
(1,32)	1:68:A:GLU:C	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	2	7.56	2.62	7.56
(1,27)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:LEU:N	2	6.54	0.91	6.54
(1,97)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:THR:N	2	5.16	2.41	5.16
(1,104)	1:120:A:ARG:C	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	2	2.9	0.55	2.9
(1,1)	1:48:A:PRO:N	1:48:A:PRO:CA	1:48:A:PRO:C	1:49:A:VAL:N	2	2.89	0.56	2.89
(1,16)	1:56:A:GLU:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	2	2.82	1.5	2.82
(1,14)	1:55:A:ALA:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	2	2.62	0.07	2.62
(1,88)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:LEU:N	2	1.38	0.25	1.38

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 (°)
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	6	55.28
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	10	54.69
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	24	54.65
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	17	54.58
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	7	54.47
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	2	54.42
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	9	54.07
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	25	53.96
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	21	53.84
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	18	53.2
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	12	51.49
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	22	50.38
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	11	48.67
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	20	44.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	16	43.84
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	4	43.51
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	3	41.15
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	20	41.06
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	14	40.48
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	19	40.44
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	11	39.97
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	16	39.95
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	1	39.7
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	12	39.58
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	3	39.31
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	13	37.65
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	15	36.73
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	16	35.95
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	6	35.57
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	21	34.81
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	5	34.35
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	12	33.63
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	4	33.45
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	9	33.42
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	25	33.28
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	15	33.15
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	8	33.08
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	21	33.0
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	22	32.79
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	15	32.68
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	15	32.53
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	7	32.28
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	14	32.26
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	25	32.01
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	11	31.92
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	10	31.39
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	24	31.35
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	14	31.33
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	18	30.93
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	19	30.73
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	4	30.71
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	15	30.51
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	5	30.46
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	8	30.25
(1,96)	1:110:A:GLU:C	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	10	30.22
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	16	30.04
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	19	29.44
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	17	28.56
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	7	27.85
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	2	27.78
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	11	27.69
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	3	27.69
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	10	27.63
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	6	27.48
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	22	26.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	13	25.94
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	17	25.9
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	2	25.86
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	14	25.58
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	22	25.4
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	25	25.35
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	24	25.0
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	7	24.54
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	23	24.44
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	12	24.17
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	17	23.99
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1	23.8
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	25	23.28
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	19	23.21
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	6	23.1
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	13	23.05
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	19	23.01
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	24	22.55
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	3	22.4
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	5	22.36
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	20	22.27
(1,43)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:ALA:N	13	22.14
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	19	21.96
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	9	21.95
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	3	21.93
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	13	21.92
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	7	21.8
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	21	21.65
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	15	21.01
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	4	20.93
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	19	20.76
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	22	20.72
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	19	20.61
(1,96)	1:110:A:GLU:C	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	7	20.46
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	9	20.4
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	9	20.38
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	15	20.33
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	15	20.29
(1,101)	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	1:114:A:GLY:N	23	20.24
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	18	20.18
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	21	19.97
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	19	19.91
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	22	19.86
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	11	19.83
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	5	19.61
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	19	19.47
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	2	19.36
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	10	19.19
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	10	19.17
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	3	19.07
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	11	19.03

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	17	18.96
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	8	18.77
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	20	18.59
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	18	18.57
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	7	18.35
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	1	18.31
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	6	18.13
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	15	18.02
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	11	18.0
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	15	17.98
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	9	17.96
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	23	17.93
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	17	17.78
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	1	17.74
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	15	17.72
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	21	17.71
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	13	17.63
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	18	17.58
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	5	17.48
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	21	17.47
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	4	17.24
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	6	17.15
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	7	17.12
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	24	17.06
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	8	16.94
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	21	16.79
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	5	16.76
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	5	16.32
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	2	16.23
(1,45)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:SER:N	19	16.16
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	10	15.94
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	6	15.94
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	14	15.74
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	2	15.58
(1,45)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:SER:N	24	15.49
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	22	15.38
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	24	15.22
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	20	15.22
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	21	15.2
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	10	15.14
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	2	15.05
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	17	14.95
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	25	14.93
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	4	14.71
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	22	14.64
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	24	14.58
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	14	14.45
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	19	14.44
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	9	14.29
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	7	14.14
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	12	14.12

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	24	14.04
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	24	13.97
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	14	13.84
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	6	13.73
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	25	13.7
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	7	13.57
(1,123)	1:130:A:ASN:N	1:130:A:ASN:CA	1:130:A:ASN:C	1:131:A:ILE:N	6	13.53
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	1	13.5
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	12	13.49
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	17	13.37
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	23	13.35
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	4	13.32
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	7	13.31
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	16	13.28
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	10	13.18
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	20	13.16
(1,11)	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	1:54:A:ASN:N	8	13.09
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	11	13.05
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	14	13.04
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	8	13.0
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	14	12.99
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	17	12.96
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	10	12.95
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	3	12.8
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	4	12.73
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	6	12.65
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	15	12.44
(1,10)	1:52:A:TYR:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	14	12.29
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	18	12.2
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	1	12.11
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	20	11.97
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	14	11.86
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	10	11.78
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	24	11.77
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	2	11.69
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	9	11.67
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	3	11.63
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	23	11.56
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	14	11.55
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	17	11.54
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	11	11.42
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	3	11.41
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	7	11.4
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	22	11.18
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	23	11.18
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	24	11.17
(1,41)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	22	11.16
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	4	11.05
(1,29)	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	1:68:A:GLU:N	23	11.03
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	5	11.01
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	12	11.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	21	10.96
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	23	10.92
(1,96)	1:110:A:GLU:C	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	18	10.92
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	13	10.92
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	2	10.87
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	9	10.87
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	25	10.77
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	2	10.72
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	16	10.7
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	18	10.64
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	20	10.61
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	25	10.52
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	15	10.52
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	6	10.5
(1,10)	1:52:A:TYR:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	16	10.48
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	4	10.45
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	9	10.42
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	18	10.27
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	22	10.21
(1,119)	1:128:A:ALA:N	1:128:A:ALA:CA	1:128:A:ALA:C	1:129:A:LEU:N	15	10.2
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	22	10.2
(1,32)	1:68:A:GLU:C	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	3	10.18
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	20	10.11
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	6	10.11
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	20	10.07
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	10	10.06
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	2	10.05
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	19	10.03
(1,108)	1:122:A:ALA:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	8	10.02
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	23	10.01
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	7	9.96
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	11	9.95
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	21	9.8
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	17	9.72
(1,45)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:SER:N	25	9.72
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	10	9.66
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	16	9.58
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	2	9.54
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	19	9.53
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	3	9.47
(1,108)	1:122:A:ALA:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	11	9.4
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	24	9.38
(1,25)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:ASP:N	6	9.37
(1,10)	1:52:A:TYR:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	23	9.29
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	2	9.26
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	16	9.23
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	8	9.21
(1,101)	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	1:114:A:GLY:N	4	9.11
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	19	9.11
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	19	9.06
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	11	8.98

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:ALA:N	15	8.97
(1,45)	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	1:77:A:SER:N	11	8.84
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	13	8.83
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	19	8.79
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	16	8.79
(1,99)	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	1:113:A:SER:N	13	8.76
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	23	8.75
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	16	8.72
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	21	8.67
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	12	8.63
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	15	8.61
(1,24)	1:63:A:PHE:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	25	8.55
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	14	8.54
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	9	8.46
(1,43)	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1:76:A:ALA:N	24	8.45
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	18	8.42
(1,127)	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	1:133:A:ALA:N	23	8.39
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	6	8.39
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	15	8.36
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	22	8.34
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	12	8.33
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	18	8.23
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	10	8.23
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	18	8.21
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	5	8.19
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	4	8.17
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	25	8.14
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	15	8.12
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	24	8.1
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	21	7.87
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	13	7.85
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	16	7.77
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	6	7.7
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	18	7.68
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	10	7.67
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	17	7.67
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	13	7.64
(1,97)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:THR:N	5	7.57
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	11	7.48
(1,27)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:LEU:N	4	7.44
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	1	7.42
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	11	7.29
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	16	7.29
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	20	7.25
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	17	7.2
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	15	7.17
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	13	7.12
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	11	7.04
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	9	6.98
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	11	6.89
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	7	6.85

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	15	6.85
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	9	6.83
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	9	6.82
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	11	6.82
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	2	6.77
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	18	6.76
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	7	6.71
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	8	6.66
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	7	6.65
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	2	6.63
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	20	6.61
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	2	6.61
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	11	6.6
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	12	6.59
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	18	6.58
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	25	6.49
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	20	6.48
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	14	6.47
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	16	6.47
(1,46)	1:76:A:ALA:C	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	10	6.4
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	1	6.36
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	12	6.34
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	10	6.3
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	22	6.25
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	10	6.21
(1,77)	1:95:A:ASN:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	18	6.21
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	5	6.21
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	9	6.21
(1,106)	1:121:A:GLN:C	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	13	6.17
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	23	6.15
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	16	6.12
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	9	6.08
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	7	6.07
(1,105)	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	1:122:A:ALA:N	17	5.93
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	16	5.85
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	22	5.85
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	12	5.78
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	1	5.73
(1,28)	1:66:A:LEU:C	1:67:A:GLY:N	1:67:A:GLY:CA	1:67:A:GLY:C	8	5.73
(1,25)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:ASP:N	22	5.72
(1,27)	1:65:A:ASP:N	1:65:A:ASP:CA	1:65:A:ASP:C	1:66:A:LEU:N	17	5.63
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	2	5.6
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	17	5.54
(1,35)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLY:N	3	5.51
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	25	5.49
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	8	5.49
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	16	5.48
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	24	5.46
(1,108)	1:122:A:ALA:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	7	5.38
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	20	5.37
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	12	5.29

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	7	5.25
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	18	5.25
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	13	5.24
(1,105)	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	1:122:A:ALA:N	21	5.23
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	20	5.22
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	18	5.22
(1,10)	1:52:A:TYR:C	1:53:A:THR:N	1:53:A:THR:CA	1:53:A:THR:C	11	5.16
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	14	5.15
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	11	5.03
(1,24)	1:63:A:PHE:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	21	4.99
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	10	4.99
(1,76)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:96:A:ALA:N	18	4.95
(1,98)	1:111:A:VAL:C	1:112:A:THR:N	1:112:A:THR:CA	1:112:A:THR:C	13	4.94
(1,32)	1:68:A:GLU:C	1:69:A:VAL:N	1:69:A:VAL:CA	1:69:A:VAL:C	13	4.94
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	13	4.92
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	11	4.92
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	23	4.91
(1,96)	1:110:A:GLU:C	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	4	4.86
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	13	4.85
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	20	4.82
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	19	4.79
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	11	4.76
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	6	4.72
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	4	4.7
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	19	4.64
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1	4.61
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	14	4.59
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	20	4.57
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	19	4.54
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	11	4.53
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	8	4.44
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	7	4.36
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	14	4.34
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	5	4.33
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	25	4.33
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	19	4.33
(1,16)	1:56:A:GLU:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	14	4.32
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	17	4.31
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	1	4.28
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	20	4.26
(1,2)	1:48:A:PRO:C	1:49:A:VAL:N	1:49:A:VAL:CA	1:49:A:VAL:C	7	4.21
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	19	4.2
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	11	4.19
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	15	4.14
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	5	4.12
(1,24)	1:63:A:PHE:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	22	4.12
(1,24)	1:63:A:PHE:C	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	2	4.09
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	7	4.07
(1,37)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	22	4.07
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	8	4.03
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	8	4.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	2	3.95
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	5	3.93
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	10	3.93
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	12	3.92
(1,72)	1:93:A:GLN:N	1:93:A:GLN:CA	1:93:A:GLN:C	1:94:A:ILE:N	9	3.92
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	3	3.92
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	4	3.92
(1,95)	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	1:111:A:VAL:N	2	3.84
(1,48)	1:77:A:SER:C	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	17	3.77
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	12	3.71
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	16	3.71
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	24	3.66
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	24	3.65
(1,35)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLY:N	22	3.64
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	12	3.6
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	15	3.6
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	24	3.55
(1,44)	1:75:A:GLN:C	1:76:A:ALA:N	1:76:A:ALA:CA	1:76:A:ALA:C	12	3.48
(1,104)	1:120:A:ARG:C	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	16	3.45
(1,40)	1:73:A:SER:C	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	15	3.45
(1,1)	1:48:A:PRO:N	1:48:A:PRO:CA	1:48:A:PRO:C	1:49:A:VAL:N	18	3.45
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	13	3.4
(1,102)	1:119:A:TYR:C	1:120:A:ARG:N	1:120:A:ARG:CA	1:120:A:ARG:C	15	3.37
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	7	3.36
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	2	3.3
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	10	3.28
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	7	3.28
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	14	3.27
(1,8)	1:51:A:ILE:C	1:52:A:TYR:N	1:52:A:TYR:CA	1:52:A:TYR:C	9	3.24
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	5	3.21
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	6	3.21
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	12	3.18
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	16	3.14
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	4	3.13
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	23	3.13
(1,77)	1:95:A:ASN:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	20	3.1
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	9	3.09
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	7	3.09
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	1	3.08
(1,25)	1:64:A:ARG:N	1:64:A:ARG:CA	1:64:A:ARG:C	1:65:A:ASP:N	24	3.07
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	25	3.06
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	23	2.95
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	20	2.88
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	15	2.83
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	25	2.81
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	18	2.81
(1,51)	1:79:A:GLN:N	1:79:A:GLN:CA	1:79:A:GLN:C	1:80:A:ASP:N	12	2.79
(1,108)	1:122:A:ALA:C	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	18	2.78
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	5	2.76
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	14	2.76
(1,97)	1:111:A:VAL:N	1:111:A:VAL:CA	1:111:A:VAL:C	1:112:A:THR:N	25	2.75

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	18	2.74
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	20	2.72
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	20	2.68
(1,14)	1:55:A:ALA:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	18	2.68
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	2	2.66
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	16	2.65
(1,37)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	21	2.63
(1,49)	1:78:A:ASN:N	1:78:A:ASN:CA	1:78:A:ASN:C	1:79:A:GLN:N	19	2.62
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	8	2.6
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	5	2.6
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	21	2.6
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	6	2.59
(1,100)	1:112:A:THR:C	1:113:A:SER:N	1:113:A:SER:CA	1:113:A:SER:C	16	2.56
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	14	2.55
(1,14)	1:55:A:ALA:C	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	25	2.55
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	6	2.54
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	18	2.51
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	17	2.49
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	18	2.49
(1,104)	1:120:A:ARG:C	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	4	2.36
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	21	2.36
(1,1)	1:48:A:PRO:N	1:48:A:PRO:CA	1:48:A:PRO:C	1:49:A:VAL:N	3	2.33
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	25	2.31
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	23	2.27
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	22	2.26
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	2	2.14
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	9	2.14
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	4	2.1
(1,94)	1:109:A:CYS:C	1:110:A:GLU:N	1:110:A:GLU:CA	1:110:A:GLU:C	1	2.09
(1,76)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:96:A:ALA:N	16	2.09
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	22	2.07
(1,23)	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	1:64:A:ARG:N	4	2.07
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	6	2.06
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	19	2.02
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	22	2.02
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	24	2.01
(1,42)	1:74:A:CYS:C	1:75:A:GLN:N	1:75:A:GLN:CA	1:75:A:GLN:C	1	2.0
(1,41)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	9	2.0
(1,123)	1:130:A:ASN:N	1:130:A:ASN:CA	1:130:A:ASN:C	1:131:A:ILE:N	1	1.95
(1,77)	1:95:A:ASN:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	16	1.93
(1,36)	1:71:A:GLY:C	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	22	1.88
(1,21)	1:59:A:VAL:N	1:59:A:VAL:CA	1:59:A:VAL:C	1:60:A:GLY:N	24	1.87
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	17	1.85
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	18	1.83
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	25	1.81
(1,38)	1:72:A:ASP:C	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	18	1.78
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	7	1.76
(1,77)	1:95:A:ASN:C	1:96:A:ALA:N	1:96:A:ALA:CA	1:96:A:ALA:C	8	1.68
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	18	1.68
(1,39)	1:73:A:SER:N	1:73:A:SER:CA	1:73:A:SER:C	1:74:A:CYS:N	23	1.65
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	12	1.65

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,105)	1:121:A:GLN:N	1:121:A:GLN:CA	1:121:A:GLN:C	1:122:A:ALA:N	20	1.64
(1,111)	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	1:125:A:ILE:N	3	1.63
(1,64)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LYS:N	19	1.63
(1,58)	1:86:A:PRO:N	1:86:A:PRO:CA	1:86:A:PRO:C	1:87:A:THR:N	12	1.63
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	13	1.63
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	22	1.62
(1,88)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:LEU:N	1	1.62
(1,22)	1:62:A:PRO:C	1:63:A:PHE:N	1:63:A:PHE:CA	1:63:A:PHE:C	5	1.6
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	10	1.59
(1,64)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LYS:N	6	1.56
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	4	1.55
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	9	1.52
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	10	1.52
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	3	1.47
(1,35)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLY:N	12	1.46
(1,85)	1:103:A:ALA:C	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	18	1.44
(1,37)	1:72:A:ASP:N	1:72:A:ASP:CA	1:72:A:ASP:C	1:73:A:SER:N	9	1.43
(1,129)	1:133:A:ALA:N	1:133:A:ALA:CA	1:133:A:ALA:C	1:134:A:LYS:N	17	1.42
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	7	1.39
(1,41)	1:74:A:CYS:N	1:74:A:CYS:CA	1:74:A:CYS:C	1:75:A:GLN:N	5	1.39
(1,114)	1:125:A:ILE:C	1:126:A:GLY:N	1:126:A:GLY:CA	1:126:A:GLY:C	7	1.34
(1,110)	1:123:A:VAL:C	1:124:A:CYS:N	1:124:A:CYS:CA	1:124:A:CYS:C	8	1.34
(1,126)	1:131:A:ILE:C	1:132:A:THR:N	1:132:A:THR:CA	1:132:A:THR:C	22	1.33
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	6	1.33
(1,92)	1:108:A:SER:C	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	23	1.31
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	4	1.31
(1,16)	1:56:A:GLU:C	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	8	1.31
(1,109)	1:123:A:VAL:N	1:123:A:VAL:CA	1:123:A:VAL:C	1:124:A:CYS:N	9	1.24
(1,93)	1:109:A:CYS:N	1:109:A:CYS:CA	1:109:A:CYS:C	1:110:A:GLU:N	14	1.24
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	6	1.23
(1,59)	1:86:A:PRO:C	1:87:A:THR:N	1:87:A:THR:CA	1:87:A:THR:C	2	1.21
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	15	1.19
(1,64)	1:89:A:ARG:N	1:89:A:ARG:CA	1:89:A:ARG:C	1:90:A:LYS:N	7	1.17
(1,53)	1:80:A:ASP:N	1:80:A:ASP:CA	1:80:A:ASP:C	1:81:A:SER:N	19	1.15
(1,35)	1:70:A:SER:N	1:70:A:SER:CA	1:70:A:SER:C	1:71:A:GLY:N	21	1.15
(1,15)	1:56:A:GLU:N	1:56:A:GLU:CA	1:56:A:GLU:C	1:57:A:GLU:N	8	1.14
(1,88)	1:105:A:LEU:N	1:105:A:LEU:CA	1:105:A:LEU:C	1:106:A:LEU:N	7	1.13
(1,76)	1:95:A:ASN:N	1:95:A:ASN:CA	1:95:A:ASN:C	1:96:A:ALA:N	8	1.11
(1,86)	1:104:A:VAL:N	1:104:A:VAL:CA	1:104:A:VAL:C	1:105:A:LEU:N	1	1.09
(1,30)	1:67:A:GLY:C	1:68:A:GLU:N	1:68:A:GLU:CA	1:68:A:GLU:C	5	1.07
(1,47)	1:77:A:SER:N	1:77:A:SER:CA	1:77:A:SER:C	1:78:A:ASN:N	3	1.06
(1,19)	1:58:A:LEU:N	1:58:A:LEU:CA	1:58:A:LEU:C	1:59:A:VAL:N	5	1.05
(1,17)	1:57:A:GLU:N	1:57:A:GLU:CA	1:57:A:GLU:C	1:58:A:LEU:N	7	1.05
(1,107)	1:122:A:ALA:N	1:122:A:ALA:CA	1:122:A:ALA:C	1:123:A:VAL:N	20	1.01