



Full wwPDB NMR Structure Validation Report ⓘ

Mar 21, 2026 – 03:36 PM UTC

PDB ID : 8FG1 / pdb_00008fg1
BMRB ID : 31064
Title : Human diaphanous inhibitory domain bound to diaphanous autoregulatory domain
Authors : Ramirez, L.M.S.; Theophall, G.; Premo, A.; Manigrasso, M.; Yepuri, G.; Burz, D.; Ramasamy, R.; Schmidt, A.M.; Shekhtman, A.
Deposited on : 2022-12-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

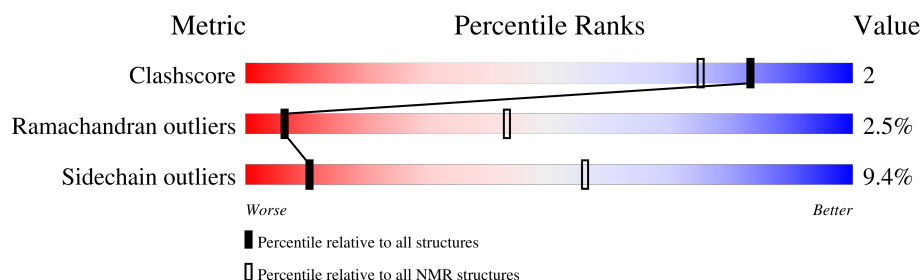
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 64%.

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	256	
2	B	29	

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:145-A:199, A:209-A:301, A:307-A:373, B:1196- B:1199, B:1120-B:1132 (232)	0.33	5

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

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

The models can be grouped into 3 clusters and 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4307 atoms, of which 2166 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms						Trace
1	A	243	Total	C	H	N	O	S	0
			3861	1196	1942	331	375	17	

There are 17 discrepancies between the modelled and reference sequences:

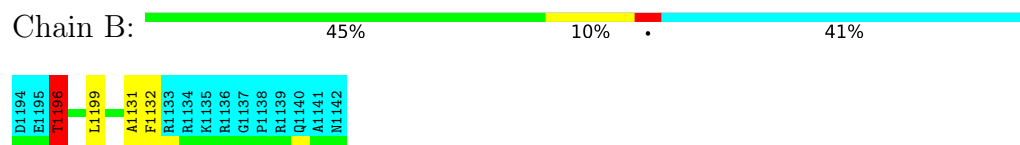
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	MET	-	initiating methionine	UNP O60610
A	126	GLY	-	expression tag	UNP O60610
A	127	SER	-	expression tag	UNP O60610
A	128	SER	-	expression tag	UNP O60610
A	129	GLU	-	expression tag	UNP O60610
A	130	ARG	-	expression tag	UNP O60610
A	131	SER	-	expression tag	UNP O60610
A	132	HIS	-	expression tag	UNP O60610
A	133	HIS	-	expression tag	UNP O60610
A	134	HIS	-	expression tag	UNP O60610
A	135	HIS	-	expression tag	UNP O60610
A	136	HIS	-	expression tag	UNP O60610
A	137	HIS	-	expression tag	UNP O60610
A	138	SER	-	expression tag	UNP O60610
A	139	GLY	-	expression tag	UNP O60610
A	140	SER	-	expression tag	UNP O60610
A	141	GLU	-	expression tag	UNP O60610

- Molecule 2 is a protein called Protein diaphanous homolog 1.

Mol	Chain	Residues	Atoms					Trace
2	B	29	Total	C	H	N	O	0
			446	133	224	45	44	

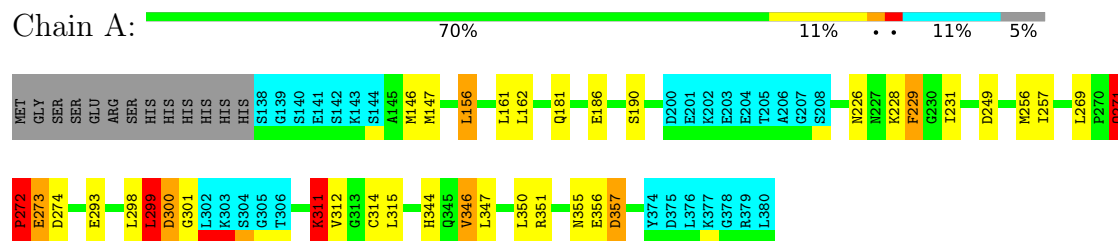
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1199	LEU	MET	engineered mutation	UNP O60610

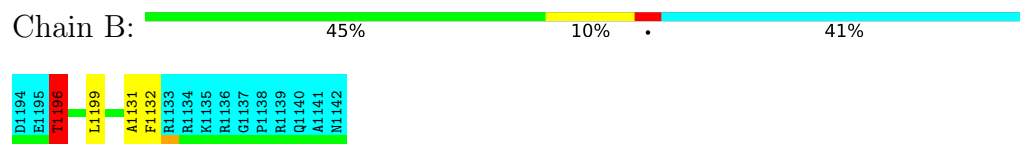


4.2.2 Score per residue for model 2

- Molecule 1: Protein diaphanous homolog 1

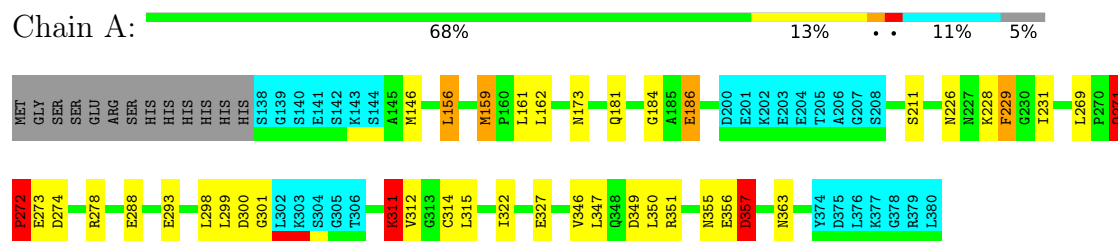


- Molecule 2: Protein diaphanous homolog 1

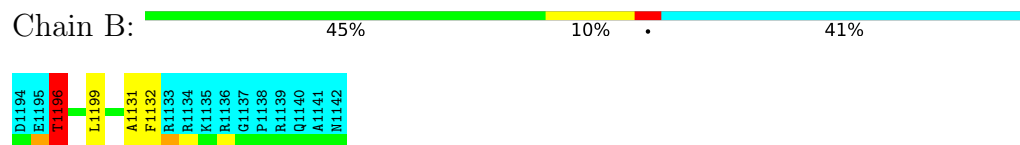


4.2.3 Score per residue for model 3

- Molecule 1: Protein diaphanous homolog 1

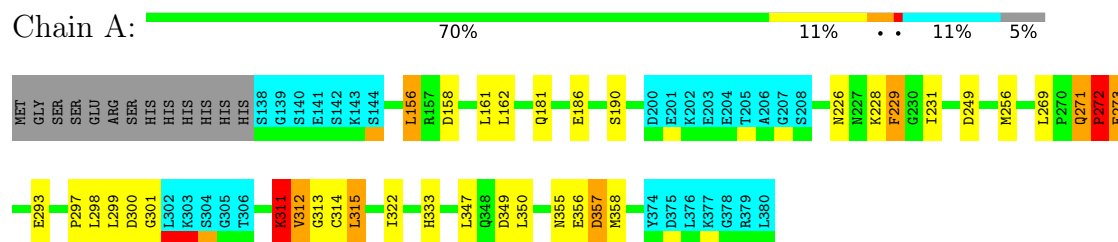


- Molecule 2: Protein diaphanous homolog 1

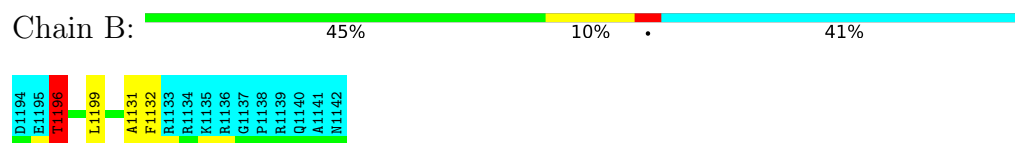


4.2.4 Score per residue for model 4

- Molecule 1: Protein diaphanous homolog 1

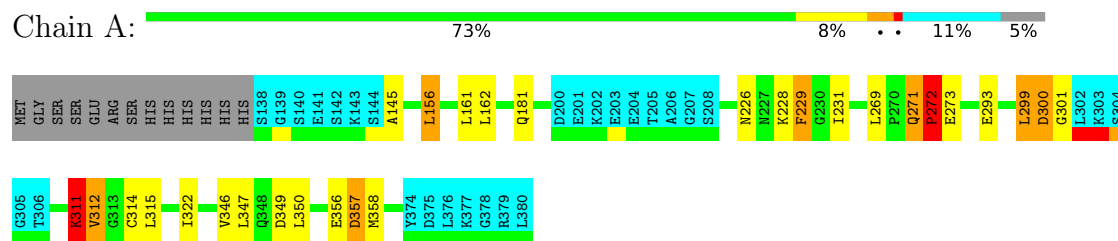


- Molecule 2: Protein diaphanous homolog 1

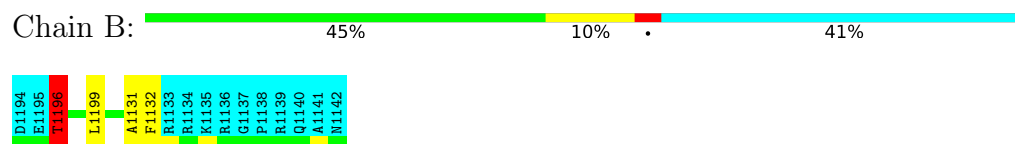


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Protein diaphanous homolog 1

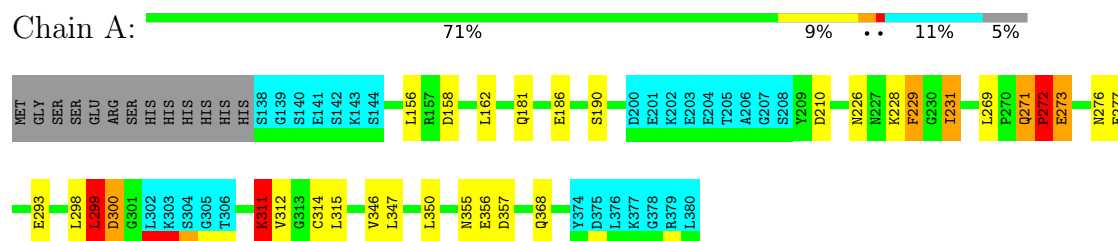


- Molecule 2: Protein diaphanous homolog 1

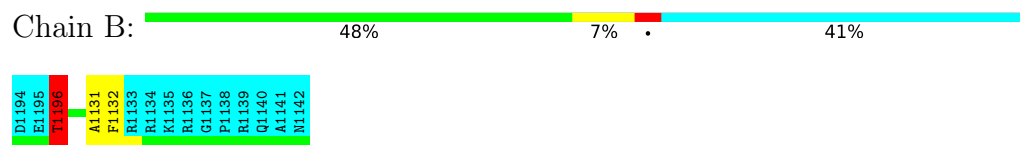


4.2.6 Score per residue for model 6

- Molecule 1: Protein diaphanous homolog 1

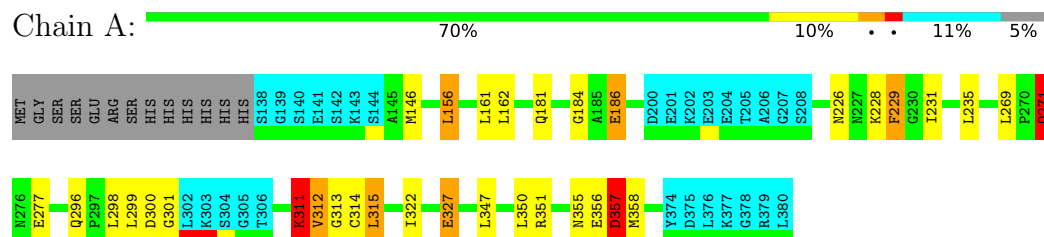


- Molecule 2: Protein diaphanous homolog 1

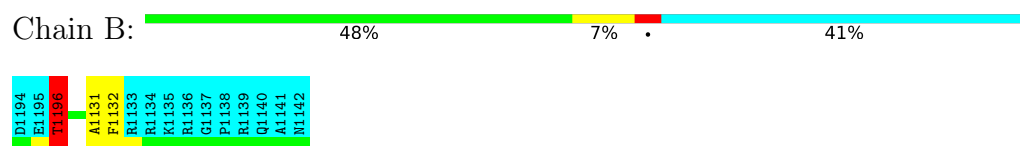


4.2.7 Score per residue for model 7

- Molecule 1: Protein diaphanous homolog 1

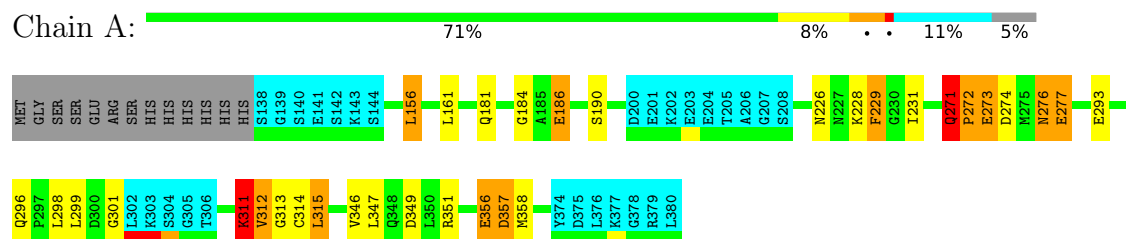


- Molecule 2: Protein diaphanous homolog 1

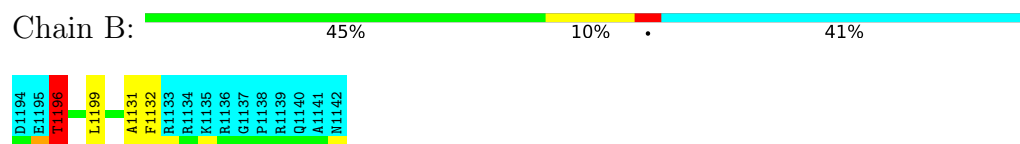


4.2.8 Score per residue for model 8

- Molecule 1: Protein diaphanous homolog 1



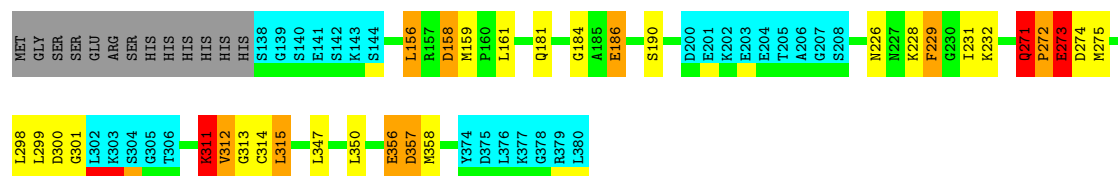
- Molecule 2: Protein diaphanous homolog 1



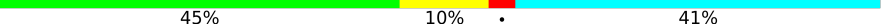
4.2.9 Score per residue for model 9

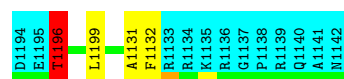
- Molecule 1: Protein diaphanous homolog 1

Chain A: 



- Molecule 2: Protein diaphanous homolog 1

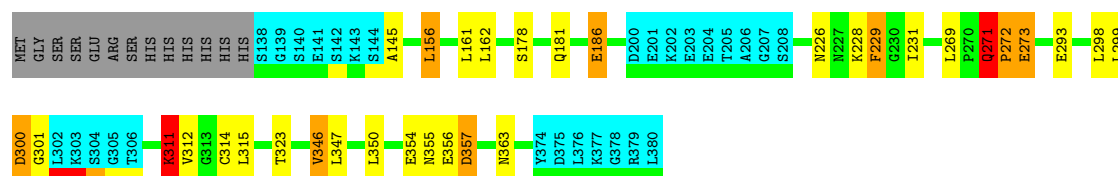
Chain B: 



4.2.10 Score per residue for model 10

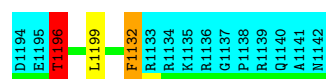
- Molecule 1: Protein diaphanous homolog 1

Chain A: 



- Molecule 2: Protein diaphanous homolog 1

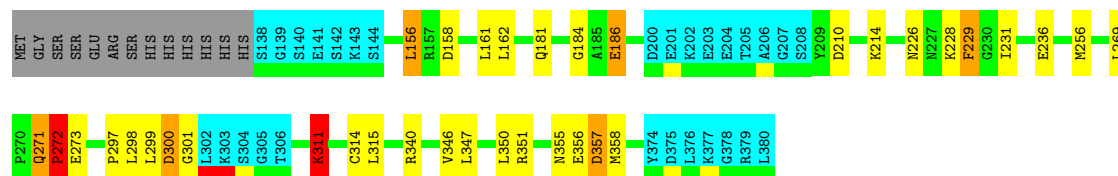
Chain B: 



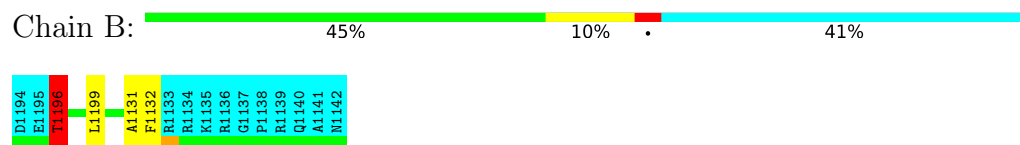
4.2.11 Score per residue for model 11

- Molecule 1: Protein diaphanous homolog 1

Chain A: 

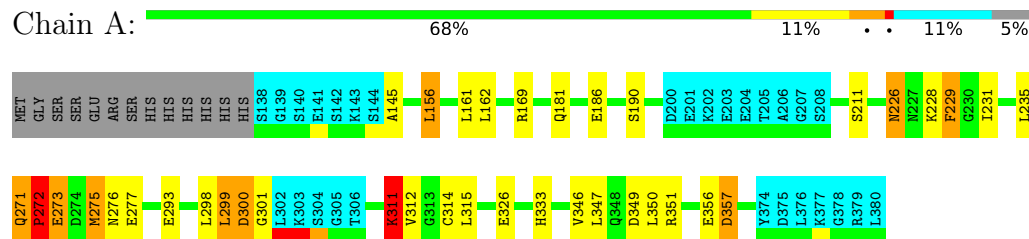


- Molecule 2: Protein diaphanous homolog 1

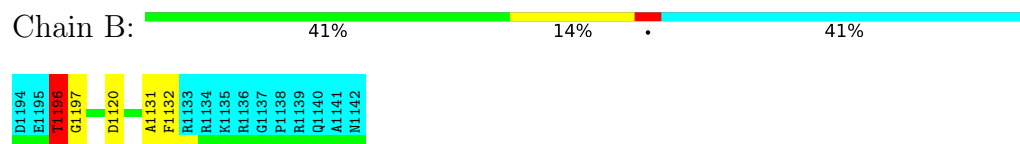


4.2.12 Score per residue for model 12

- Molecule 1: Protein diaphanous homolog 1

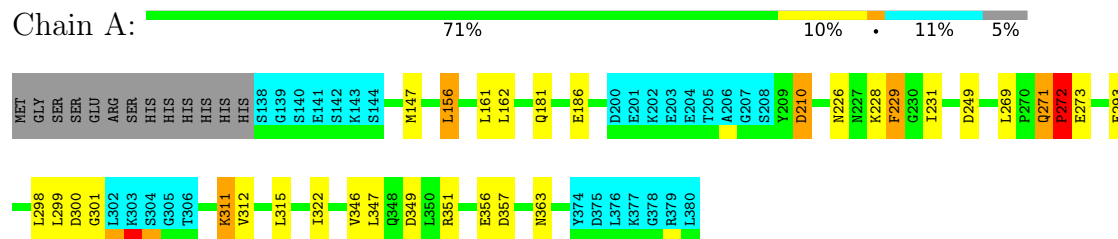


- Molecule 2: Protein diaphanous homolog 1

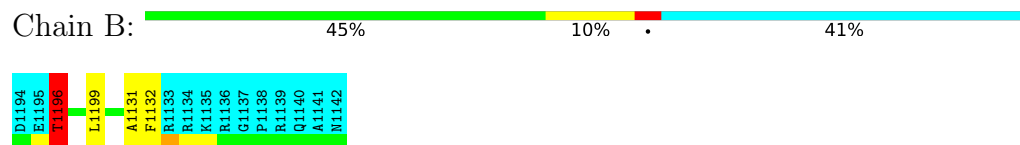


4.2.13 Score per residue for model 13

- Molecule 1: Protein diaphanous homolog 1

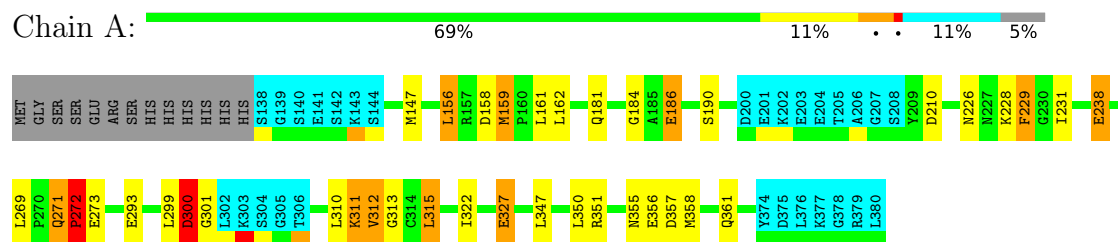


- Molecule 2: Protein diaphanous homolog 1

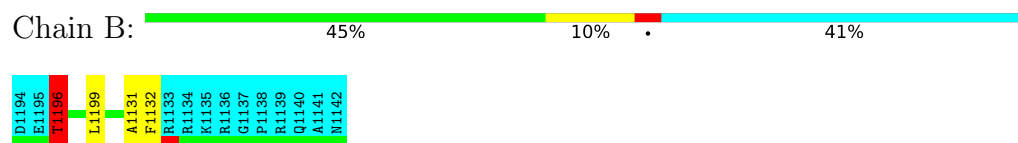


4.2.14 Score per residue for model 14

- Molecule 1: Protein diaphanous homolog 1

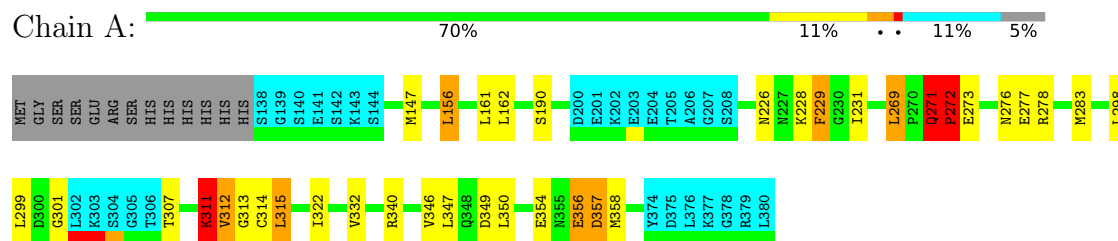


- Molecule 2: Protein diaphanous homolog 1

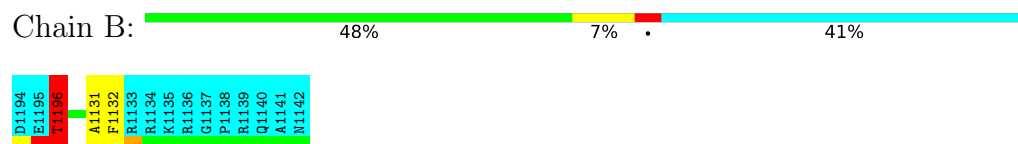


4.2.15 Score per residue for model 15

- Molecule 1: Protein diaphanous homolog 1

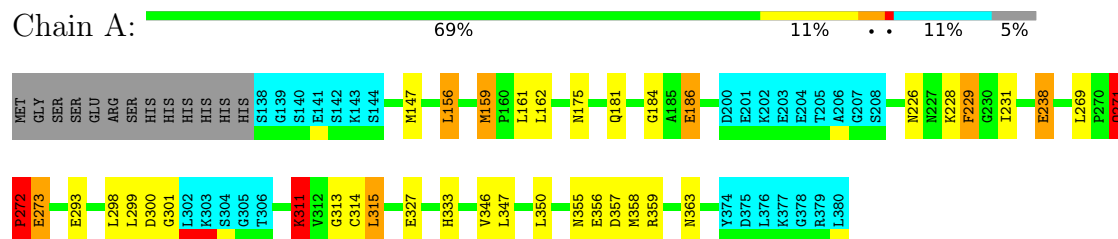


- Molecule 2: Protein diaphanous homolog 1

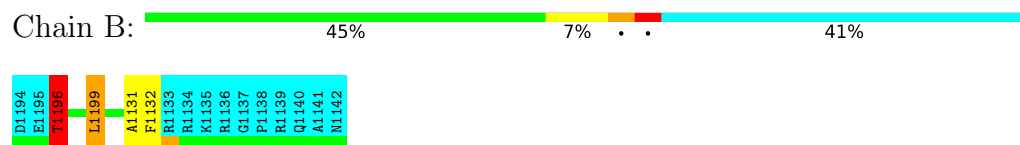


4.2.16 Score per residue for model 16

- Molecule 1: Protein diaphanous homolog 1

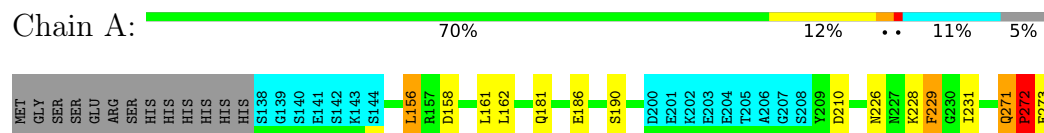


- Molecule 2: Protein diaphanous homolog 1

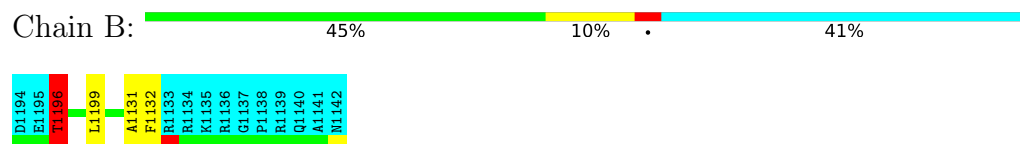


4.2.17 Score per residue for model 17

- Molecule 1: Protein diaphanous homolog 1

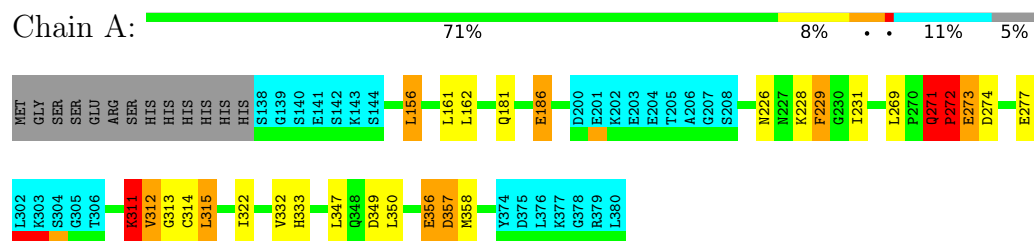


- Molecule 2: Protein diaphanous homolog 1



4.2.18 Score per residue for model 18

- Molecule 1: Protein diaphanous homolog 1



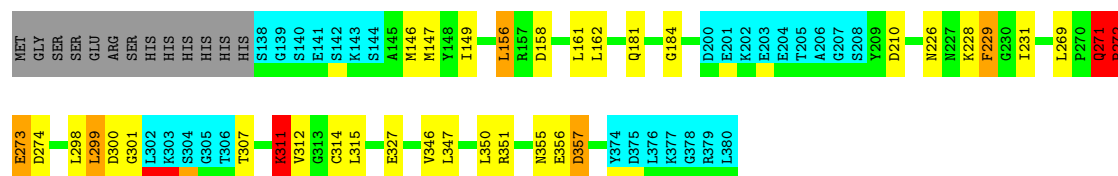
- Molecule 2: Protein diaphanous homolog 1



4.2.19 Score per residue for model 19

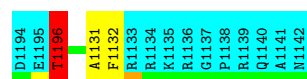
- Molecule 1: Protein diaphanous homolog 1

Chain A: 



- Molecule 2: Protein diaphanous homolog 1

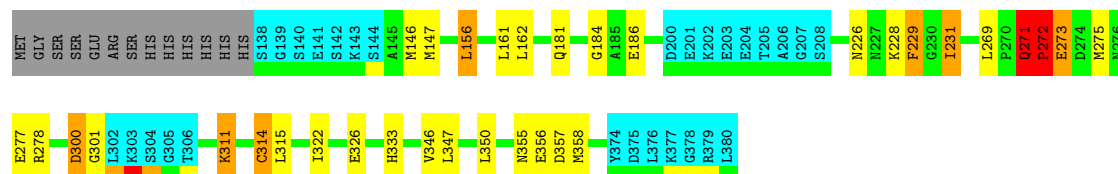
Chain B: 



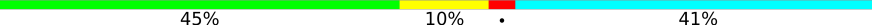
4.2.20 Score per residue for model 20

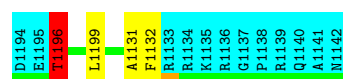
- Molecule 1: Protein diaphanous homolog 1

Chain A: 



- Molecule 2: Protein diaphanous homolog 1

Chain B: 



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure calculation	
YASARA	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	2422
Number of shifts mapped to atoms	2418
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	64%

6 Model quality

6.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.94±0.02	5±1/1734 (0.3± 0.1%)	1.21±0.09	16±2/2339 (0.7± 0.1%)
2	B	1.15±0.05	1±0/119 (0.8± 0.0%)	1.30±0.05	1±0/162 (0.6± 0.1%)
All	All	0.96	119/37060 (0.3%)	1.22	344/50020 (0.7%)

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.9±0.2
All	All	0	39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	311	LYS	CA-C	-9.37	1.41	1.52	14	17
2	B	1196	THR	C-O	-8.56	1.12	1.24	12	20
1	A	273	GLU	CA-CB	-8.47	1.40	1.53	10	16
1	A	311	LYS	C-O	7.86	1.33	1.24	9	9
1	A	299	LEU	C-O	-7.82	1.15	1.24	6	18
1	A	273	GLU	CA-C	-7.72	1.43	1.52	20	14
1	A	300	ASP	C-O	-7.04	1.13	1.24	14	1
1	A	311	LYS	CB-CG	-6.37	1.33	1.52	13	1
1	A	312	VAL	CA-CB	6.21	1.63	1.54	9	6
1	A	273	GLU	CB-CG	-6.02	1.34	1.52	15	7
1	A	226	ASN	CG-ND2	-5.96	1.20	1.33	12	1
1	A	311	LYS	CA-CB	-5.49	1.44	1.53	13	1
1	A	231	ILE	CA-CB	5.43	1.60	1.54	20	3
1	A	300	ASP	CA-CB	-5.36	1.44	1.53	10	1
1	A	346	VAL	CA-CB	5.32	1.61	1.54	10	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	271	GLN	CA-C	-5.19	1.46	1.52	10	1
1	A	272	PRO	C-N	-5.14	1.26	1.33	7	1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	271	GLN	CA-C-O	-36.32	70.40	120.16	10	1
1	A	271	GLN	O-C-N	-29.74	87.12	121.32	10	1
1	A	271	GLN	CA-C-N	-19.92	94.94	119.84	8	9
1	A	271	GLN	C-N-CA	-19.92	94.94	119.84	8	9
1	A	311	LYS	O-C-N	14.05	136.70	122.09	7	20
1	A	273	GLU	N-CA-CB	-11.14	91.67	110.49	8	20
1	A	272	PRO	CA-N-CD	-10.67	97.07	112.00	8	19
1	A	273	GLU	N-CA-C	10.33	129.10	113.61	6	20
1	A	301	GLY	N-CA-C	-10.09	101.95	114.16	13	1
1	A	272	PRO	N-CA-C	10.02	133.12	112.47	8	19
1	A	299	LEU	N-CA-C	-9.50	100.90	111.07	18	11
2	B	1132	PHE	N-CA-C	-9.13	102.25	112.57	4	20
1	A	271	GLN	C-N-CD	-9.07	100.65	120.60	10	3
1	A	300	ASP	N-CA-C	9.01	123.59	112.23	10	9
1	A	311	LYS	N-CA-C	8.77	121.80	111.71	13	2
1	A	311	LYS	CA-C-N	8.37	134.03	120.30	15	20
1	A	311	LYS	C-N-CA	8.37	134.03	120.30	15	20
1	A	273	GLU	CB-CA-C	-8.16	97.81	111.02	13	12
1	A	159	MET	CA-C-N	-6.72	111.89	119.28	1	4
1	A	159	MET	C-N-CA	-6.72	111.89	119.28	1	4
1	A	274	ASP	N-CA-C	-6.50	96.95	110.80	2	4
1	A	313	GLY	N-CA-C	-6.21	105.11	113.24	17	10
1	A	276	ASN	N-CA-C	-6.11	104.70	111.36	15	4
1	A	312	VAL	CB-CA-C	-6.00	102.54	112.26	15	16
2	B	1196	THR	N-CA-C	5.83	123.22	110.80	10	1
1	A	357	ASP	N-CA-C	5.81	123.18	110.80	18	8
1	A	296	GLN	CA-C-N	-5.79	113.71	119.56	7	2
1	A	296	GLN	C-N-CA	-5.79	113.71	119.56	7	2
1	A	355	ASN	CA-C-N	5.79	132.59	121.54	2	12
1	A	355	ASN	C-N-CA	5.79	132.59	121.54	2	12
1	A	357	ASP	CB-CA-C	-5.76	98.96	110.42	2	13
1	A	322	ILE	N-CA-C	5.75	116.40	110.82	18	9
1	A	355	ASN	O-C-N	5.73	129.43	122.96	20	3
1	A	362	LEU	CB-CA-C	-5.62	102.06	110.88	17	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	311	LYS	CB-CA-C	-5.58	100.31	110.63	13	1
1	A	184	GLY	N-CA-C	5.55	126.34	113.18	11	9
1	A	356	GLU	N-CA-C	-5.55	98.97	110.80	18	4
1	A	145	ALA	N-CA-C	-5.49	104.72	111.75	10	4
1	A	314	CYS	CA-CB-SG	-5.36	102.06	114.40	20	1
1	A	210	ASP	N-CA-C	5.27	117.71	111.33	13	1
1	A	301	GLY	CA-C-O	5.12	125.54	119.50	13	1
1	A	257	ILE	CB-CA-C	-5.06	105.49	111.97	2	1
1	A	271	GLN	CB-CA-C	5.03	120.07	110.17	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	271	GLN	Peptide,Mainchain	20
1	A	273	GLU	Peptide	2

6.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1712	1742	1742	9±3
2	B	118	118	118	1±1
All	All	36600	37200	37200	175

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:VAL:HG22	1:A:358:MET:HE2	0.69	1.64	7	4
1:A:301:GLY:HA3	1:A:314:CYS:SG	0.63	2.34	20	17
1:A:235:LEU:HD22	1:A:275:MET:HE1	0.62	1.70	7	2
1:A:186:GLU:H	1:A:186:GLU:CD	0.57	2.07	3	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:LEU:HD13	1:A:161:LEU:HD13	0.56	1.77	2	19
1:A:350:LEU:HD22	1:A:358:MET:SD	0.55	2.40	18	3
1:A:350:LEU:HD22	1:A:358:MET:HE3	0.55	1.77	15	4
1:A:226:ASN:CG	2:B:1196:THR:O	0.55	2.50	20	20
1:A:226:ASN:ND2	2:B:1120:ASP:H	0.54	2.00	12	1
1:A:226:ASN:ND2	2:B:1197:GLY:C	0.50	2.70	12	1
1:A:301:GLY:O	1:A:311:LYS:HA	0.49	2.08	20	9
2:B:1197:GLY:HA2	2:B:1120:ASP:OD2	0.48	2.07	12	1
1:A:315:LEU:HD12	1:A:361:GLN:HB3	0.48	1.86	14	1
1:A:229:PHE:CD2	1:A:229:PHE:C	0.48	2.92	1	20
1:A:310:LEU:O	1:A:311:LYS:C	0.48	2.57	14	1
1:A:226:ASN:HD21	2:B:1120:ASP:H	0.48	1.52	12	1
1:A:238:GLU:H	1:A:238:GLU:CD	0.47	2.17	14	2
1:A:256:MET:HE1	1:A:297:PRO:O	0.47	2.08	4	3
1:A:311:LYS:O	1:A:314:CYS:HB2	0.46	2.11	8	9
1:A:312:VAL:HG22	1:A:358:MET:SD	0.46	2.51	9	4
1:A:181:GLN:HA	1:A:229:PHE:CE2	0.46	2.46	14	19
1:A:312:VAL:CG2	1:A:358:MET:HE2	0.46	2.39	7	1
1:A:273:GLU:CD	1:A:275:MET:HE3	0.45	2.37	12	2
1:A:327:GLU:H	1:A:327:GLU:CD	0.45	2.20	7	1
1:A:271:GLN:O	1:A:272:PRO:C	0.44	2.60	10	1
1:A:276:ASN:CG	1:A:277:GLU:N	0.43	2.76	8	1
1:A:273:GLU:CD	1:A:273:GLU:H	0.43	2.21	9	1
1:A:273:GLU:C	1:A:275:MET:H	0.43	2.21	9	1
1:A:269:LEU:C	1:A:271:GLN:H	0.42	2.22	15	2
1:A:158:ASP:CG	1:A:159:MET:H	0.42	2.22	9	1
1:A:146:MET:HA	1:A:149:ILE:HD12	0.42	1.92	19	1
1:A:323:THR:HG21	2:B:1132:PHE:HA	0.41	1.93	10	1
1:A:226:ASN:ND2	2:B:1197:GLY:CA	0.41	2.84	12	1
1:A:226:ASN:HA	2:B:1199:LEU:HB2	0.41	1.93	16	1
1:A:327:GLU:CD	1:A:327:GLU:H	0.40	2.23	14	1
1:A:271:GLN:NE2	1:A:271:GLN:HA	0.40	2.32	16	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/256 (84%)	204±1 (95±1%)	6±1 (3±1%)	6±1 (3±0%)	6	42
2	B	17/29 (59%)	17±0 (99±2%)	0±0 (0±0%)	0±0 (1±2%)	16	66
All	All	4640/5700 (81%)	4408 (95%)	117 (3%)	115 (2%)	6	43

All 11 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	228	LYS	20
1	A	229	PHE	20
1	A	272	PRO	20
1	A	356	GLU	20
1	A	357	ASP	20
1	A	158	ASP	7
2	B	1196	THR	3
1	A	274	ASP	2
1	A	300	ASP	1
1	A	271	GLN	1
1	A	354	GLU	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/227 (85%)	175±3 (91±2%)	17±3 (9±2%)	11	57
2	B	12/22 (55%)	10±0 (86±4%)	2±0 (14±4%)	5	44
All	All	4080/4980 (82%)	3698 (91%)	382 (9%)	10	56

All 53 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	156	LEU	20
1	A	231	ILE	20
1	A	315	LEU	20
1	A	347	LEU	20
2	B	1196	THR	20

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Mol	Chain	Res	Type	Models (Total)
1	A	271	GLN	19
1	A	162	LEU	18
1	A	269	LEU	17
1	A	272	PRO	17
1	A	311	LYS	17
1	A	298	LEU	16
1	A	346	VAL	15
2	B	1199	LEU	14
1	A	293	GLU	13
1	A	349	ASP	10
1	A	351	ARG	10
1	A	190	SER	9
1	A	186	GLU	9
1	A	273	GLU	8
1	A	327	GLU	7
1	A	333	HIS	7
1	A	147	MET	7
1	A	277	GLU	7
1	A	210	ASP	6
1	A	159	MET	4
1	A	278	ARG	4
1	A	363	ASN	4
1	A	358	MET	4
1	A	249	ASP	3
1	A	275	MET	3
1	A	238	GLU	3
1	A	299	LEU	2
1	A	211	SER	2
1	A	288	GLU	2
1	A	357	ASP	2
1	A	340	ARG	2
1	A	326	GLU	2
1	A	300	ASP	2
1	A	307	THR	2
1	A	332	VAL	2
1	A	256	MET	1
1	A	344	HIS	1
1	A	173	ASN	1
1	A	368	GLN	1
1	A	232	LYS	1
1	A	178	SER	1
1	A	354	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	214	LYS	1
1	A	236	GLU	1
1	A	169	ARG	1
1	A	283	MET	1
1	A	175	ASN	1
1	A	359	ARG	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 64% for the well-defined parts and 64% 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	2146
Number of shifts mapped to atoms	2142
Number of unparsed shifts	0
Number of shifts with mapping errors	4
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

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

- No matching atom found in the structure. All 4 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	MET	CA	58.346	0.300	1
1	A	126	GLY	H	8.362	0.020	1
1	A	126	GLY	CA	45.226	0.300	1
1	A	126	GLY	N	112.333	0.300	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	239	-1.25 ± 0.09	Should be checked
$^{13}\text{C}_\beta$	155	-0.05 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	226	0.62 ± 0.17	Should be applied

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 59%, i.e. 1932 atoms were assigned a chemical shift out of a possible 3253. 0 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	823/1155 (71%)	412/467 (88%)	211/464 (45%)	200/224 (89%)
Sidechain	1079/1970 (55%)	944/1286 (73%)	135/611 (22%)	0/73 (0%)
Aromatic	30/128 (23%)	29/65 (45%)	0/58 (0%)	1/5 (20%)
Overall	1932/3253 (59%)	1385/1818 (76%)	346/1133 (31%)	201/302 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 57%, i.e. 2142 atoms were assigned a chemical shift out of a possible 3773. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	922/1358 (68%)	460/551 (83%)	237/544 (44%)	225/263 (86%)
Sidechain	1190/2278 (52%)	1035/1478 (70%)	155/705 (22%)	0/95 (0%)
Aromatic	30/137 (22%)	29/69 (42%)	0/63 (0%)	1/5 (20%)
Overall	2142/3773 (57%)	1524/2098 (73%)	392/1312 (30%)	226/363 (62%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

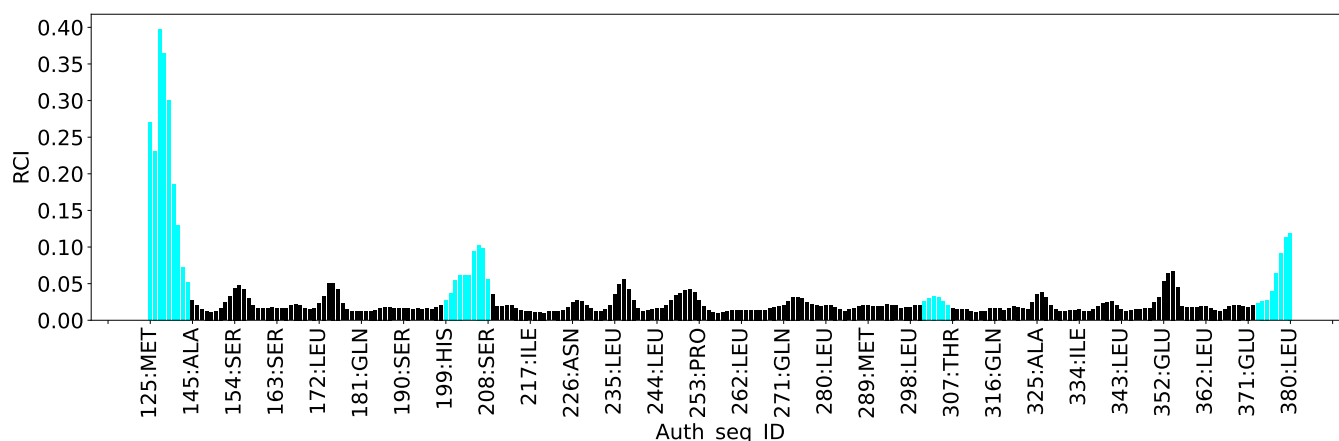
List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	319	ASN	HB2	0.59	1.27 – 4.34	-7.2
1	A	184	GLY	N	128.26	91.59 – 127.52	5.2
1	A	340	ARG	CB	39.75	21.74 – 39.52	5.1
1	A	306	THR	HG21	0.07	0.08 – 2.19	-5.0
1	A	306	THR	HG22	0.07	0.08 – 2.19	-5.0
1	A	306	THR	HG23	0.07	0.08 – 2.19	-5.0

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 Bookkeeping [i](#)

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

Total number of shifts	276
Number of shifts mapped to atoms	276
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

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	28	-0.37 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	23	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	26	-0.14 ± 0.75	None needed (< 0.5 ppm)

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 5%, i.e. 163 atoms were assigned a chemical shift out of a possible 3253. 0 out of 52 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	70/1155 (6%)	36/467 (8%)	17/464 (4%)	17/224 (8%)
Sidechain	88/1970 (4%)	71/1286 (6%)	17/611 (3%)	0/73 (0%)
Aromatic	5/128 (4%)	5/65 (8%)	0/58 (0%)	0/5 (0%)
Overall	163/3253 (5%)	112/1818 (6%)	34/1133 (3%)	17/302 (6%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 276 atoms were assigned a chemical shift out of a possible 3773. 0 out of 55 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	110/1358 (8%)	56/551 (10%)	28/544 (5%)	26/263 (10%)
Sidechain	161/2278 (7%)	120/1478 (8%)	41/705 (6%)	0/95 (0%)
Aromatic	5/137 (4%)	5/69 (7%)	0/63 (0%)	0/5 (0%)
Overall	276/3773 (7%)	181/2098 (9%)	69/1312 (5%)	26/363 (7%)

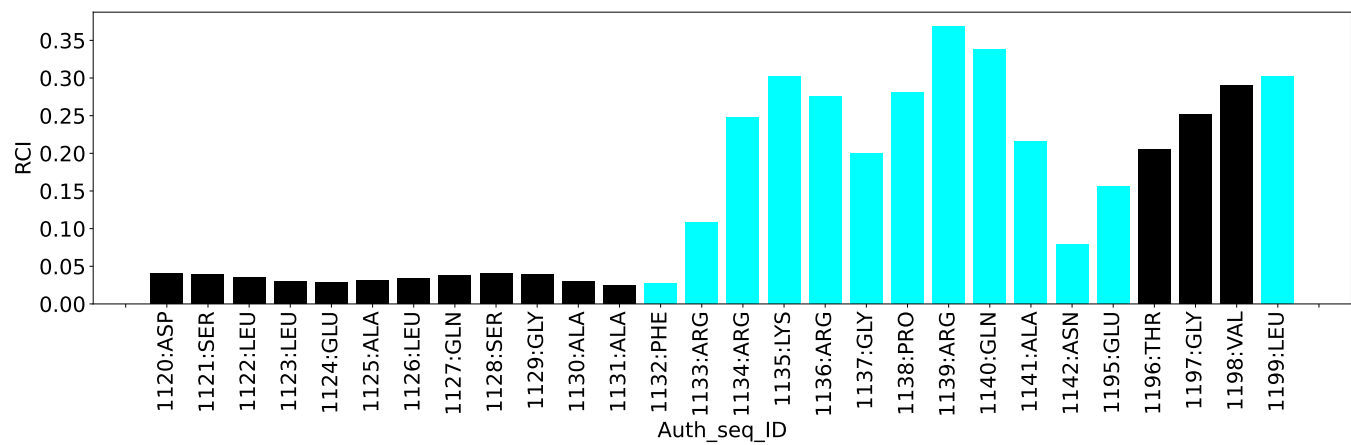
7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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 B:



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	1508
Intra-residue ($ i-j =0$)	673
Sequential ($ i-j =1$)	571
Medium range ($ i-j >1$ and $ i-j <5$)	102
Long range ($ i-j \geq 5$)	146
Inter-chain	16
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	443
Number of unmapped restraints	0
Number of restraints per residue	6.8
Number of long range restraints per residue ¹	0.5

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)	2.2	0.2
0.2-0.5 (Medium)	6.4	0.5
>0.5 (Large)	18.9	2.26

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)	9.3	9.93
10.0-20.0 (Medium)	4.5	19.91
>20.0 (Large)	5.0	75.71

9 Distance violation analysis ⓘ

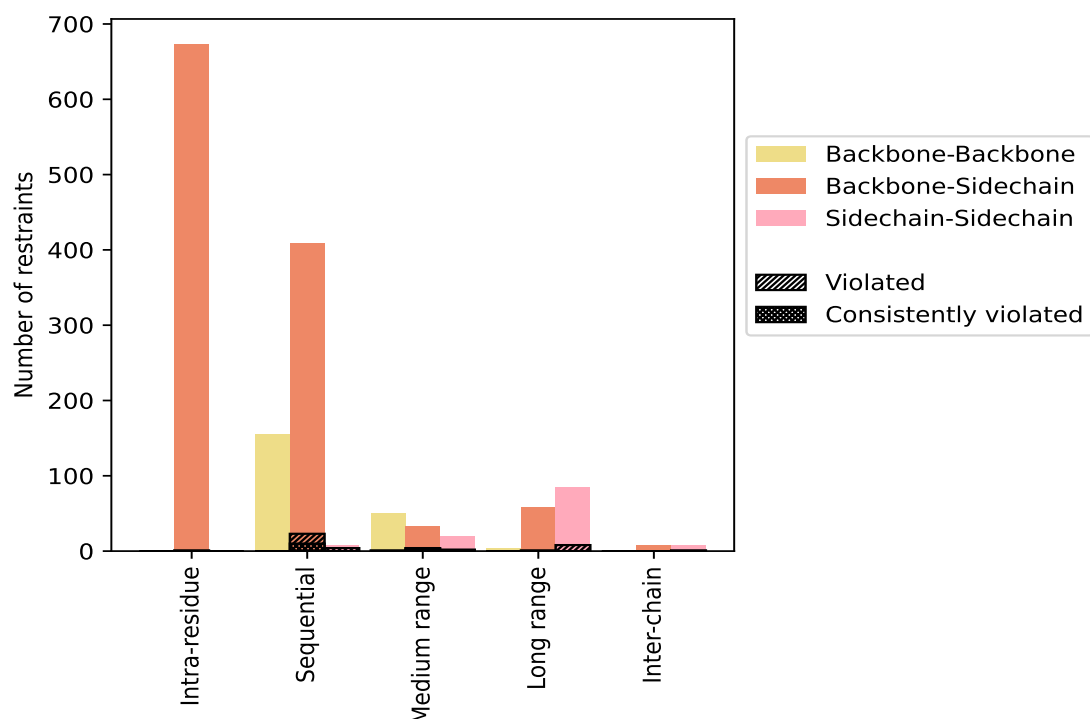
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	673	44.6	1	0.1	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	673	44.6	1	0.1	0.1	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	571	37.9	27	4.7	1.8	10	1.8	0.7
Backbone-Backbone	155	10.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	408	27.1	23	5.6	1.5	10	2.5	0.7
Sidechain-Sidechain	8	0.5	4	50.0	0.3	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	102	6.8	7	6.9	0.5	2	2.0	0.1
Backbone-Backbone	50	3.3	1	2.0	0.1	0	0.0	0.0
Backbone-Sidechain	33	2.2	4	12.1	0.3	2	6.1	0.1
Sidechain-Sidechain	19	1.3	2	10.5	0.1	0	0.0	0.0
Long range ($i-j \geq 5$)	146	9.7	9	6.2	0.6	0	0.0	0.0
Backbone-Backbone	3	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	58	3.8	1	1.7	0.1	0	0.0	0.0
Sidechain-Sidechain	85	5.6	8	9.4	0.5	0	0.0	0.0
Inter-chain	16	1.1	1	6.2	0.1	0	0.0	0.0
Backbone-Backbone	1	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	8	0.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.5	1	14.3	0.1	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1508	100.0	45	3.0	3.0	12	0.8	0.8
Backbone-Backbone	209	13.9	1	0.5	0.1	0	0.0	0.0
Backbone-Sidechain	1180	78.2	29	2.5	1.9	12	1.0	0.8
Sidechain-Sidechain	119	7.9	15	12.6	1.0	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	20	3	4	0	28	0.84	2.26	0.53	0.78
2	1	21	2	3	0	27	0.99	2.02	0.53	1.14
3	1	20	2	4	0	27	0.98	2.06	0.54	1.02
4	1	20	3	4	0	28	0.81	2.26	0.55	0.66
5	1	21	2	3	0	27	0.99	2.07	0.52	1.17
6	1	19	2	4	0	26	1.0	2.0	0.52	1.04
7	1	19	3	3	0	26	0.86	2.26	0.55	0.88
8	1	21	3	3	1	29	0.8	2.26	0.56	0.72
9	1	20	3	4	0	28	0.8	2.25	0.56	0.59
10	1	21	2	3	0	27	0.95	1.98	0.54	1.0

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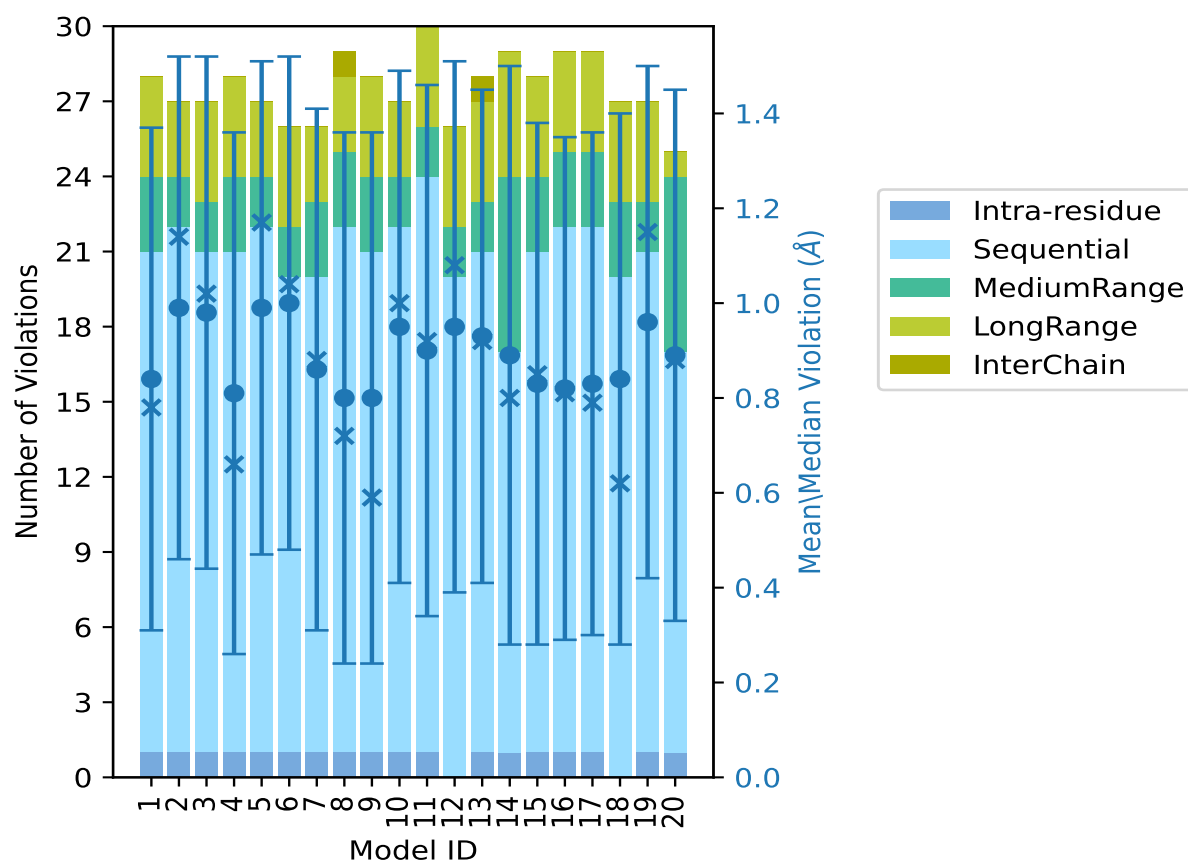
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	1	23	2	4	0	30	0.9	2.06	0.56	0.92
12	0	20	2	4	0	26	0.95	2.05	0.56	1.08
13	1	20	2	4	1	28	0.93	2.24	0.52	0.92
14	1	16	7	5	0	29	0.89	2.22	0.61	0.8
15	1	20	3	4	0	28	0.83	2.26	0.55	0.85
16	1	21	3	4	0	29	0.82	2.26	0.53	0.81
17	1	21	3	4	0	29	0.83	2.25	0.53	0.79
18	0	20	3	4	0	27	0.84	2.25	0.56	0.62
19	1	20	2	4	0	27	0.96	2.05	0.54	1.15
20	1	16	7	1	0	25	0.89	2.05	0.56	0.88

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

⁵Inter-chain restraints, ⁶Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

9.3 Distance violation statistics for the ensemble

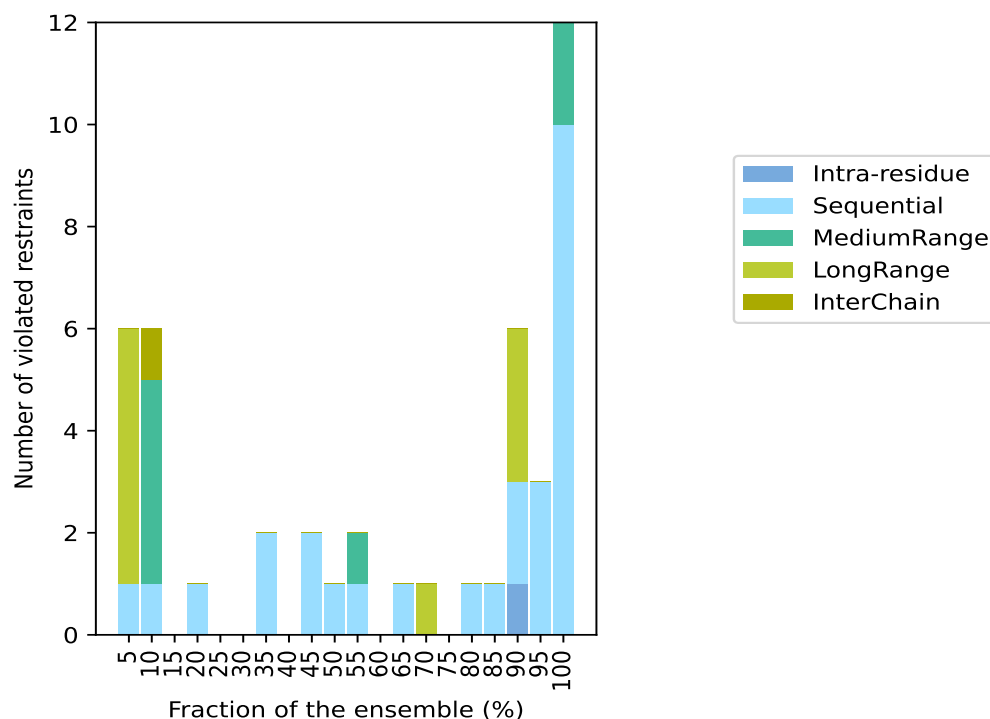
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1463(IR:672, SQ:544, MR:95, LR:137, IC:15) restraints are 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	%
0	1	0	5	0	6	1	5.0
0	1	4	0	1	6	2	10.0
0	0	0	0	0	0	3	15.0
0	1	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	2	0	0	0	2	7	35.0
0	0	0	0	0	0	8	40.0
0	2	0	0	0	2	9	45.0
0	1	0	0	0	1	10	50.0
0	1	1	0	0	2	11	55.0
0	0	0	0	0	0	12	60.0
0	1	0	0	0	1	13	65.0
0	0	0	1	0	1	14	70.0
0	0	0	0	0	0	15	75.0
0	1	0	0	0	1	16	80.0
0	1	0	0	0	1	17	85.0
1	2	0	3	0	6	18	90.0
0	3	0	0	0	3	19	95.0
0	10	2	0	0	12	20	100.0

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

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

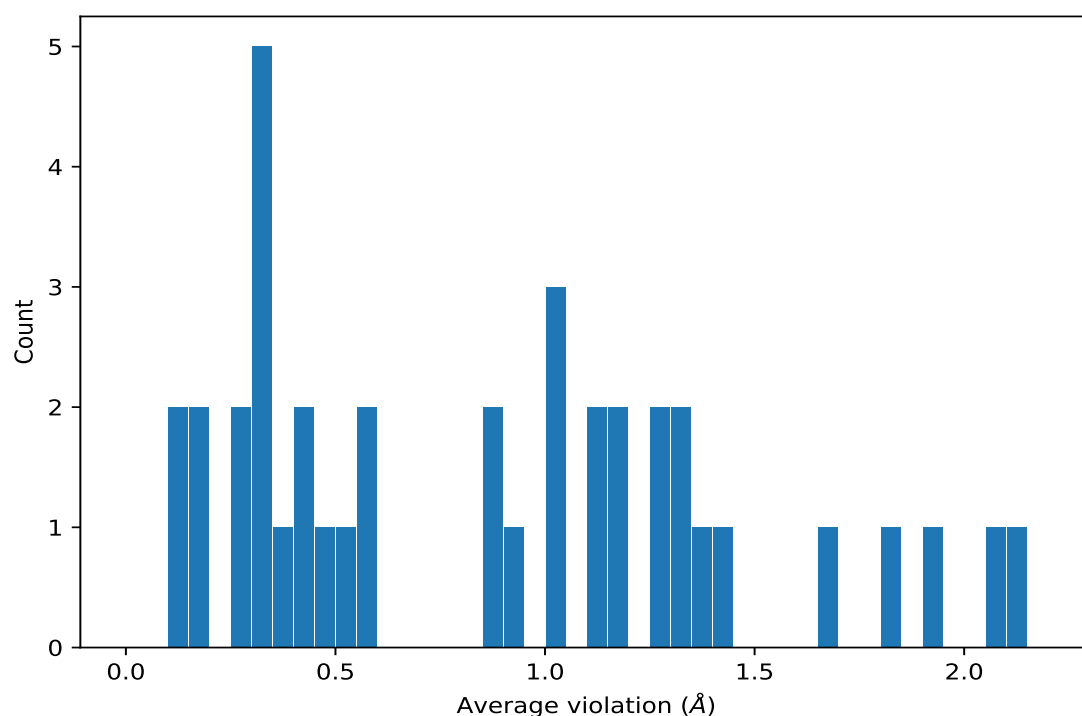
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	20	1.36	0.02	1.36
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	20	1.33	0.07	1.35
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	20	1.29	0.04	1.31
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	20	1.28	0.04	1.29
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	20	1.19	0.02	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	20	1.19	0.02	1.19
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	20	0.91	0.29	1.01
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	20	0.56	0.02	0.56
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	20	0.43	0.1	0.46
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	20	0.34	0.03	0.36
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	20	0.33	0.06	0.34
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	20	0.19	0.05	0.18
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	19	2.06	0.43	2.24
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	19	1.95	0.21	1.91
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	19	0.53	0.02	0.53
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	18	1.32	0.46	1.34

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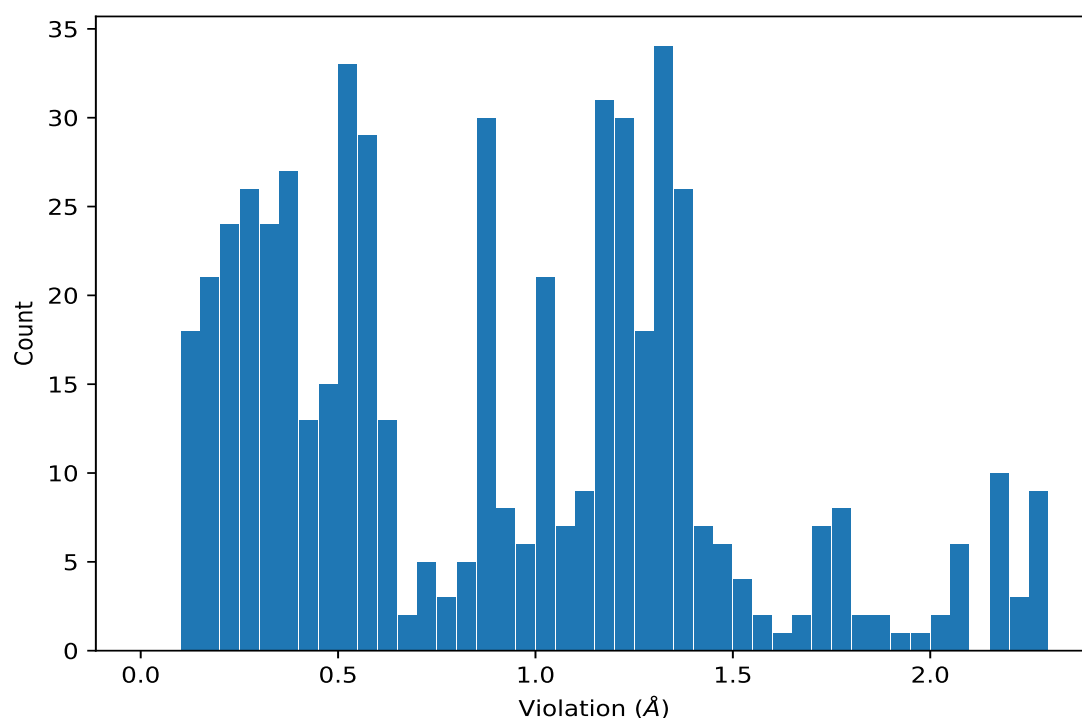
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	18	1.15	0.15	1.12
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	18	1.1	0.4	1.12
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	18	1.04	0.18	0.92
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	18	0.88	0.01	0.88
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	18	0.58	0.05	0.57
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	17	0.25	0.07	0.26
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	16	0.45	0.1	0.48
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	14	0.19	0.07	0.18
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	13	1.0	0.06	1.01
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	11	0.86	0.41	1.01
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	11	0.32	0.05	0.32
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	10	0.4	0.19	0.44
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	9	1.41	0.41	1.5
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	9	0.27	0.03	0.28
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	7	1.04	0.07	1.04
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	7	0.31	0.09	0.3
(5,1245)	1:167:A:SER:H	1:168:A:LEU:HB2	4	0.14	0.02	0.14
(2,32)	1:303:A:LYS:NZ	1:306:A:THR:CG2	2	2.12	0.08	2.12
(2,24)	1:303:A:LYS:NZ	1:301:A:GLY:CA	2	1.82	0.35	1.82
(2,31)	1:303:A:LYS:NZ	1:306:A:THR:CB	2	1.66	0.17	1.66
(2,30)	1:303:A:LYS:NZ	1:306:A:THR:CA	2	0.38	0.27	0.38
(2,129)	1:228:A:LYS:NZ	2:1198:B:VAL:CG2	2	0.35	0.15	0.35
(5,1153)	1:278:A:ARG:HG2	1:279:A:VAL:H	2	0.14	0.02	0.14

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)
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	1	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	4	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	7	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	8	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	15	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	16	2.26
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	9	2.25
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	17	2.25
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	18	2.25
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	13	2.24
(2,37)	1:303:A:LYS:NZ	1:310:A:LEU:CD2	14	2.22
(2,32)	1:303:A:LYS:NZ	1:306:A:THR:CG2	14	2.2
(2,24)	1:303:A:LYS:NZ	1:301:A:GLY:CA	14	2.17
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	1	2.16
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	4	2.16
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	15	2.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	18	2.16
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	7	2.15
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	8	2.15
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	9	2.15
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	16	2.15
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	17	2.15
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	5	2.07
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	3	2.06
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	11	2.06
(2,32)	1:303:A:LYS:NZ	1:306:A:THR:CG2	20	2.05
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	12	2.05
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	19	2.05
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	2	2.02
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	6	2.0
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	10	1.98
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	11	1.91
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	5	1.89
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	3	1.86
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	12	1.84
(2,31)	1:303:A:LYS:NZ	1:306:A:THR:CB	20	1.82
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	3	1.79
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	13	1.78
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	19	1.78
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	2	1.77
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	6	1.77
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	12	1.77
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	19	1.76
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	11	1.75
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	10	1.74
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	20	1.74
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	5	1.73
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	6	1.73
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	13	1.73
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	2	1.72
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	10	1.71
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	2	1.69
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	6	1.67
(2,25)	1:303:A:LYS:NZ	1:302:A:LEU:CA	10	1.62
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	13	1.59
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	3	1.55
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	19	1.54
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	6	1.51

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	19	1.51
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	3	1.5
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	2	1.49
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	10	1.49
(2,31)	1:303:A:LYS:NZ	1:306:A:THR:CB	14	1.49
(2,24)	1:303:A:LYS:NZ	1:301:A:GLY:CA	20	1.47
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	3	1.46
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	11	1.45
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	12	1.44
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	12	1.43
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	5	1.41
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	11	1.41
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	4	1.4
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	11	1.4
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	12	1.4
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	2	1.38
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	6	1.38
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	20	1.38
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	8	1.38
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	12	1.38
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	18	1.38
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	15	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	7	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	9	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	13	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	16	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	19	1.37
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	20	1.37
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	10	1.36
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	18	1.36
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	5	1.36
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	10	1.36
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	15	1.36
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	8	1.35
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	9	1.35
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	17	1.35
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	1	1.35
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	11	1.35
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	17	1.35
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	6	1.35
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	11	1.35
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	3	1.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	6	1.34
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	14	1.34
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	9	1.34
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	1	1.33
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	13	1.33
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	5	1.33
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	8	1.33
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	15	1.33
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	1	1.33
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	12	1.33
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	12	1.33
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	5	1.33
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	5	1.32
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	2	1.32
(5,1256)	1:242:A:LEU:H	1:243:A:LEU:HB3	4	1.32
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	3	1.32
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	18	1.32
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	13	1.32
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	5	1.32
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	16	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	2	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	5	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	6	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	7	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	13	1.31
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	3	1.31
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	14	1.31
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	15	1.31
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	14	1.3
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	7	1.3
(2,35)	1:303:A:LYS:NZ	1:310:A:LEU:CG	14	1.3
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	2	1.3
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	10	1.3
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	20	1.29
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	4	1.29
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	9	1.29
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	18	1.29
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	6	1.29
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	19	1.28
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	11	1.28
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	19	1.28
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	12	1.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	1	1.26
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	2	1.26
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	5	1.26
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	8	1.26
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	18	1.25
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	11	1.25
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	17	1.25
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	20	1.25
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	19	1.25
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	3	1.24
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	14	1.24
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	10	1.24
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	16	1.24
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	19	1.24
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	10	1.24
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	10	1.24
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	17	1.24
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	3	1.24
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	3	1.23
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	10	1.23
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	19	1.23
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	5	1.22
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	13	1.22
(5,1106)	1:320:A:ALA:H	1:321:A:LEU:HB3	4	1.22
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	20	1.22
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	10	1.21
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	16	1.21
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	17	1.21
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	18	1.21
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	12	1.21
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	11	1.2
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	15	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	1	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	2	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	4	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	8	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	16	1.2
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	19	1.2
(5,930)	1:165:A:LEU:H	1:166:A:GLU:HB3	16	1.2
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	14	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	3	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	4	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	5	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	6	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	13	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	20	1.19
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	2	1.19
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	11	1.19
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	9	1.19
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	11	1.19
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	12	1.19
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	20	1.19
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	1	1.19
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	1	1.18
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	2	1.18
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	8	1.18
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	9	1.18
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	19	1.18
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	7	1.18
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	15	1.18
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	17	1.18
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	11	1.18
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	7	1.17
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	16	1.17
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	6	1.17
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	5	1.17
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	17	1.16
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	14	1.16
(5,1294)	1:192:A:LEU:H	1:193:A:ASP:HB3	12	1.15
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	19	1.15
(5,1315)	1:330:A:PHE:H	1:331:A:ARG:HB3	7	1.14
(5,1141)	1:220:A:CYS:H	1:221:A:LEU:HB3	18	1.14
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	2	1.14
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	7	1.14
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	18	1.13
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	8	1.12
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	8	1.12
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	18	1.12
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	9	1.11
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	9	1.09
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	16	1.08
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	7	1.07
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	14	1.06
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	15	1.06

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	6	1.06
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	2	1.05
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	20	1.04
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	5	1.04
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	19	1.04
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	17	1.04
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	14	1.03
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	7	1.03
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	12	1.02
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	3	1.02
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	4	1.02
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	6	1.02
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	8	1.01
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	6	1.01
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	4	1.01
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	3	1.01
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	13	1.01
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	13	1.0
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	1	1.0
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	10	1.0
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	17	1.0
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	2	1.0
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	10	1.0
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	4	0.99
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	11	0.98
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	1	0.98
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	13	0.98
(2,45)	1:303:A:LYS:NZ	1:346:A:VAL:CG1	15	0.98
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	13	0.96
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	5	0.93
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	9	0.92
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	16	0.91
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	5	0.9
(5,1207)	1:276:A:ASN:H	1:277:A:GLU:HG3	15	0.9
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	16	0.9
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	7	0.9
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	15	0.9
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	1	0.89
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	7	0.89
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	10	0.89
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	15	0.89
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	16	0.89

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	19	0.89
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	1	0.89
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	8	0.89
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	17	0.89
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	3	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	4	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	13	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	14	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	17	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	20	0.88
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	7	0.88
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	15	0.88
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	16	0.88
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	6	0.87
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	8	0.87
(5,1206)	1:276:A:ASN:H	1:277:A:GLU:HB3	13	0.87
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	4	0.87
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	8	0.87
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	9	0.87
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	2	0.86
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	11	0.86
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	1	0.86
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	17	0.86
(2,27)	1:303:A:LYS:NZ	1:302:A:LEU:CG	18	0.86
(5,1246)	1:169:A:ARG:H	1:169:A:ARG:HD3	11	0.85
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	12	0.83
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	15	0.82
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	9	0.81
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	16	0.81
(2,57)	1:202:A:LYS:NZ	1:201:A:GLU:CA	14	0.8
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	18	0.79
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	17	0.79
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	7	0.76
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	16	0.73
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	13	0.73
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	8	0.72
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	1	0.71
(2,47)	1:303:A:LYS:NZ	1:346:A:VAL:CB	4	0.7
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	17	0.66
(2,30)	1:303:A:LYS:NZ	1:306:A:THR:CA	20	0.65
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	9	0.63
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	3	0.63

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	18	0.62
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	11	0.62
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	4	0.61
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	6	0.61
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	2	0.61
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	19	0.61
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	2	0.6
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	13	0.6
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	18	0.6
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	6	0.6
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	10	0.6
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	18	0.59
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	12	0.59
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	15	0.58
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	11	0.58
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	7	0.58
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	8	0.57
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	6	0.57
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	20	0.57
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	15	0.57
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	7	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	11	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	15	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	16	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	19	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	20	0.56
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	19	0.56
(2,46)	1:303:A:LYS:NZ	1:346:A:VAL:CG2	4	0.56
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	5	0.56
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	8	0.56
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	16	0.56
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	3	0.55
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	5	0.55
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	9	0.55
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	10	0.55
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	14	0.55
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	17	0.55
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	2	0.55
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	13	0.55
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	4	0.55
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	1	0.54
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	6	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	17	0.54
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	7	0.54
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	8	0.54
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	9	0.54
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	15	0.54
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	19	0.54
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	9	0.54
(5,1297)	1:219:A:ARG:HB3	1:221:A:LEU:H	12	0.53
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	18	0.53
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	3	0.53
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	4	0.53
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	6	0.53
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	12	0.53
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	18	0.53
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	17	0.53
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	14	0.52
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	19	0.52
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	1	0.52
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	5	0.52
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	10	0.52
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	14	0.52
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	18	0.52
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	12	0.51
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	20	0.51
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	3	0.51
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	5	0.51
(2,5)	1:303:A:LYS:NZ	1:250:A:PRO:CB	14	0.51
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	17	0.5
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	16	0.5
(5,1091)	1:269:A:LEU:H	1:270:A:PRO:HD2	17	0.5
(2,129)	1:228:A:LYS:NZ	2:1198:B:VAL:CG2	13	0.5
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	2	0.49
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	17	0.49
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	1	0.48
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	13	0.48
(2,28)	1:303:A:LYS:NZ	1:302:A:LEU:CD1	1	0.48
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	3	0.47
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	8	0.47
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	1	0.46
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	11	0.46
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	13	0.46
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	5	0.46

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	10	0.46
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	4	0.45
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	9	0.45
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	16	0.45
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	6	0.44
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	9	0.44
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	1	0.43
(2,34)	1:303:A:LYS:NZ	1:310:A:LEU:CB	14	0.43
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	10	0.41
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	15	0.41
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	2	0.4
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	6	0.4
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	19	0.4
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	4	0.4
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	9	0.4
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	14	0.4
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	14	0.4
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	16	0.39
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	15	0.39
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	17	0.39
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	11	0.39
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	12	0.38
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	13	0.38
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	10	0.38
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	14	0.38
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	9	0.38
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	3	0.37
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	1	0.37
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	3	0.37
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	3	0.37
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	12	0.37
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	1	0.37
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	6	0.36
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	11	0.36
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	12	0.36
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	14	0.36
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	16	0.36
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	20	0.36
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	5	0.36
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	9	0.36
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	16	0.36
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	18	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	14	0.35
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	1	0.35
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	13	0.34
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	18	0.34
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	11	0.34
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	18	0.34
(2,29)	1:303:A:LYS:NZ	1:302:A:LEU:CD2	13	0.34
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	16	0.33
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	9	0.33
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	19	0.33
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	17	0.33
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	8	0.33
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	8	0.32
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	2	0.32
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	5	0.32
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	16	0.32
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	20	0.32
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	1	0.31
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	4	0.31
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	20	0.31
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	7	0.3
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	3	0.3
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	11	0.3
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	12	0.3
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	4	0.3
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	15	0.3
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	17	0.29
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	4	0.29
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	16	0.29
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	18	0.29
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	20	0.29
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	7	0.29
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	15	0.29
(2,26)	1:303:A:LYS:NZ	1:302:A:LEU:CB	20	0.29
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	8	0.28
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	13	0.28
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	15	0.28
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	10	0.28
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	8	0.28
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	10	0.28
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	7	0.28
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	5	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1187)	1:175:A:ASN:H	1:176:A:PRO:HD3	2	0.27
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	8	0.27
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	10	0.27
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	1	0.26
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	18	0.26
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	7	0.26
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	5	0.26
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	7	0.25
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	13	0.25
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	4	0.25
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	9	0.24
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	17	0.24
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	19	0.24
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	19	0.24
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	7	0.24
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	14	0.24
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	13	0.24
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	1	0.24
(5,991)	1:313:A:GLY:HA3	1:317:A:LEU:H	17	0.23
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	4	0.22
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	1	0.22
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	15	0.22
(5,1281)	1:369:A:GLY:H	1:370:A:GLU:HB3	15	0.22
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	4	0.22
(5,1308)	1:292:A:VAL:H	1:291:A:GLU:HG3	2	0.21
(5,1284)	1:157:A:ARG:HB3	1:161:A:LEU:H	8	0.21
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	12	0.21
(5,1094)	1:275:A:MET:HG3	1:276:A:ASN:H	20	0.21
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	8	0.21
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	20	0.2
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	7	0.2
(5,1149)	1:248:A:MET:HG3	1:249:A:ASP:H	8	0.2
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	2	0.2
(2,129)	1:228:A:LYS:NZ	2:1198:B:VAL:CG2	8	0.2
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	4	0.19
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	11	0.19
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	7	0.19
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	15	0.19
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	18	0.19
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	11	0.18
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	17	0.18
(5,1325)	1:368:A:GLN:HG3	1:369:A:GLY:H	11	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	15	0.17
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	17	0.17
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	12	0.16
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	16	0.16
(5,1245)	1:167:A:SER:H	1:168:A:LEU:HB2	10	0.16
(5,1245)	1:167:A:SER:H	1:168:A:LEU:HB2	16	0.16
(5,1153)	1:278:A:ARG:HG2	1:279:A:VAL:H	19	0.16
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	3	0.16
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	4	0.16
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	9	0.16
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	10	0.15
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	18	0.15
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	16	0.15
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	12	0.14
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	9	0.14
(2,36)	1:303:A:LYS:NZ	1:310:A:LEU:CD1	14	0.14
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	3	0.13
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	19	0.13
(5,1153)	1:278:A:ARG:HG2	1:279:A:VAL:H	8	0.12
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	6	0.12
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	14	0.12
(5,1116)	1:361:A:GLN:HG3	1:362:A:LEU:H	20	0.12
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	11	0.12
(5,946)	1:268:A:ILE:H	1:269:A:LEU:HB3	9	0.12
(5,1322)	1:351:A:ARG:HG2	1:352:A:GLU:H	2	0.11
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	6	0.11
(5,1313)	1:321:A:LEU:H	1:267:A:CYS:HB2	9	0.11
(5,1245)	1:167:A:SER:H	1:168:A:LEU:HB2	5	0.11
(5,1245)	1:167:A:SER:H	1:168:A:LEU:HB2	11	0.11
(5,1114)	1:352:A:GLU:HG3	1:353:A:ILE:H	18	0.11
(2,30)	1:303:A:LYS:NZ	1:306:A:THR:CA	14	0.11

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

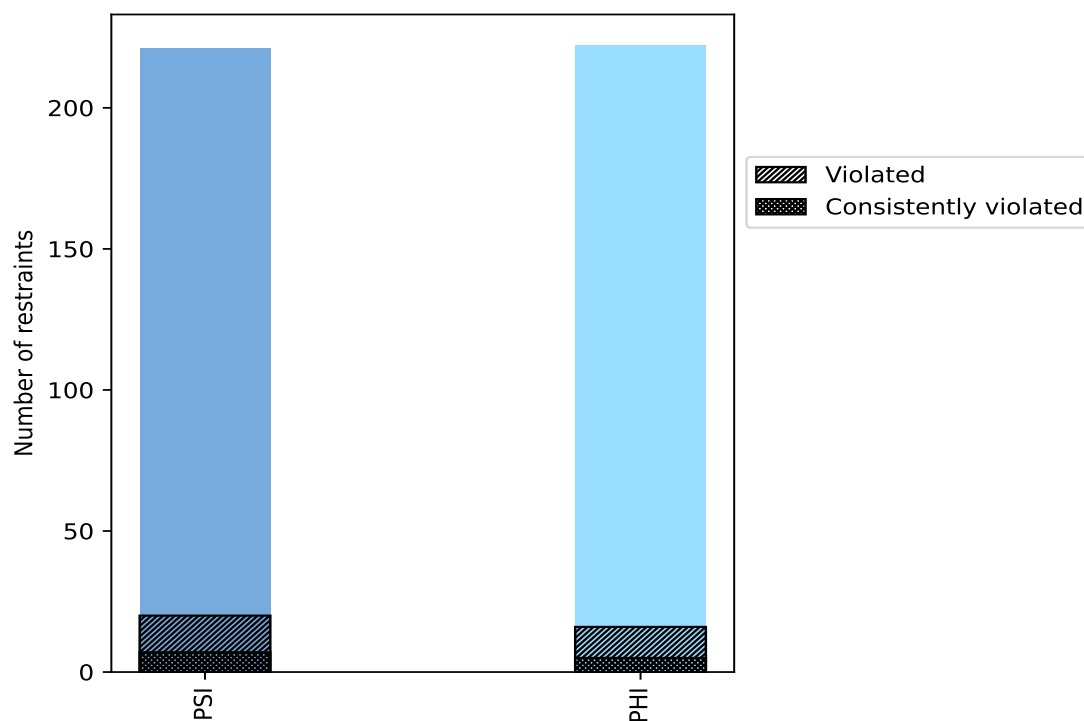
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PSI	221	49.9	20	9.0	4.5	7	3.2	1.6
PHI	222	50.1	16	7.2	3.6	5	2.3	1.1
Total	443	100.0	36	8.1	8.1	12	2.7	2.7

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

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



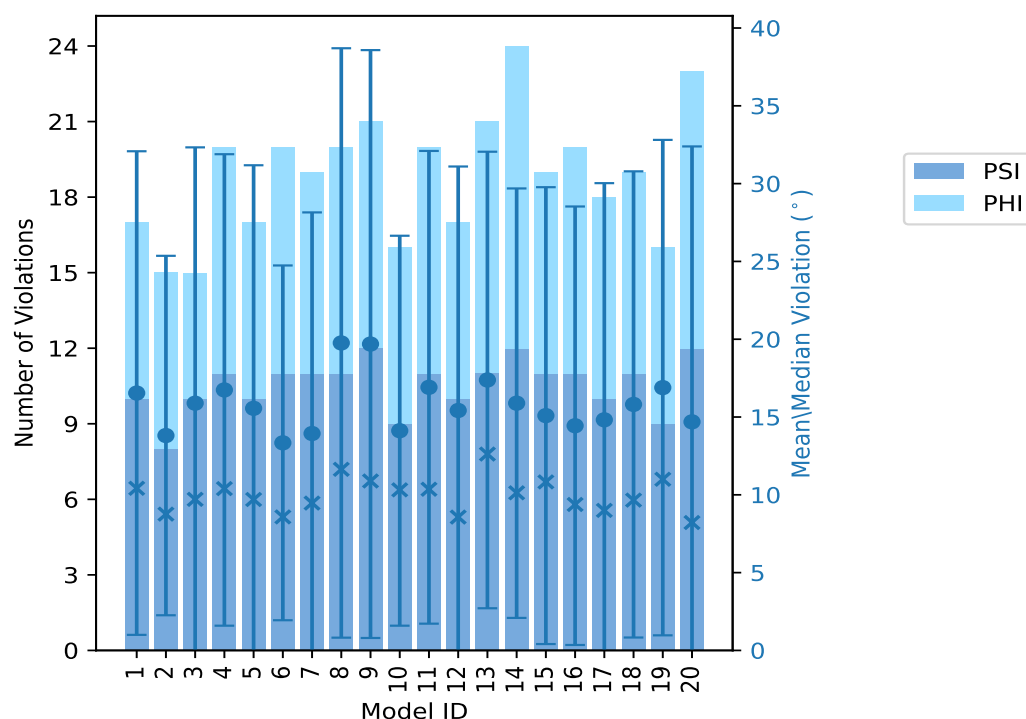
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	10	7	17	16.54	55.05	15.54	10.42
2	8	7	15	13.81	45.06	11.55	8.76
3	10	5	15	15.89	58.54	16.44	9.71
4	11	9	20	16.74	56.55	15.15	10.4
5	10	7	17	15.56	55.15	15.62	9.7
6	11	9	20	13.34	45.29	11.4	8.58
7	11	8	19	13.94	52.06	14.21	9.47
8	11	9	20	19.76	75.23	18.94	11.64
9	12	9	21	19.69	75.71	18.89	10.89
10	9	7	16	14.12	48.49	12.53	10.32
11	11	9	20	16.91	55.3	15.19	10.36
12	10	7	17	15.42	57.35	15.68	8.57
13	11	10	21	17.38	62.54	14.67	12.62
14	12	12	24	15.89	49.43	13.8	10.13
15	11	8	19	15.09	55.86	14.68	10.83
16	11	9	20	14.44	52.89	14.09	9.38
17	10	8	18	14.82	56.41	15.21	9.0
18	11	8	19	15.81	56.29	14.98	9.66
19	9	7	16	16.89	58.69	15.92	11.0
20	12	11	23	14.69	75.3	17.7	8.22

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



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

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

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

Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
3	1	4	1	5.0
3	3	6	2	10.0
1	0	1	3	15.0
1	1	2	4	20.0
1	0	1	5	25.0
0	2	2	6	30.0
1	0	1	7	35.0
0	1	1	8	40.0
0	1	1	9	45.0
0	0	0	10	50.0
1	1	2	11	55.0

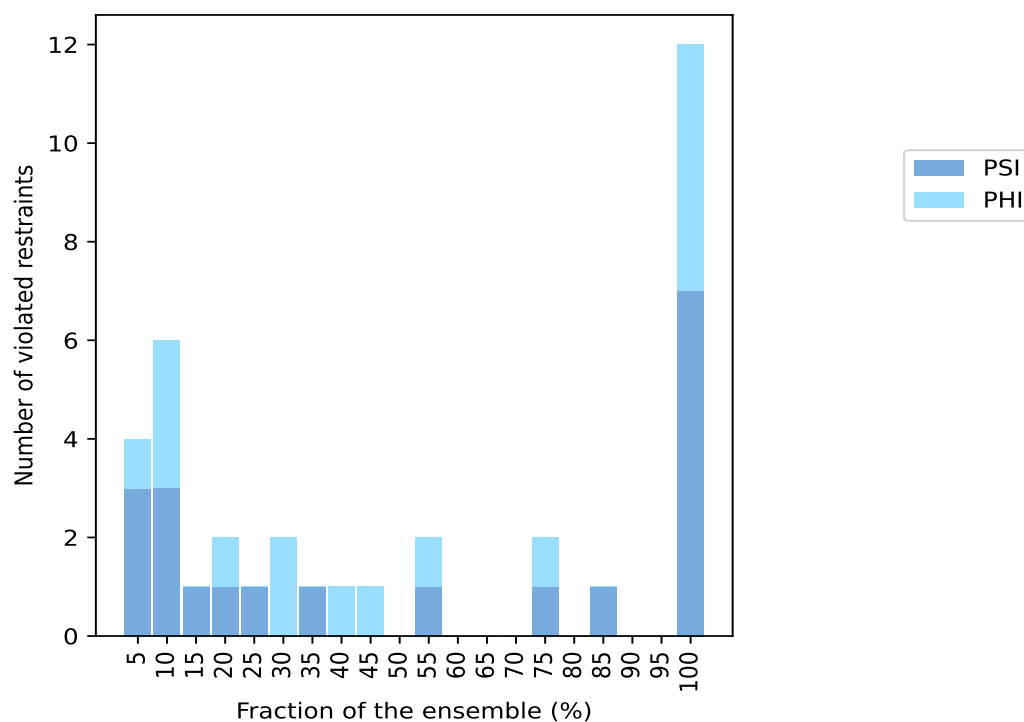
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Number of violated restraints			Fraction of the ensemble	
PSI	PHI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
1	1	2	15	75.0
0	0	0	16	80.0
1	0	1	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
7	5	12	20	100.0

¹ Number of models with violations

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

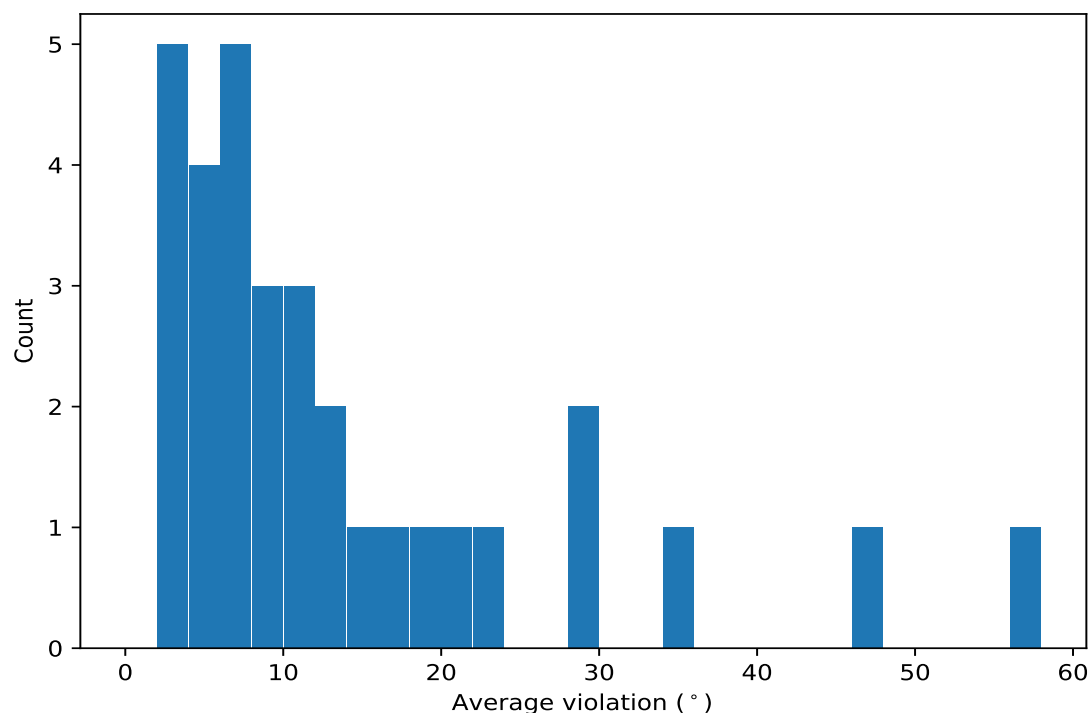


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	20	46.03	1.18	45.60
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	20	35.13	2.33	34.98
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	20	20.1	0.18	20.14
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	20	18.07	2.07	18.29
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	20	14.05	8.99	17.29
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	20	11.95	6.85	9.25
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	20	11.64	1.14	11.79
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	20	10.67	0.53	10.72
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	20	9.84	8.01	5.18
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	20	9.16	1.32	9.56
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	20	6.42	1.84	5.8
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	20	5.24	0.4	5.14
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	17	56.79	5.42	55.86
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	15	13.34	24.46	3.65
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	15	4.77	1.5	4.77
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	11	7.92	6.72	4.83
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	11	2.78	0.86	2.63
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	9	4.33	1.8	5.24
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	8	3.37	0.58	3.39
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	7	8.9	9.91	3.05

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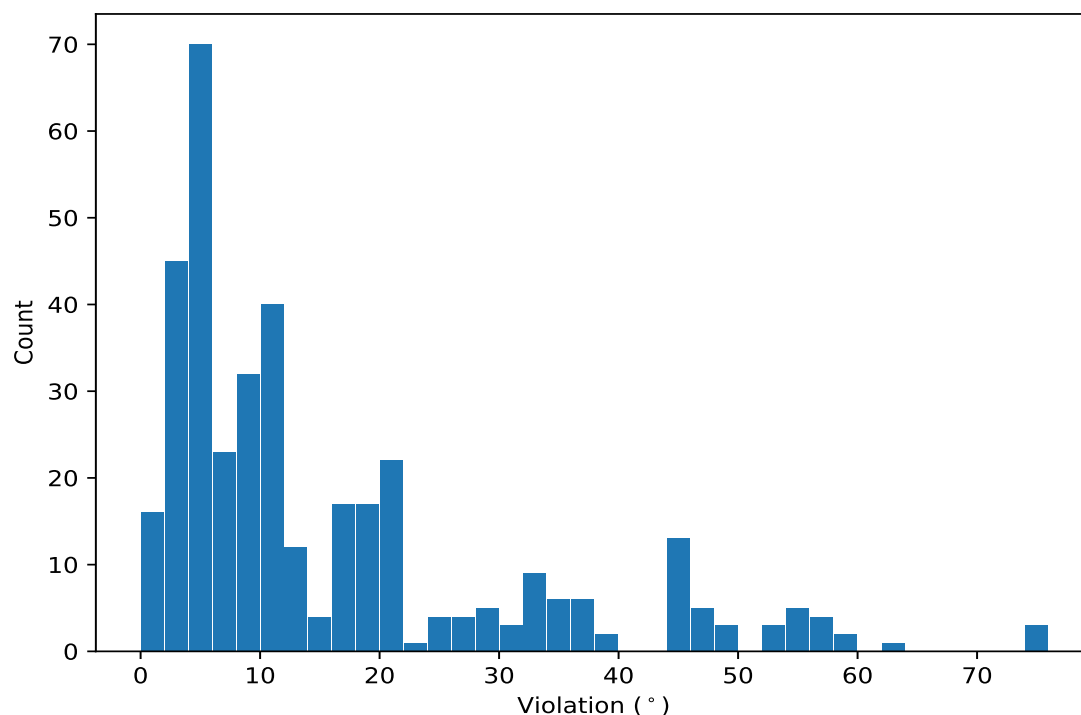
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Media
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	6	22.34	9.53	25.39
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	6	4.7	2.79	5.19
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	5	28.95	5.32	32.08
(1,3)	1:143:A:LYS:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	4	6.18	2.46	6.84
(1,30)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:ASP:N	4	2.54	0.04	2.54
(1,296)	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	1:305:A:GLY:N	3	17.77	0.55	17.84
(1,236)	1:273:A:GLU:N	1:273:A:GLU:CA	1:273:A:GLU:C	1:274:A:ASP:N	2	29.58	3.38	29.58
(1,111)	1:201:A:GLU:C	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	2	12.07	1.06	12.07
(1,234)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:PRO:N	2	7.12	1.73	7.12
(1,114)	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	1:204:A:GLU:N	2	6.13	0.12	6.13
(1,297)	1:304:A:SER:C	1:305:A:GLY:N	1:305:A:GLY:CA	1:305:A:GLY:C	2	3.0	1.0	3.0
(1,309)	1:310:A:LEU:C	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	2	2.9	1.12	2.9

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 (°)
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	9	75.71
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	20	75.3
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	8	75.23
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	13	62.54
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	19	58.69
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	3	58.54
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	12	57.35
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	4	56.55
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	17	56.41
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	18	56.29
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	15	55.86
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	11	55.3
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	5	55.15
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	1	55.05
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	8	54.41
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	9	53.62
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	16	52.89
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	7	52.06
(1,294)	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	1:304:A:SER:N	14	49.43
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	8	49.34
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	10	48.49
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	11	47.3
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	7	46.75
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	19	46.69
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	15	46.29
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	3	46.09
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	20	45.75
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	16	45.71
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	12	45.66
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	4	45.65
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	18	45.65
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	13	45.63
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	1	45.56
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	14	45.43
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	6	45.29
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	2	45.06
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	17	45.01
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	9	44.91
(1,158)	1:228:A:LYS:N	1:228:A:LYS:CA	1:228:A:LYS:C	1:229:A:PHE:N	5	44.32
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	14	38.98
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	20	38.85
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	6	37.86
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	1	37.66
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	17	37.29
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	12	37.01
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	16	36.24
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	11	36.01

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	2	35.6
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	9	35.0
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	5	34.96
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	19	34.55
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	18	34.49
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	13	34.28
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	15	33.91
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	11	33.33
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	3	33.12
(1,236)	1:273:A:GLU:N	1:273:A:GLU:CA	1:273:A:GLU:C	1:274:A:ASP:N	9	32.95
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	4	32.66
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	4	32.56
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	8	32.25
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	4	32.13
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	14	32.08
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	10	31.22
(1,396)	1:356:A:GLU:N	1:356:A:GLU:CA	1:356:A:GLU:C	1:357:A:ASP:N	7	30.82
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	11	30.16
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	20	29.36
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	14	29.18
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	1	28.88
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	18	28.3
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	10	28.23
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	5	27.84
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	20	27.57
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	13	27.56
(1,236)	1:273:A:GLU:N	1:273:A:GLU:CA	1:273:A:GLU:C	1:274:A:ASP:N	8	26.2
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	9	25.65
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	14	25.13
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	6	24.47
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	13	24.45
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	14	23.49
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	18	21.84
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	6	21.36
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	9	21.19
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	19	21.05
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	8	20.93
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	12	20.39
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	13	20.29
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	20	20.28
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	7	20.26
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	4	20.25
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	11	20.23
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	2	20.2
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	10	20.2
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	5	20.17
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	16	20.16
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	19	20.12
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	8	20.09
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	15	20.09
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	14	20.08

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	9	20.06
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	6	20.05
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	1	20.04
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	15	19.91
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	3	19.87
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	12	19.75
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	17	19.74
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	4	19.72
(2,2)	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2:1198:B:VAL:N	18	19.7
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	13	19.66
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	8	19.4
(1,112)	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	1:203:A:GLU:N	9	19.12
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	7	19.03
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	11	18.88
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	16	18.84
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	5	18.8
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	1	18.64
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	9	18.44
(1,296)	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	1:305:A:GLY:N	10	18.4
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	11	18.4
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	10	17.94
(1,296)	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	1:305:A:GLY:N	6	17.84
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	15	17.75
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	17	17.7
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	4	17.68
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	18	17.34
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	8	17.29
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	16	17.29
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	3	17.16
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	13	17.12
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	7	17.1
(1,296)	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	1:305:A:GLY:N	2	17.07
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	13	17.04
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	16	16.7
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	14	16.62
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	19	16.57
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	2	16.26
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	13	15.97
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	6	15.66
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	17	15.26
(1,397)	1:356:A:GLU:C	1:357:A:ASP:N	1:357:A:ASP:CA	1:357:A:ASP:C	20	14.44
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	19	13.48
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	15	13.37
(1,111)	1:201:A:GLU:C	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	14	13.13
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	4	13.1
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	5	12.8
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	13	12.62
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	2	12.35
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	15	12.33
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	18	12.32
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	6	12.15

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	8	12.13
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	1	12.05
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	15	11.89
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	12	11.85
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	14	11.8
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	17	11.73
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	20	11.41
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	10	11.28
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	10	11.21
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	8	11.16
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	19	11.16
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	12	11.13
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	7	11.06
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	4	11.03
(1,111)	1:201:A:GLU:C	1:202:A:LYS:N	1:202:A:LYS:CA	1:202:A:LYS:C	11	11.01
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	16	10.97
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	9	10.89
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	15	10.83
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	19	10.83
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	11	10.81
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	19	10.8
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	7	10.73
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	17	10.72
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	13	10.72
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	9	10.71
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	20	10.69
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	14	10.65
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	8	10.63
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	1	10.62
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	12	10.52
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	2	10.47
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	16	10.46
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	13	10.45
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	1	10.42
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	15	10.39
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	3	10.37
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	20	10.36
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	3	10.35
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	6	10.33
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	18	10.31
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	5	10.07
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	16	10.05
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	7	9.93
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	11	9.9
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	4	9.76
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	3	9.71
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	8	9.71
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	5	9.7
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	18	9.66
(1,159)	1:228:A:LYS:C	1:229:A:PHE:N	1:229:A:PHE:CA	1:229:A:PHE:C	17	9.61
(1,78)	1:184:A:GLY:N	1:184:A:GLY:CA	1:184:A:GLY:C	1:185:A:ALA:N	14	9.61

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	15	9.6
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	14	9.53
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	7	9.47
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	10	9.43
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	4	9.4
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	3	9.37
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	13	9.35
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	14	9.32
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	20	9.18
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	1	9.16
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	11	9.13
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	1	9.06
(1,234)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:PRO:N	7	8.85
(1,2)	1:143:A:LYS:N	1:143:A:LYS:CA	1:143:A:LYS:C	1:144:A:SER:N	6	8.83
(1,3)	1:143:A:LYS:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	18	8.82
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	2	8.76
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	16	8.7
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	13	8.59
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	12	8.57
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	17	8.38
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	6	8.33
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	8	8.25
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	20	8.22
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	9	7.93
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	12	7.89
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	2	7.69
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	2	7.54
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	10	7.5
(1,76)	1:183:A:PHE:N	1:183:A:PHE:CA	1:183:A:PHE:C	1:184:A:GLY:N	11	7.5
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	10	7.46
(1,3)	1:143:A:LYS:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	13	7.39
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	6	7.33
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	9	6.8
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	6	6.74
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	4	6.69
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	1	6.6
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	17	6.55
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	18	6.4
(1,3)	1:143:A:LYS:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	2	6.3
(1,295)	1:303:A:LYS:C	1:304:A:SER:N	1:304:A:SER:CA	1:304:A:SER:C	2	6.28
(1,114)	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	1:204:A:GLU:N	12	6.25
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	19	6.24
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	3	6.23
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	5	6.11
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	5	6.1
(1,114)	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	1:204:A:GLU:N	6	6.01
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	14	5.98
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	19	5.97
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	7	5.93
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	10	5.93
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	19	5.93

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	6	5.92
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	8	5.9
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	8	5.89
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	18	5.88
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	17	5.86
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	2	5.74
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	11	5.73
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	15	5.72
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	18	5.7
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	9	5.67
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	12	5.63
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	6	5.6
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	12	5.55
(1,290)	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	1:302:A:LEU:N	20	5.53
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	1	5.53
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	11	5.52
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	14	5.48
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	1	5.47
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	9	5.47
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	4	5.44
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	16	5.41
(1,234)	1:271:A:GLN:N	1:271:A:GLN:CA	1:271:A:GLN:C	1:272:A:PRO:N	20	5.39
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	17	5.39
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	3	5.27
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	16	5.27
(1,311)	1:311:A:LYS:C	1:312:A:VAL:N	1:312:A:VAL:CA	1:312:A:VAL:C	13	5.25
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	4	5.24
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	15	5.24
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	16	5.24
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	13	5.23
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	13	5.21
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	8	5.16
(2,1)	2:1196:B:THR:C	2:1197:B:GLY:N	2:1197:B:GLY:CA	2:1197:B:GLY:C	20	5.14
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	5	5.13
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	12	5.13
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	20	5.08
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	3	5.06
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	14	5.05
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	2	5.03
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	19	5.02
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	9	4.99
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	9	4.98
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	16	4.94
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	16	4.87
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	6	4.85
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	18	4.83
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	14	4.8
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	11	4.77
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	16	4.72
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	15	4.7
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	11	4.68

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,79)	1:184:A:GLY:C	1:185:A:ALA:N	1:185:A:ALA:CA	1:185:A:ALA:C	7	4.62
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	5	4.49
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	9	4.41
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	17	4.34
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	17	4.34
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	4	4.33
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	11	4.33
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	8	4.27
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	20	4.26
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	7	4.2
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	16	4.14
(1,289)	1:300:A:ASP:C	1:301:A:GLY:N	1:301:A:GLY:CA	1:301:A:GLY:C	7	4.12
(1,309)	1:310:A:LEU:C	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	14	4.02
(1,297)	1:304:A:SER:C	1:305:A:GLY:N	1:305:A:GLY:CA	1:305:A:GLY:C	14	4.01
(1,110)	1:200:A:ASP:N	1:200:A:ASP:CA	1:200:A:ASP:C	1:201:A:GLU:N	18	3.9
(1,113)	1:202:A:LYS:C	1:203:A:GLU:N	1:203:A:GLU:CA	1:203:A:GLU:C	6	3.86
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	12	3.78
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	18	3.76
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	4	3.74
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	8	3.68
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	11	3.68
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	4	3.65
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	13	3.41
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	8	3.25
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	16	3.1
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	7	3.08
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	12	3.05
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	10	3.05
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	16	3.03
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	14	2.99
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	17	2.92
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	6	2.88
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	17	2.85
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	2	2.77
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	15	2.76
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	4	2.73
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	18	2.68
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	3	2.65
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	7	2.64
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	17	2.64
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	14	2.63
(1,287)	1:299:A:LEU:C	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	7	2.62
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	5	2.61
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	1	2.6
(1,30)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:ASP:N	3	2.58
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	12	2.58
(1,30)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:ASP:N	5	2.57
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	18	2.55
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	9	2.55
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	10	2.53
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	9	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:ASP:N	15	2.5
(1,30)	1:157:A:ARG:N	1:157:A:ARG:CA	1:157:A:ARG:C	1:158:A:ASP:N	20	2.5
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	5	2.48
(1,4)	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	1:145:A:ALA:N	4	2.43
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	13	2.24
(1,3)	1:143:A:LYS:C	1:144:A:SER:N	1:144:A:SER:CA	1:144:A:SER:C	20	2.22
(1,292)	1:302:A:LEU:N	1:302:A:LEU:CA	1:302:A:LEU:C	1:303:A:LYS:N	3	2.03
(1,297)	1:304:A:SER:C	1:305:A:GLY:N	1:305:A:GLY:CA	1:305:A:GLY:C	20	2.0
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	1	1.93
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	1	1.92
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	10	1.91
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	14	1.91
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	15	1.81
(1,309)	1:310:A:LEU:C	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	20	1.78
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	15	1.74
(1,310)	1:311:A:LYS:N	1:311:A:LYS:CA	1:311:A:LYS:C	1:312:A:VAL:N	7	1.61
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	19	1.58
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	19	1.57
(1,120)	1:208:A:SER:N	1:208:A:SER:CA	1:208:A:SER:C	1:209:A:TYR:N	11	1.57
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	6	1.42
(1,237)	1:273:A:GLU:C	1:274:A:ASP:N	1:274:A:ASP:CA	1:274:A:ASP:C	20	1.32
(1,293)	1:302:A:LEU:C	1:303:A:LYS:N	1:303:A:LYS:CA	1:303:A:LYS:C	5	1.28
(1,5)	1:144:A:SER:C	1:145:A:ALA:N	1:145:A:ALA:CA	1:145:A:ALA:C	20	1.19
(1,288)	1:300:A:ASP:N	1:300:A:ASP:CA	1:300:A:ASP:C	1:301:A:GLY:N	10	1.09