



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 09:52 AM UTC

PDB ID : 2LOX / pdb_00002lox
BMRB ID : 18229
Title : NMR structure of the complex between the PH domain of the Tfb1 subunit from TFIID and Rad2
Authors : Lafrance-Vanasse, J.; Legault, P.; Omichinski, J.
Deposited on : 2012-01-27

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

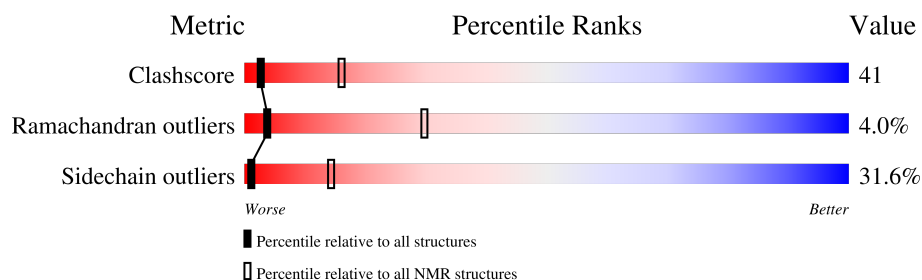
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

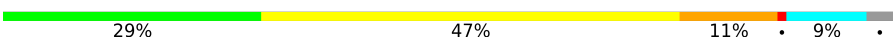
The overall completeness of chemical shifts assignment is 92%.

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	119	
2	B	52	

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:3-A:51, A:58-A:64, A:86-A:114 (85)	0.23	13
2	A:66-A:84 (19)	1.07	12

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

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

The models can be grouped into 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2132 atoms, of which 1072 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RNA polymerase II transcription factor B subunit 1.

Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1820	559	919	161	176	5	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PRO	-	expression tag	UNP P32776
A	116	GLY	-	expression tag	UNP P32776
A	117	ASN	-	expression tag	UNP P32776
A	118	SER	-	expression tag	UNP P32776
A	119	SER	-	expression tag	UNP P32776

- Molecule 2 is a protein called DNA repair protein RAD2.

Mol	Chain	Residues	Atoms					Trace
2	B	20	Total	C	H	N	O	0
			312	100	153	22	37	

There are 3 discrepancies between the modelled and reference sequences:

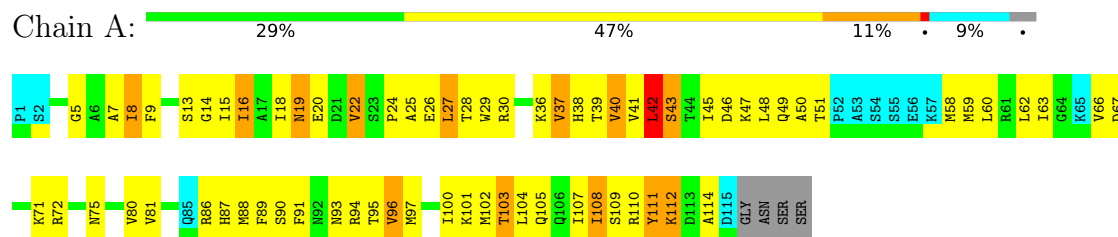
Chain	Residue	Modelled	Actual	Comment	Reference
B	640	GLY	-	expression tag	UNP P07276
B	641	SER	-	expression tag	UNP P07276
B	691	TYR	-	expression tag	UNP P07276

4 Residue-property plots

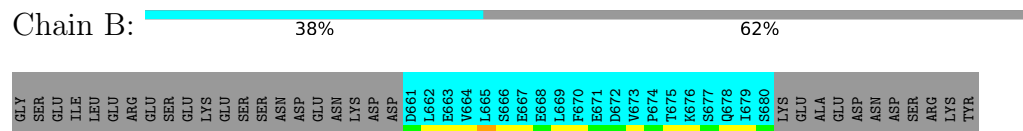
4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: RNA polymerase II transcription factor B subunit 1



- Molecule 2: DNA repair protein RAD2

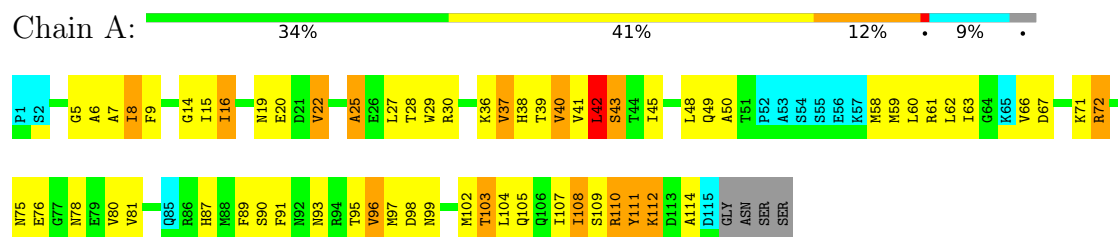


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

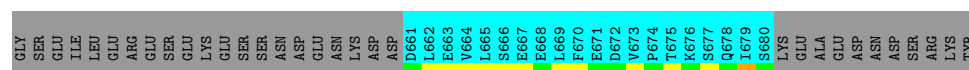
4.2.1 Score per residue for model 1

- Molecule 1: RNA polymerase II transcription factor B subunit 1



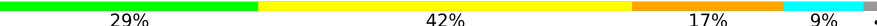
- Molecule 2: DNA repair protein RAD2

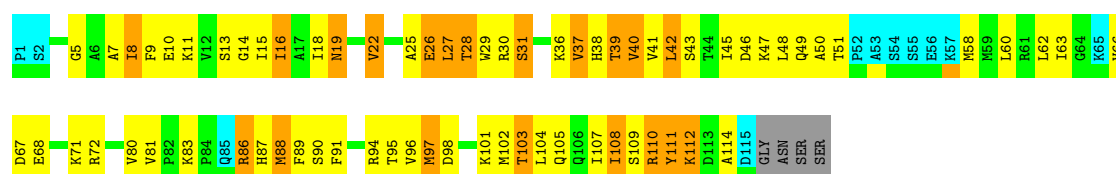
Chain B: 



4.2.2 Score per residue for model 2

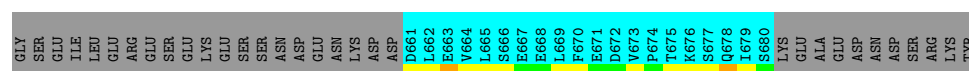
- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 



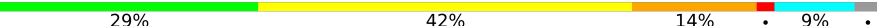
- Molecule 2: DNA repair protein RAD2

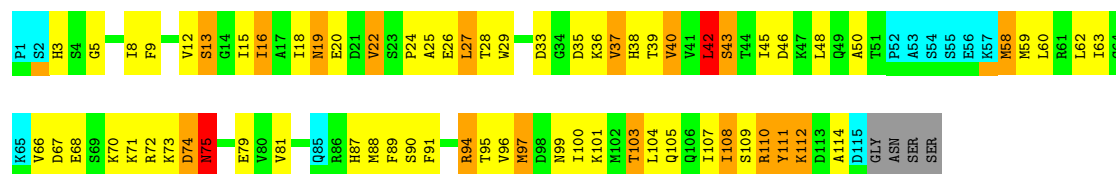
Chain B: 



4.2.3 Score per residue for model 3

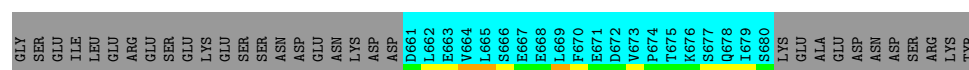
- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 



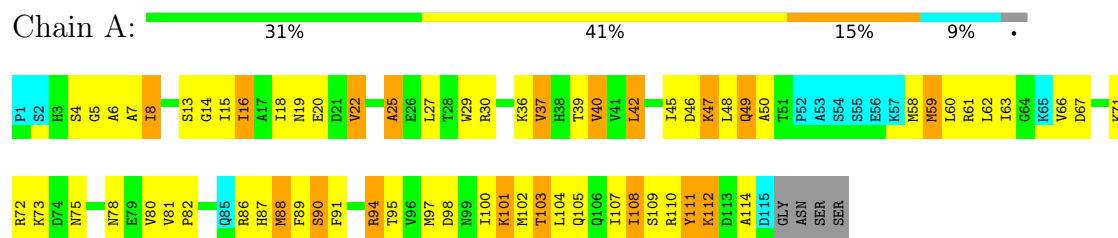
- Molecule 2: DNA repair protein RAD2

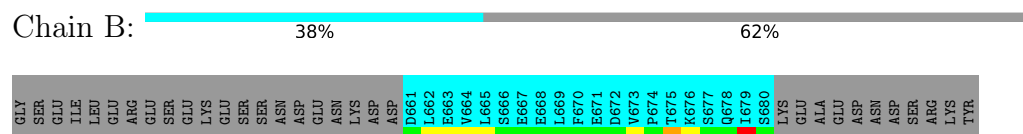
Chain B: 



4.2.4 Score per residue for model 4

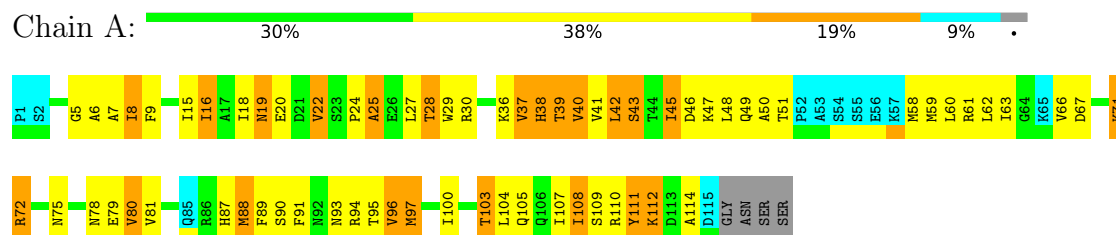
- Molecule 1: RNA polymerase II transcription factor B subunit 1



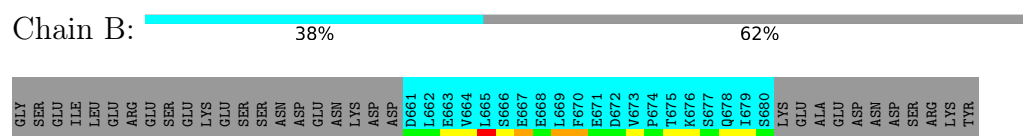


4.2.7 Score per residue for model 7

- Molecule 1: RNA polymerase II transcription factor B subunit 1

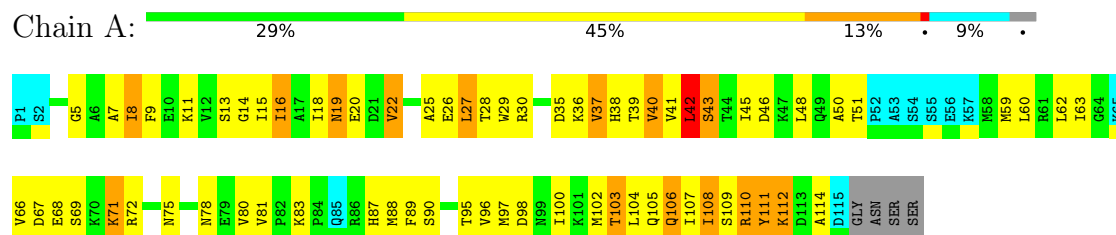


- Molecule 2: DNA repair protein RAD2

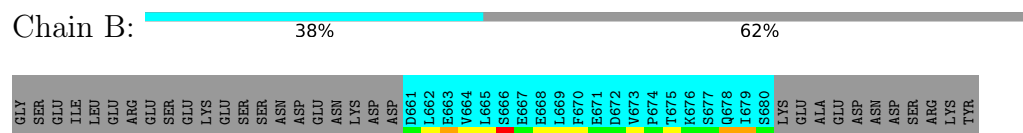


4.2.8 Score per residue for model 8

- Molecule 1: RNA polymerase II transcription factor B subunit 1

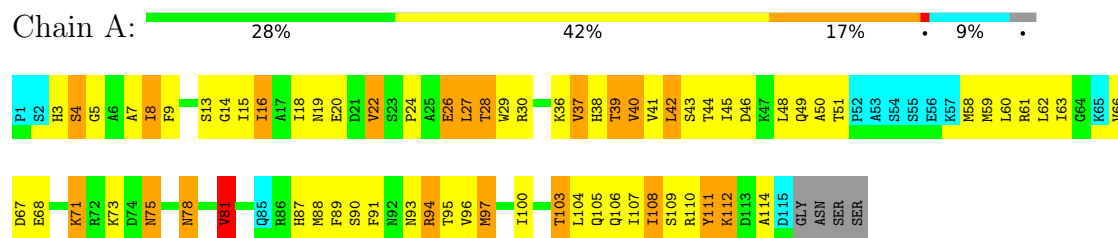


- Molecule 2: DNA repair protein RAD2

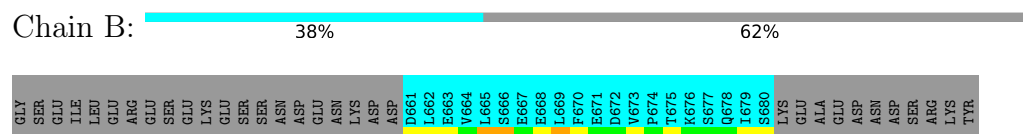


4.2.9 Score per residue for model 9

- Molecule 1: RNA polymerase II transcription factor B subunit 1

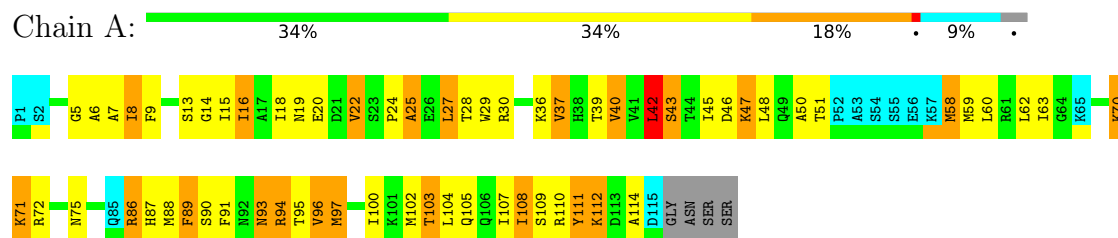


- Molecule 2: DNA repair protein RAD2

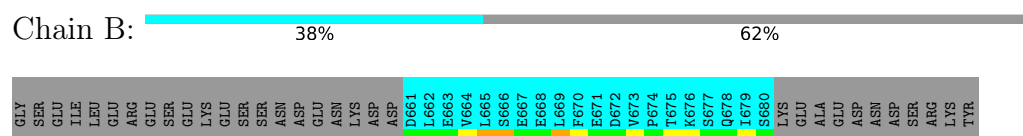


4.2.10 Score per residue for model 10

- Molecule 1: RNA polymerase II transcription factor B subunit 1

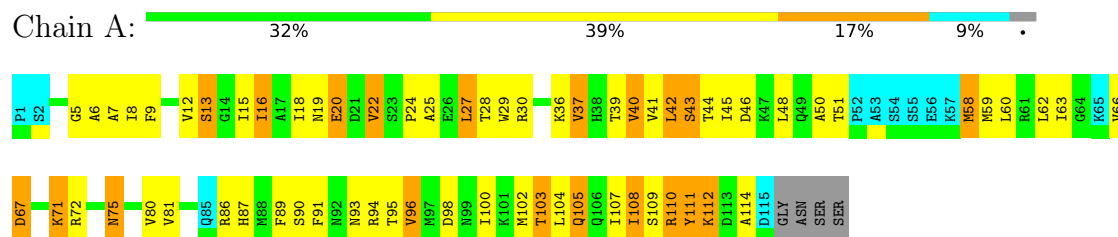


- Molecule 2: DNA repair protein RAD2

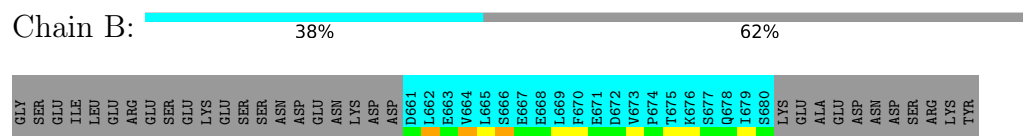


4.2.11 Score per residue for model 11

- Molecule 1: RNA polymerase II transcription factor B subunit 1

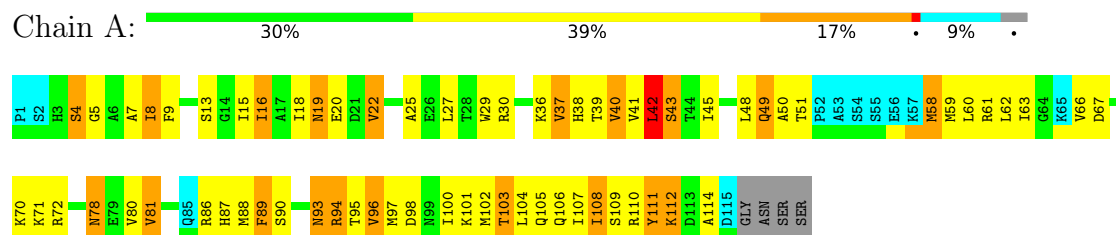


- Molecule 2: DNA repair protein RAD2

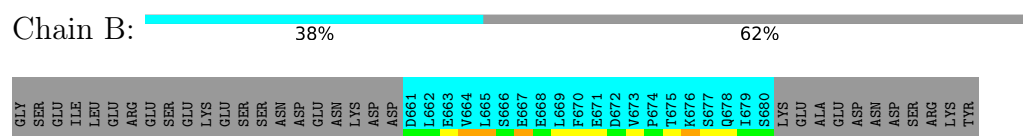


4.2.12 Score per residue for model 12

- Molecule 1: RNA polymerase II transcription factor B subunit 1

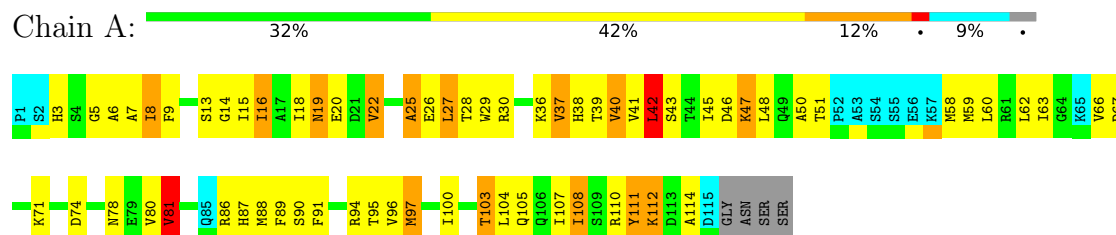


- Molecule 2: DNA repair protein RAD2

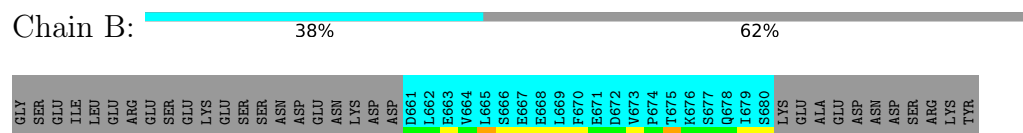


4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: RNA polymerase II transcription factor B subunit 1

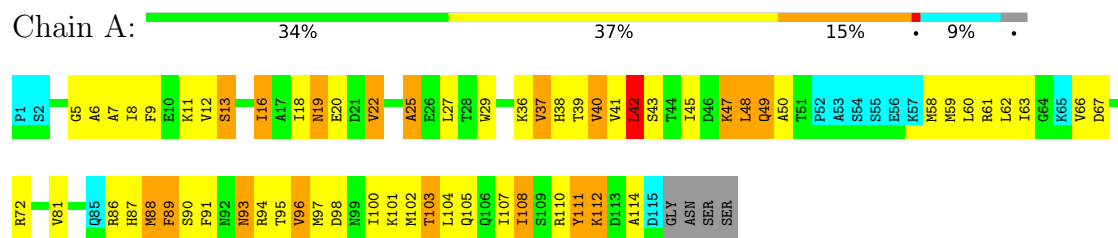


- Molecule 2: DNA repair protein RAD2

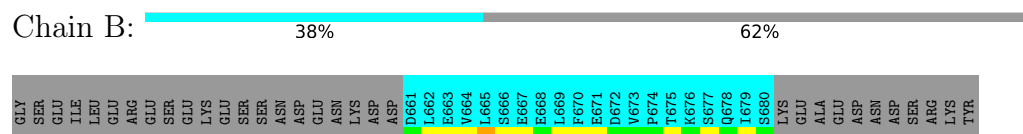


4.2.14 Score per residue for model 14

- Molecule 1: RNA polymerase II transcription factor B subunit 1

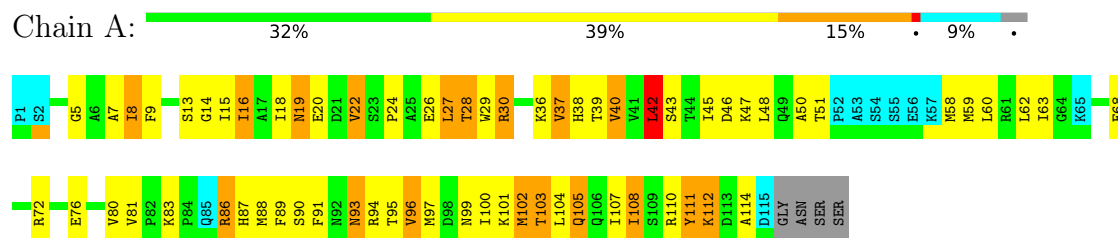


- Molecule 2: DNA repair protein RAD2

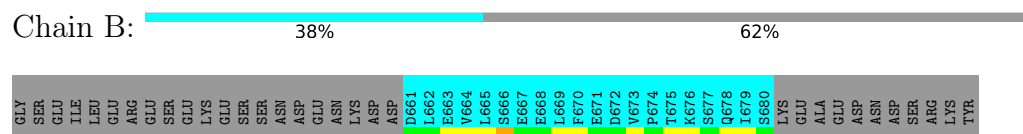


4.2.15 Score per residue for model 15

- Molecule 1: RNA polymerase II transcription factor B subunit 1

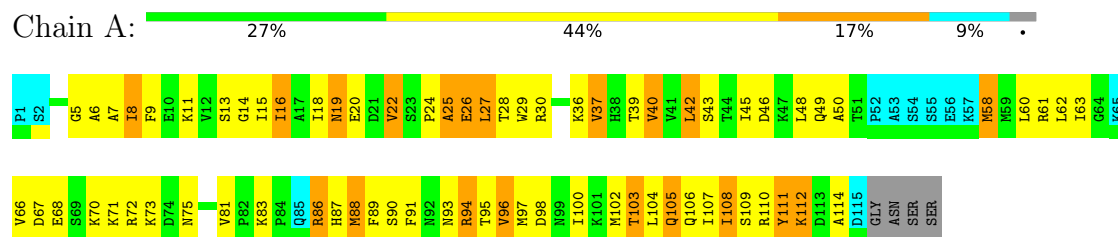


- Molecule 2: DNA repair protein RAD2



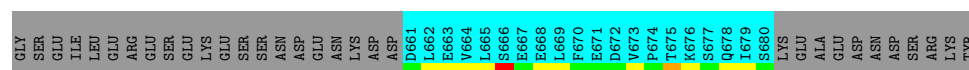
4.2.16 Score per residue for model 16

- Molecule 1: RNA polymerase II transcription factor B subunit 1



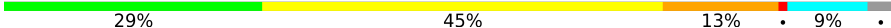
- Molecule 2: DNA repair protein RAD2

Chain B: 



4.2.17 Score per residue for model 17

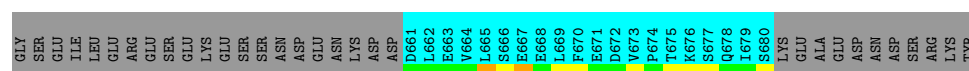
- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 



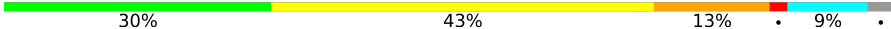
- Molecule 2: DNA repair protein RAD2

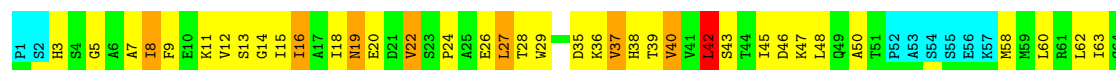
Chain B: 



4.2.18 Score per residue for model 18

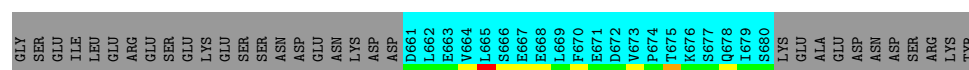
- Molecule 1: RNA polymerase II transcription factor B subunit 1

Chain A: 



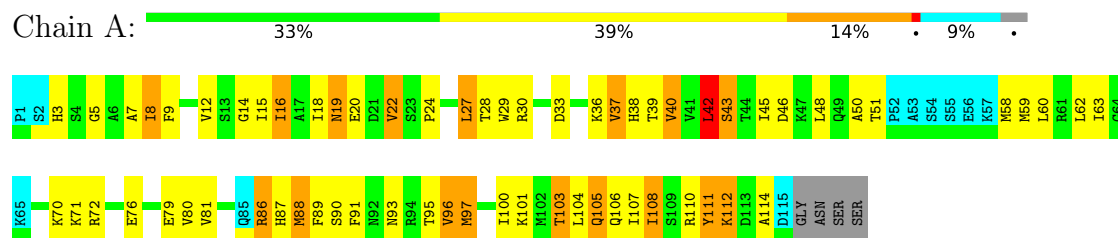
- Molecule 2: DNA repair protein RAD2

Chain B: 

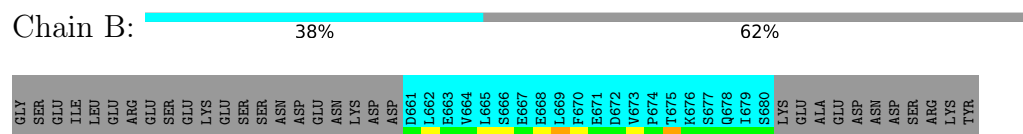


4.2.19 Score per residue for model 19

- Molecule 1: RNA polymerase II transcription factor B subunit 1

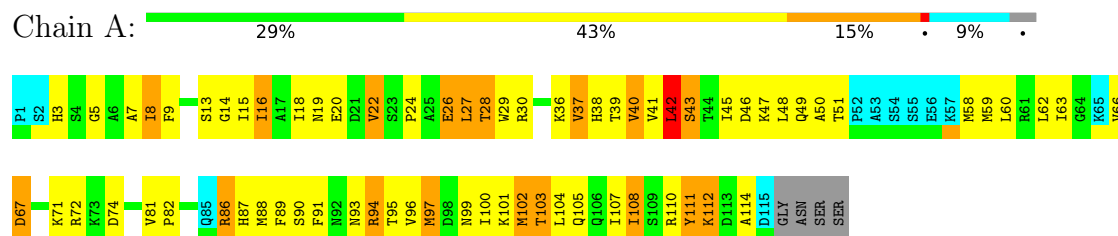


- Molecule 2: DNA repair protein RAD2

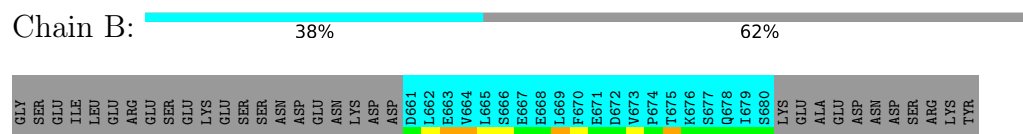


4.2.20 Score per residue for model 20

- Molecule 1: RNA polymerase II transcription factor B subunit 1



- Molecule 2: DNA repair protein RAD2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	
CNS	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1955
Number of shifts mapped to atoms	1703
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	820	839	836	69±5
2	B	0	0	0	0±0
All	All	16400	16780	16720	1372

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 41.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:A:104:LEU:HD13	0.99	1.34	1	18
1:A:107:ILE:HG22	1:A:111:TYR:CE1	0.85	2.07	7	20
1:A:16:ILE:HD11	1:A:89:PHE:CD2	0.84	2.06	19	9
1:A:16:ILE:HD11	1:A:89:PHE:CD1	0.84	2.06	13	11
1:A:107:ILE:HG22	1:A:111:TYR:HE1	0.83	1.33	7	20
1:A:27:LEU:HD12	1:A:27:LEU:C	0.81	1.99	10	15
1:A:48:LEU:HD22	1:A:105:GLN:NE2	0.81	1.90	14	1
1:A:42:LEU:HD11	1:A:104:LEU:CD2	0.80	2.07	4	19
1:A:45:ILE:HD12	1:A:62:LEU:HB3	0.79	1.52	1	20
1:A:14:GLY:O	1:A:15:ILE:HD13	0.79	1.78	6	15
1:A:18:ILE:HD13	1:A:103:THR:HG22	0.77	1.56	8	10
1:A:42:LEU:HD11	1:A:104:LEU:HD23	0.75	1.57	4	2
1:A:49:GLN:HG3	1:A:63:ILE:HD11	0.74	1.60	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:ILE:HD12	1:A:62:LEU:CB	0.73	2.14	1	20
1:A:16:ILE:HD11	1:A:89:PHE:CG	0.73	2.19	10	20
1:A:48:LEU:CD1	1:A:104:LEU:HD13	0.72	2.14	9	10
1:A:51:THR:OG1	1:A:97:MET:HE1	0.72	1.84	19	1
1:A:28:THR:HG22	1:A:37:VAL:CG2	0.70	2.16	20	15
1:A:58:MET:HE2	1:A:94:ARG:N	0.70	2.01	2	4
1:A:112:LYS:N	1:A:112:LYS:HD2	0.70	2.02	1	20
1:A:51:THR:O	1:A:97:MET:HE1	0.69	1.87	10	4
1:A:18:ILE:HD11	1:A:100:ILE:HG23	0.67	1.67	11	4
1:A:18:ILE:HD13	1:A:103:THR:CG2	0.67	2.20	11	10
1:A:100:ILE:HG22	1:A:104:LEU:HD11	0.67	1.65	8	8
1:A:48:LEU:HD11	1:A:104:LEU:CD1	0.67	2.17	1	9
1:A:42:LEU:HD11	1:A:104:LEU:HD22	0.67	1.66	17	17
1:A:63:ILE:HG23	1:A:86:ARG:HG2	0.66	1.67	2	7
1:A:41:VAL:HG12	1:A:43:SER:OG	0.66	1.89	2	1
1:A:62:LEU:HD21	1:A:104:LEU:HD22	0.65	1.67	12	2
1:A:94:ARG:HD2	1:A:97:MET:HE3	0.65	1.68	5	1
1:A:63:ILE:HD12	1:A:86:ARG:HD3	0.65	1.69	12	3
1:A:58:MET:HE3	1:A:94:ARG:HD3	0.65	1.68	16	1
1:A:58:MET:HE3	1:A:94:ARG:N	0.65	2.05	20	6
1:A:50:ALA:HB1	1:A:60:LEU:CD2	0.65	2.22	1	20
1:A:18:ILE:HD13	1:A:103:THR:HB	0.65	1.66	9	2
1:A:59:MET:HE3	1:A:88:MET:CE	0.64	2.21	4	1
1:A:48:LEU:HD23	1:A:105:GLN:HE21	0.64	1.53	6	1
1:A:98:ASP:O	1:A:102:MET:HE3	0.64	1.93	18	6
1:A:7:ALA:HB2	1:A:91:PHE:CZ	0.62	2.28	13	11
1:A:48:LEU:HD21	1:A:104:LEU:HB2	0.62	1.70	13	2
1:A:81:VAL:O	1:A:81:VAL:HG13	0.62	1.93	20	2
1:A:27:LEU:C	1:A:27:LEU:CD1	0.62	2.73	10	15
1:A:81:VAL:HG12	1:A:81:VAL:O	0.62	1.94	9	4
1:A:27:LEU:HD12	1:A:27:LEU:O	0.62	1.94	6	11
1:A:8:ILE:N	1:A:8:ILE:HD13	0.61	2.10	4	17
1:A:7:ALA:HB2	1:A:91:PHE:CE1	0.61	2.30	2	10
1:A:48:LEU:HD12	1:A:62:LEU:HD23	0.60	1.71	14	1
1:A:27:LEU:HB3	1:A:40:VAL:CG1	0.60	2.25	12	5
1:A:108:ILE:HA	1:A:111:TYR:CE2	0.60	2.31	6	20
1:A:59:MET:SD	1:A:88:MET:HE2	0.60	2.37	7	1
1:A:80:VAL:HG12	1:A:82:PRO:HD3	0.60	1.72	4	1
1:A:19:ASN:O	1:A:22:VAL:HG23	0.59	1.97	3	19
1:A:58:MET:HE2	1:A:94:ARG:H	0.59	1.57	12	6
1:A:68:GLU:HA	1:A:81:VAL:HG13	0.59	1.73	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:TYR:N	1:A:111:TYR:CD1	0.58	2.71	5	20
1:A:50:ALA:CB	1:A:60:LEU:HD22	0.58	2.28	1	20
1:A:48:LEU:HD22	1:A:105:GLN:CD	0.58	2.23	14	1
1:A:18:ILE:HD12	1:A:103:THR:HB	0.57	1.75	13	7
1:A:60:LEU:HD12	1:A:91:PHE:CZ	0.57	2.35	19	1
1:A:58:MET:HE3	1:A:94:ARG:HG3	0.57	1.74	10	1
1:A:25:ALA:HB2	1:A:107:ILE:HG21	0.57	1.75	14	9
1:A:58:MET:HE3	1:A:94:ARG:HB2	0.57	1.75	11	2
1:A:93:ASN:HB3	1:A:96:VAL:HG23	0.57	1.76	14	6
1:A:14:GLY:C	1:A:15:ILE:HD13	0.56	2.24	6	12
1:A:48:LEU:HD22	1:A:108:ILE:CD1	0.56	2.31	7	1
1:A:8:ILE:HD12	1:A:13:SER:HA	0.56	1.76	11	3
1:A:62:LEU:HD12	1:A:89:PHE:CE1	0.56	2.36	14	2
1:A:16:ILE:HD11	1:A:89:PHE:CE1	0.55	2.36	3	3
1:A:48:LEU:HD23	1:A:105:GLN:HG2	0.55	1.78	5	3
1:A:19:ASN:OD1	1:A:22:VAL:HG22	0.54	2.02	20	1
1:A:28:THR:HG23	1:A:39:THR:HG23	0.54	1.80	7	3
1:A:27:LEU:HB3	1:A:40:VAL:HG12	0.54	1.79	4	5
1:A:7:ALA:C	1:A:8:ILE:HD13	0.54	2.28	1	17
1:A:98:ASP:O	1:A:102:MET:HE2	0.54	2.03	17	4
1:A:62:LEU:HD12	1:A:89:PHE:HE1	0.54	1.63	14	2
1:A:58:MET:HE3	1:A:94:ARG:H	0.53	1.62	15	4
1:A:89:PHE:CD1	1:A:89:PHE:N	0.53	2.77	10	5
1:A:49:GLN:O	1:A:61:ARG:N	0.53	2.39	14	8
1:A:40:VAL:CG2	1:A:87:HIS:CD2	0.53	2.92	5	20
1:A:16:ILE:CD1	1:A:89:PHE:CD1	0.53	2.92	3	8
1:A:16:ILE:CG2	1:A:100:ILE:HD12	0.53	2.34	16	13
1:A:49:GLN:NE2	1:A:63:ILE:HD11	0.53	2.19	7	1
1:A:5:GLY:O	1:A:16:ILE:N	0.52	2.40	2	14
1:A:49:GLN:CG	1:A:63:ILE:HD11	0.52	2.31	1	1
1:A:50:ALA:HB1	1:A:60:LEU:HD22	0.52	1.79	1	5
1:A:100:ILE:HG22	1:A:104:LEU:HD12	0.52	1.81	12	2
1:A:71:LYS:HG2	1:A:81:VAL:HG23	0.52	1.80	11	1
1:A:51:THR:HG23	1:A:59:MET:HB2	0.51	1.82	17	7
1:A:63:ILE:HD12	1:A:86:ARG:HG2	0.51	1.82	17	4
1:A:15:ILE:N	1:A:30:ARG:O	0.51	2.43	16	17
1:A:16:ILE:O	1:A:16:ILE:HG22	0.50	2.05	14	5
1:A:112:LYS:N	1:A:112:LYS:CD	0.50	2.72	13	19
1:A:81:VAL:O	1:A:81:VAL:CG1	0.50	2.59	9	5
1:A:59:MET:SD	1:A:88:MET:HE1	0.50	2.46	4	1
1:A:49:GLN:OE1	1:A:63:ILE:HD11	0.50	2.06	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:ILE:HD12	1:A:86:ARG:CD	0.50	2.37	6	1
1:A:27:LEU:HD22	1:A:40:VAL:HB	0.50	1.83	7	5
1:A:9:PHE:CZ	1:A:38:HIS:CD2	0.50	3.00	7	6
1:A:59:MET:HE3	1:A:88:MET:HE2	0.49	1.84	4	1
1:A:50:ALA:CB	1:A:60:LEU:CD2	0.49	2.91	12	20
1:A:8:ILE:N	1:A:8:ILE:CD1	0.49	2.75	20	17
1:A:27:LEU:HD21	1:A:62:LEU:CD1	0.49	2.37	20	9
1:A:8:ILE:HG23	1:A:12:VAL:O	0.49	2.07	18	5
1:A:27:LEU:HG	1:A:40:VAL:CG1	0.49	2.38	5	15
1:A:29:TRP:O	1:A:37:VAL:HA	0.48	2.07	2	19
1:A:48:LEU:HD13	1:A:108:ILE:HD11	0.48	1.84	7	2
1:A:50:ALA:HB3	1:A:101:LYS:HD2	0.48	1.85	3	3
1:A:9:PHE:CE1	1:A:38:HIS:CD2	0.48	3.00	20	2
1:A:3:HIS:HA	1:A:103:THR:HG21	0.48	1.85	9	1
1:A:66:VAL:HG22	1:A:67:ASP:N	0.48	2.24	14	16
1:A:9:PHE:CE1	1:A:38:HIS:CE1	0.48	3.02	14	7
1:A:93:ASN:CB	1:A:96:VAL:HG23	0.48	2.38	12	10
1:A:9:PHE:HB3	1:A:29:TRP:CE2	0.48	2.43	7	14
1:A:45:ILE:CG2	1:A:62:LEU:HB3	0.47	2.38	12	20
1:A:46:ASP:N	1:A:63:ILE:O	0.47	2.48	2	17
1:A:9:PHE:CB	1:A:29:TRP:CE2	0.47	2.97	18	3
1:A:42:LEU:CB	1:A:111:TYR:OH	0.47	2.63	7	12
1:A:48:LEU:HD22	1:A:108:ILE:HG13	0.47	1.84	7	1
1:A:110:ARG:O	1:A:114:ALA:CB	0.47	2.63	18	20
1:A:112:LYS:HD2	1:A:112:LYS:H	0.47	1.69	12	19
1:A:51:THR:HG23	1:A:59:MET:HB3	0.47	1.86	7	1
1:A:16:ILE:HG22	1:A:100:ILE:HD12	0.47	1.87	9	11
1:A:25:ALA:CB	1:A:107:ILE:HG21	0.46	2.40	7	7
1:A:107:ILE:O	1:A:110:ARG:HB2	0.46	2.10	3	5
1:A:100:ILE:HG22	1:A:104:LEU:CD1	0.46	2.40	16	4
1:A:26:GLU:OE1	1:A:41:VAL:HG22	0.46	2.10	13	1
1:A:58:MET:HE3	1:A:94:ARG:CD	0.46	2.39	16	1
1:A:9:PHE:CE2	1:A:38:HIS:CB	0.46	2.99	2	2
1:A:15:ILE:O	1:A:29:TRP:HA	0.46	2.10	8	13
1:A:27:LEU:HD13	1:A:62:LEU:HD11	0.46	1.87	4	4
1:A:26:GLU:HA	1:A:40:VAL:O	0.46	2.10	6	10
1:A:7:ALA:HB1	1:A:89:PHE:HB3	0.46	1.88	20	2
1:A:5:GLY:N	1:A:16:ILE:O	0.46	2.49	4	5
1:A:58:MET:HE3	1:A:94:ARG:CG	0.46	2.41	10	1
1:A:16:ILE:CD1	1:A:89:PHE:CD2	0.46	2.93	19	5
1:A:112:LYS:H	1:A:112:LYS:CD	0.45	2.23	4	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:HIS:O	1:A:18:ILE:N	0.45	2.47	20	7
1:A:40:VAL:HG22	1:A:45:ILE:HD11	0.45	1.87	7	4
1:A:102:MET:HG3	1:A:103:THR:N	0.45	2.26	5	1
1:A:48:LEU:HD23	1:A:105:GLN:NE2	0.45	2.26	6	2
1:A:24:PRO:CB	1:A:43:SER:CB	0.45	2.94	9	12
1:A:40:VAL:CG2	1:A:87:HIS:CG	0.45	2.99	20	8
1:A:112:LYS:CD	1:A:112:LYS:H	0.45	2.23	11	9
1:A:9:PHE:CZ	1:A:38:HIS:ND1	0.45	2.85	6	2
1:A:104:LEU:O	1:A:108:ILE:HG13	0.45	2.12	16	4
1:A:5:GLY:O	1:A:16:ILE:O	0.45	2.34	2	1
1:A:5:GLY:HA3	1:A:96:VAL:HG12	0.45	1.86	14	1
1:A:80:VAL:O	1:A:81:VAL:C	0.44	2.60	11	8
1:A:108:ILE:O	1:A:112:LYS:HD3	0.44	2.12	16	15
1:A:5:GLY:O	1:A:16:ILE:HB	0.44	2.12	8	10
1:A:71:LYS:HG2	1:A:81:VAL:HG22	0.44	1.88	7	1
1:A:68:GLU:CG	1:A:81:VAL:HG11	0.44	2.42	16	1
1:A:47:LYS:CG	1:A:63:ILE:CG1	0.44	2.96	13	9
1:A:58:MET:HE3	1:A:93:ASN:CA	0.44	2.43	20	2
1:A:6:ALA:O	1:A:91:PHE:CD2	0.44	2.70	7	8
1:A:4:SER:C	1:A:100:ILE:HD11	0.44	2.38	12	3
1:A:107:ILE:O	1:A:111:TYR:CE1	0.44	2.71	13	20
1:A:16:ILE:CD1	1:A:89:PHE:CG	0.44	3.00	14	3
1:A:28:THR:HG22	1:A:37:VAL:HG21	0.44	1.89	19	2
1:A:99:ASN:O	1:A:103:THR:OG1	0.44	2.35	5	6
1:A:9:PHE:CB	1:A:29:TRP:CD2	0.44	3.01	2	3
1:A:9:PHE:HB2	1:A:29:TRP:CE2	0.43	2.48	2	1
1:A:91:PHE:CD2	1:A:97:MET:CA	0.43	3.01	9	3
1:A:63:ILE:HA	1:A:86:ARG:HB3	0.43	1.88	16	1
1:A:49:GLN:CD	1:A:63:ILE:HD11	0.43	2.38	2	1
1:A:81:VAL:HG22	1:A:81:VAL:O	0.43	2.13	4	1
1:A:9:PHE:CE2	1:A:38:HIS:CG	0.43	3.05	6	1
1:A:99:ASN:O	1:A:102:MET:HE2	0.43	2.12	15	1
1:A:104:LEU:O	1:A:108:ILE:CG1	0.43	2.67	8	5
1:A:101:LYS:O	1:A:105:GLN:NE2	0.43	2.52	18	6
1:A:27:LEU:CD2	1:A:62:LEU:HD11	0.43	2.43	20	2
1:A:108:ILE:HA	1:A:111:TYR:CZ	0.43	2.48	18	12
1:A:41:VAL:CG1	1:A:44:THR:HG23	0.43	2.44	9	2
1:A:45:ILE:CD1	1:A:87:HIS:CD2	0.43	3.01	7	2
1:A:9:PHE:HB3	1:A:29:TRP:CZ2	0.43	2.49	7	2
1:A:45:ILE:CG2	1:A:47:LYS:O	0.43	2.66	5	3
1:A:48:LEU:CD1	1:A:62:LEU:HD23	0.43	2.43	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:LEU:HD12	1:A:28:THR:N	0.43	2.29	8	3
1:A:8:ILE:O	1:A:89:PHE:HA	0.43	2.13	14	1
1:A:59:MET:HG3	1:A:90:SER:HA	0.43	1.89	4	1
1:A:9:PHE:CZ	1:A:38:HIS:CG	0.43	3.07	12	1
1:A:48:LEU:HD23	1:A:105:GLN:CG	0.43	2.44	7	1
1:A:48:LEU:HD13	1:A:62:LEU:HD23	0.42	1.90	5	1
1:A:48:LEU:HD22	1:A:108:ILE:CG1	0.42	2.44	7	1
1:A:9:PHE:CD2	1:A:89:PHE:CE1	0.42	3.07	18	2
1:A:9:PHE:C	1:A:9:PHE:CD1	0.42	2.97	3	10
1:A:45:ILE:HA	1:A:63:ILE:O	0.42	2.14	13	6
1:A:9:PHE:CD1	1:A:9:PHE:C	0.42	2.97	15	2
1:A:102:MET:HG2	1:A:103:THR:N	0.42	2.29	20	1
1:A:50:ALA:HB2	1:A:60:LEU:HD22	0.42	1.91	5	8
1:A:45:ILE:CD1	1:A:62:LEU:HB3	0.42	2.40	16	5
1:A:108:ILE:O	1:A:111:TYR:N	0.42	2.49	11	2
1:A:42:LEU:N	1:A:42:LEU:CD2	0.42	2.83	9	15
1:A:47:LYS:HG2	1:A:63:ILE:CG1	0.42	2.45	5	1
1:A:18:ILE:HG21	1:A:107:ILE:CD1	0.42	2.45	20	1
1:A:8:ILE:HD12	1:A:13:SER:CA	0.42	2.44	3	2
1:A:25:ALA:O	1:A:26:GLU:CG	0.42	2.67	13	1
1:A:27:LEU:CD2	1:A:40:VAL:HB	0.41	2.45	7	4
1:A:103:THR:O	1:A:106:GLN:HG3	0.41	2.14	8	1
1:A:5:GLY:N	1:A:100:ILE:HD11	0.41	2.30	18	2
1:A:20:GLU:HG3	1:A:107:ILE:HD11	0.41	1.91	11	1
1:A:94:ARG:O	1:A:98:ASP:CB	0.41	2.69	12	1
1:A:99:ASN:O	1:A:102:MET:HG2	0.41	2.15	5	1
1:A:86:ARG:CD	1:A:86:ARG:N	0.41	2.83	16	1
1:A:58:MET:HE3	1:A:93:ASN:C	0.41	2.40	20	1
1:A:99:ASN:O	1:A:102:MET:CG	0.41	2.69	5	1
1:A:60:LEU:CD1	1:A:100:ILE:CG2	0.41	2.98	7	1
1:A:24:PRO:CB	1:A:43:SER:HB2	0.41	2.46	17	3
1:A:103:THR:O	1:A:106:GLN:CG	0.41	2.69	16	1
1:A:63:ILE:CD1	1:A:86:ARG:CG	0.41	2.98	19	1
1:A:48:LEU:CD1	1:A:62:LEU:CD2	0.41	2.98	5	1
1:A:18:ILE:CD1	1:A:103:THR:HB	0.41	2.46	20	3
1:A:72:ARG:N	1:A:80:VAL:O	0.41	2.54	7	1
1:A:48:LEU:HD22	1:A:105:GLN:CG	0.41	2.46	14	1
1:A:40:VAL:CG1	1:A:42:LEU:HD22	0.41	2.46	1	2
1:A:58:MET:HE2	1:A:93:ASN:N	0.41	2.31	6	1
1:A:60:LEU:O	1:A:89:PHE:N	0.41	2.54	9	1
1:A:49:GLN:N	1:A:61:ARG:O	0.41	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:O	1:A:81:VAL:O	0.41	2.38	13	1
1:A:48:LEU:HD22	1:A:105:GLN:HG2	0.41	1.92	14	1
1:A:80:VAL:HG12	1:A:81:VAL:N	0.41	2.31	19	1
1:A:22:VAL:HG21	1:A:26:GLU:CG	0.41	2.46	20	1
1:A:41:VAL:C	1:A:43:SER:N	0.41	2.79	20	6
1:A:3:HIS:CE1	1:A:18:ILE:O	0.40	2.73	9	1
1:A:72:ARG:CD	1:A:72:ARG:N	0.40	2.85	1	1
1:A:74:ASP:O	1:A:75:ASN:CB	0.40	2.70	3	1
1:A:7:ALA:CB	1:A:91:PHE:CE1	0.40	3.04	11	1
1:A:5:GLY:CA	1:A:96:VAL:CG1	0.40	2.99	14	1
1:A:41:VAL:O	1:A:43:SER:N	0.40	2.54	14	1
1:A:28:THR:CG2	1:A:37:VAL:CG2	0.40	2.99	5	1
1:A:24:PRO:CG	1:A:43:SER:HB2	0.40	2.46	7	1
1:A:27:LEU:CD2	1:A:62:LEU:CD1	0.40	2.99	10	1
1:A:81:VAL:HG13	1:A:81:VAL:O	0.40	2.17	11	1
1:A:12:VAL:CG1	1:A:13:SER:N	0.40	2.85	18	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	104/119 (87%)	85±2 (82±2%)	14±2 (14±2%)	4±1 (4±1%)	4	30
2	B	0	-	-	-	-	-
All	All	2080/3420 (61%)	1708 (82%)	289 (14%)	83 (4%)	4	30

All 13 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	71	LYS	18
1	A	42	LEU	13
1	A	75	ASN	11
1	A	25	ALA	10
1	A	78	ASN	8

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Mol	Chain	Res	Type	Models (Total)
1	A	93	ASN	6
1	A	81	VAL	4
1	A	79	GLU	3
1	A	45	ILE	3
1	A	70	LYS	3
1	A	82	PRO	2
1	A	31	SER	1
1	A	22	VAL	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	93/106 (88%)	64±3 (68±3%)	29±3 (32±3%)	1 14
2	B	0	-	-	-
All	All	1860/3120 (60%)	1273 (68%)	587 (32%)	1 14

All 63 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	16	ILE	20
1	A	22	VAL	20
1	A	36	LYS	20
1	A	37	VAL	20
1	A	39	THR	20
1	A	40	VAL	20
1	A	90	SER	20
1	A	95	THR	20
1	A	103	THR	20
1	A	108	ILE	20
1	A	111	TYR	20
1	A	112	LYS	20
1	A	20	GLU	19
1	A	42	LEU	19
1	A	96	VAL	19
1	A	97	MET	19

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Mol	Chain	Res	Type	Models (Total)
1	A	72	ARG	18
1	A	8	ILE	17
1	A	13	SER	15
1	A	19	ASN	15
1	A	27	LEU	15
1	A	43	SER	12
1	A	109	SER	12
1	A	94	ARG	12
1	A	58	MET	10
1	A	105	GLN	10
1	A	88	MET	9
1	A	28	THR	7
1	A	11	LYS	7
1	A	26	GLU	7
1	A	86	ARG	7
1	A	73	LYS	7
1	A	110	ARG	6
1	A	47	LYS	6
1	A	68	GLU	6
1	A	106	GLN	6
1	A	70	LYS	5
1	A	75	ASN	5
1	A	49	GLN	5
1	A	76	GLU	4
1	A	83	LYS	4
1	A	100	ILE	4
1	A	35	ASP	3
1	A	74	ASP	3
1	A	71	LYS	3
1	A	81	VAL	3
1	A	89	PHE	3
1	A	102	MET	3
1	A	33	ASP	2
1	A	38	HIS	2
1	A	61	ARG	2
1	A	79	GLU	2
1	A	4	SER	2
1	A	78	ASN	2
1	A	67	ASP	2
1	A	10	GLU	1
1	A	31	SER	1
1	A	59	MET	1

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Mol	Chain	Res	Type	Models (Total)
1	A	101	LYS	1
1	A	80	VAL	1
1	A	69	SER	1
1	A	48	LEU	1
1	A	30	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 92% for the well-defined parts and 93% 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	1955
Number of shifts mapped to atoms	1703
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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

- No matching atom found in the structure. All 252 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	GLY	H	8.217	.	1
1	A	116	GLY	HA2	4.003	0.001	1
1	A	116	GLY	HA3	4.003	0.001	1
1	A	116	GLY	C	174.366	.	1
1	A	116	GLY	CA	45.802	.	1
1	A	116	GLY	N	108.816	.	1
1	A	117	ASN	H	8.317	.	1
1	A	117	ASN	HA	4.852	0.001	1
1	A	117	ASN	HB2	2.822	0.002	2
1	A	117	ASN	HB3	2.9	0.003	2
1	A	117	ASN	HD21	7.663	.	1
1	A	117	ASN	HD22	6.941	.	1
1	A	117	ASN	C	175.359	.	1
1	A	117	ASN	CA	53.229	0.022	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	117	ASN	CB	39.193	0.012	1
1	A	117	ASN	N	118.871	.	1
1	A	117	ASN	ND2	113.528	.	1
1	A	118	SER	H	8.329	.	1
1	A	118	SER	HA	4.557	0.003	1
1	A	118	SER	HB2	3.931	0.005	2
1	A	118	SER	HB3	3.931	0.005	2
1	A	118	SER	C	173.789	.	1
1	A	118	SER	CA	58.41	0.013	1
1	A	118	SER	CB	63.939	0.001	1
1	A	118	SER	N	116.555	.	1
1	A	119	SER	H	8.016	.	1
1	A	119	SER	HA	4.306	0.002	1
1	A	119	SER	HB2	3.875	0.002	2
1	A	119	SER	HB3	3.875	0.002	2
1	A	119	SER	CA	60.007	0.019	1
1	A	119	SER	CB	64.719	0.043	1
1	A	119	SER	N	123.353	.	1
1	B	643	ILE	C	176.117	.	1
1	B	643	ILE	CA	61.194	.	1
1	B	643	ILE	CB	38.518	.	1
1	B	644	LEU	H	8.243	.	1
1	B	644	LEU	HA	4.372	.	1
1	B	644	LEU	HB2	1.685	.	1
1	B	644	LEU	HB3	1.685	.	1
1	B	644	LEU	HD11	0.967	.	1
1	B	644	LEU	HD12	0.967	.	1
1	B	644	LEU	HD13	0.967	.	1
1	B	644	LEU	HD21	0.967	.	1
1	B	644	LEU	HD22	0.967	.	1
1	B	644	LEU	HD23	0.967	.	1
1	B	644	LEU	HG	1.685	.	1
1	B	644	LEU	C	176.764	.	1
1	B	644	LEU	CA	55.212	.	1
1	B	644	LEU	CB	42.369	.	1
1	B	644	LEU	CD1	24.882	.	2
1	B	644	LEU	CD2	23.922	.	2
1	B	644	LEU	CG	27.089	.	1
1	B	644	LEU	N	126.349	.	1
1	B	645	GLU	H	8.64	.	1
1	B	645	GLU	HA	4.314	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	645	GLU	HB2	2.007	.	2
1	B	645	GLU	HB3	2.112	.	2
1	B	645	GLU	HG2	2.338	.	1
1	B	645	GLU	HG3	2.338	.	1
1	B	645	GLU	C	176.413	.	1
1	B	645	GLU	CA	56.974	.	1
1	B	645	GLU	CB	30.123	.	1
1	B	645	GLU	CG	36.33	.	1
1	B	645	GLU	N	123.191	.	1
1	B	646	ARG	H	8.307	.	1
1	B	646	ARG	HA	4.372	.	1
1	B	646	ARG	HB2	1.825	.	2
1	B	646	ARG	HB3	1.915	.	2
1	B	646	ARG	HD2	3.254	.	1
1	B	646	ARG	HD3	3.254	.	1
1	B	646	ARG	HE	7.272	.	1
1	B	646	ARG	HG2	1.685	.	1
1	B	646	ARG	HG3	1.685	.	1
1	B	646	ARG	C	176.494	.	1
1	B	646	ARG	CA	56.161	.	1
1	B	646	ARG	CB	30.988	.	1
1	B	646	ARG	CD	43.331	.	1
1	B	646	ARG	CG	27.089	.	1
1	B	646	ARG	N	121.703	.	1
1	B	646	ARG	NE	124.512	.	1
1	B	647	GLU	H	8.553	.	1
1	B	647	GLU	HA	4.314	.	1
1	B	647	GLU	HB2	2.007	.	2
1	B	647	GLU	HB3	2.112	.	2
1	B	647	GLU	HG2	2.338	.	1
1	B	647	GLU	HG3	2.338	.	1
1	B	647	GLU	C	176.799	.	1
1	B	647	GLU	CA	56.974	.	1
1	B	647	GLU	CB	30.123	.	1
1	B	647	GLU	CG	36.33	.	1
1	B	647	GLU	N	122.357	.	1
1	B	648	SER	H	8.326	.	1
1	B	648	SER	HA	4.444	.	1
1	B	648	SER	HB2	3.924	.	1
1	B	648	SER	HB3	3.924	.	1
1	B	648	SER	C	174.72	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	648	SER	CA	58.679	.	1
1	B	648	SER	CB	63.77	.	1
1	B	648	SER	N	116.353	.	1
1	B	649	GLU	H	8.43	.	1
1	B	649	GLU	HA	4.314	.	1
1	B	649	GLU	CA	56.974	.	1
1	B	649	GLU	CB	30.196	.	1
1	B	649	GLU	N	122.77	.	1
1	B	650	LYS	C	176.683	.	1
1	B	650	LYS	CA	56.443	.	1
1	B	650	LYS	CB	33.225	.	1
1	B	650	LYS	CD	29.147	.	1
1	B	650	LYS	CE	42.17	.	1
1	B	650	LYS	CG	24.739	.	1
1	B	651	GLU	H	8.459	.	1
1	B	651	GLU	C	176.624	.	1
1	B	651	GLU	CA	56.722	.	1
1	B	651	GLU	CB	30.229	.	1
1	B	651	GLU	CG	36.243	.	1
1	B	651	GLU	N	122.132	.	1
1	B	652	SER	H	8.371	.	1
1	B	652	SER	C	174.62	.	1
1	B	652	SER	CA	58.265	.	1
1	B	652	SER	CB	63.885	.	1
1	B	652	SER	N	117.099	.	1
1	B	653	SER	H	8.409	.	1
1	B	653	SER	C	174.407	.	1
1	B	653	SER	CA	58.293	.	1
1	B	653	SER	CB	63.846	.	1
1	B	653	SER	N	117.859	.	1
1	B	654	ASN	H	8.496	.	1
1	B	654	ASN	HD21	6.921	.	1
1	B	654	ASN	HD22	7.64	.	1
1	B	654	ASN	CA	53.414	.	1
1	B	654	ASN	CB	39.171	.	1
1	B	654	ASN	N	120.907	.	1
1	B	654	ASN	ND2	113.243	.	1
1	B	656	GLU	C	176.309	.	1
1	B	656	GLU	CA	56.864	.	1
1	B	656	GLU	CB	30.3	.	1
1	B	657	ASN	H	8.454	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	657	ASN	HD21	6.936	.	1
1	B	657	ASN	HD22	7.639	.	1
1	B	657	ASN	CA	53.394	.	1
1	B	657	ASN	CB	38.994	.	1
1	B	657	ASN	N	119.502	.	1
1	B	657	ASN	ND2	112.704	.	1
1	B	660	ASP	C	176.172	.	1
1	B	660	ASP	CA	54.605	.	1
1	B	660	ASP	CB	41.226	.	1
1	B	681	LYS	H	8.42	.	1
1	B	681	LYS	HA	4.359	0.0	1
1	B	681	LYS	HB2	1.812	0.0	2
1	B	681	LYS	HB3	1.896	0.0	2
1	B	681	LYS	HD2	1.728	0.002	1
1	B	681	LYS	HD3	1.728	0.002	1
1	B	681	LYS	HE2	3.038	0.001	2
1	B	681	LYS	HE3	3.038	0.002	2
1	B	681	LYS	HG2	1.48	0.003	2
1	B	681	LYS	HG3	1.479	0.003	2
1	B	681	LYS	C	176.743	.	1
1	B	681	LYS	CA	56.571	0.0	1
1	B	681	LYS	CB	33.037	0.0	1
1	B	681	LYS	CD	28.975	0.013	1
1	B	681	LYS	CE	42.143	0.013	1
1	B	681	LYS	CG	24.701	0.0	1
1	B	681	LYS	N	124.077	.	1
1	B	682	GLU	H	8.449	.	1
1	B	682	GLU	HA	4.282	0.002	1
1	B	682	GLU	HB2	2.119	0.004	2
1	B	682	GLU	HB3	1.998	0.002	2
1	B	682	GLU	HG2	2.338	0.001	1
1	B	682	GLU	HG3	2.338	0.001	1
1	B	682	GLU	C	176.442	.	1
1	B	682	GLU	CA	56.858	0.014	1
1	B	682	GLU	CB	30.059	0.013	1
1	B	682	GLU	CG	36.307	0.0	1
1	B	682	GLU	N	121.869	.	1
1	B	683	ALA	H	8.244	.	1
1	B	683	ALA	HA	4.336	.	1
1	B	683	ALA	HB1	1.45	.	1
1	B	683	ALA	HB2	1.45	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	683	ALA	HB3	1.45	.	1
1	B	683	ALA	C	177.889	.	1
1	B	683	ALA	CA	52.68	.	1
1	B	683	ALA	CB	19.346	.	1
1	B	683	ALA	N	124.346	.	1
1	B	684	GLU	H	8.313	.	1
1	B	684	GLU	HA	4.387	.	1
1	B	684	GLU	HB2	2.124	.	2
1	B	684	GLU	HB3	2.004	.	2
1	B	684	GLU	HG2	2.337	.	1
1	B	684	GLU	HG3	2.337	.	1
1	B	684	GLU	C	176.09	.	1
1	B	684	GLU	CA	56.509	.	1
1	B	684	GLU	CB	30.207	.	1
1	B	684	GLU	CG	36.282	.	1
1	B	684	GLU	N	120.022	.	1
1	B	685	ASP	H	8.506	.	1
1	B	685	ASP	HA	4.651	.	1
1	B	685	ASP	HB2	2.684	.	2
1	B	685	ASP	HB3	2.762	.	2
1	B	685	ASP	C	176.312	.	1
1	B	685	ASP	CA	54.347	.	1
1	B	685	ASP	CB	41.143	.	1
1	B	685	ASP	N	121.35	.	1
1	B	686	ASN	H	8.37	.	1
1	B	686	ASN	HA	4.662	.	1
1	B	686	ASN	HD21	7.64	.	1
1	B	686	ASN	HD22	6.96	.	1
1	B	686	ASN	CA	53.954	.	1
1	B	686	ASN	CB	39.218	.	1
1	B	686	ASN	N	119.403	.	1
1	B	686	ASN	ND2	112.412	.	1
1	B	687	ASP	C	176.631	.	1
1	B	687	ASP	CA	54.842	.	1
1	B	687	ASP	CB	41.166	.	1
1	B	688	SER	H	8.196	.	1
1	B	688	SER	HA	4.406	.	1
1	B	688	SER	HB2	3.938	.	1
1	B	688	SER	HB3	3.938	.	1
1	B	688	SER	C	175.935	.	1
1	B	688	SER	CA	58.689	.	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	B	688	SER	CB	63.591	.	1
1	B	688	SER	N	116.057	.	1
1	B	689	ARG	H	8.116	.	1
1	B	689	ARG	HA	4.317	.	1
1	B	689	ARG	HB2	1.798	.	1
1	B	689	ARG	HB3	1.798	.	1
1	B	689	ARG	HD2	3.192	.	1
1	B	689	ARG	HD3	3.192	.	1
1	B	689	ARG	HG2	1.588	.	1
1	B	689	ARG	HG3	1.588	.	1
1	B	689	ARG	C	174.692	.	1
1	B	689	ARG	CA	56.228	.	1
1	B	689	ARG	CB	30.57	.	1
1	B	689	ARG	CD	43.289	.	1
1	B	689	ARG	CG	27.055	.	1
1	B	689	ARG	N	122.433	.	1
1	B	690	LYS	H	8.124	.	1
1	B	690	LYS	HA	4.317	.	1
1	B	690	LYS	HB2	1.811	.	2
1	B	690	LYS	HB3	1.695	.	2
1	B	690	LYS	HD2	1.702	.	1
1	B	690	LYS	HD3	1.702	.	1
1	B	690	LYS	HE2	3.027	.	1
1	B	690	LYS	HE3	3.027	.	1
1	B	690	LYS	HG2	1.426	.	1
1	B	690	LYS	HG3	1.426	.	1
1	B	690	LYS	C	176.363	.	1
1	B	690	LYS	CA	56.203	.	1
1	B	690	LYS	CB	33.021	.	1
1	B	690	LYS	CD	29.046	.	1
1	B	690	LYS	CE	42.471	.	1
1	B	690	LYS	CG	24.521	.	1
1	B	690	LYS	N	122.478	.	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
$^{13}\text{C}_\alpha$	164	-0.21 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	158	-0.06 ± 0.10	None needed (< 0.5 ppm)

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}'$	154	0.05 ± 0.09	None needed (< 0.5 ppm)
^{15}N	153	-0.13 ± 0.21	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 92%, i.e. 1328 atoms were assigned a chemical shift out of a possible 1441. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	515/519 (99%)	210/210 (100%)	204/208 (98%)	101/101 (100%)
Sidechain	762/847 (90%)	522/549 (95%)	228/262 (87%)	12/36 (33%)
Aromatic	51/75 (68%)	27/37 (73%)	23/31 (74%)	1/7 (14%)
Overall	1328/1441 (92%)	759/796 (95%)	455/501 (91%)	114/144 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1703 atoms were assigned a chemical shift out of a possible 1836. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	663/668 (99%)	269/269 (100%)	265/270 (98%)	129/129 (100%)
Sidechain	981/1083 (91%)	671/700 (96%)	296/342 (87%)	14/41 (34%)
Aromatic	59/85 (69%)	31/42 (74%)	27/36 (75%)	1/7 (14%)
Overall	1703/1836 (93%)	971/1011 (96%)	588/648 (91%)	144/177 (81%)

7.1.4 Statistically unusual chemical shifts [i](#)

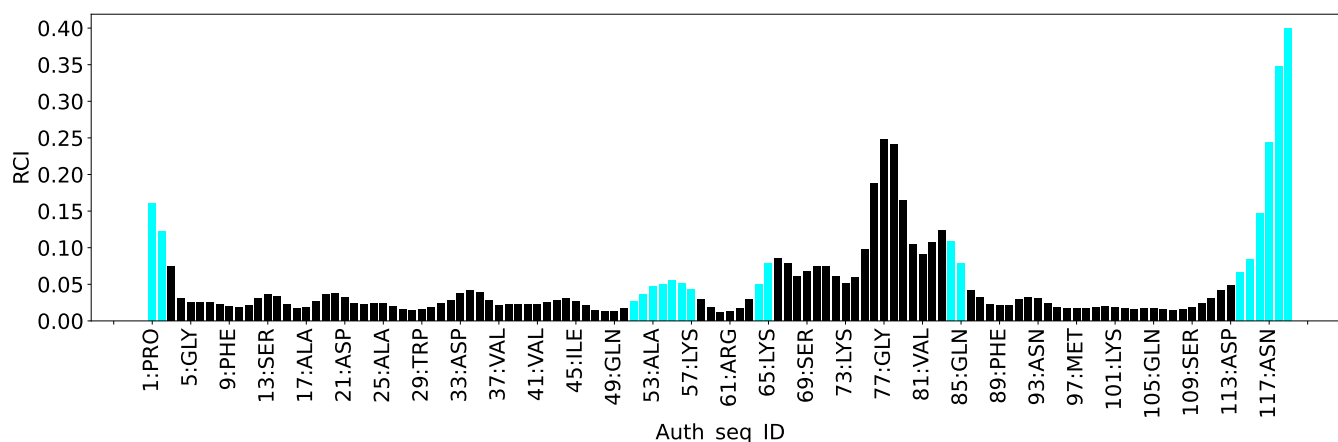
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	646	ARG	NE	124.51	76.53 – 92.65	24.8
1	A	10	GLU	HG3	0.61	1.20 – 3.30	-7.8
1	A	89	PHE	CZ	117.69	121.82 – 136.66	-7.8
1	A	10	GLU	HG2	1.11	1.24 – 3.30	-5.6
1	A	101	LYS	CG	19.14	19.35 – 30.45	-5.2

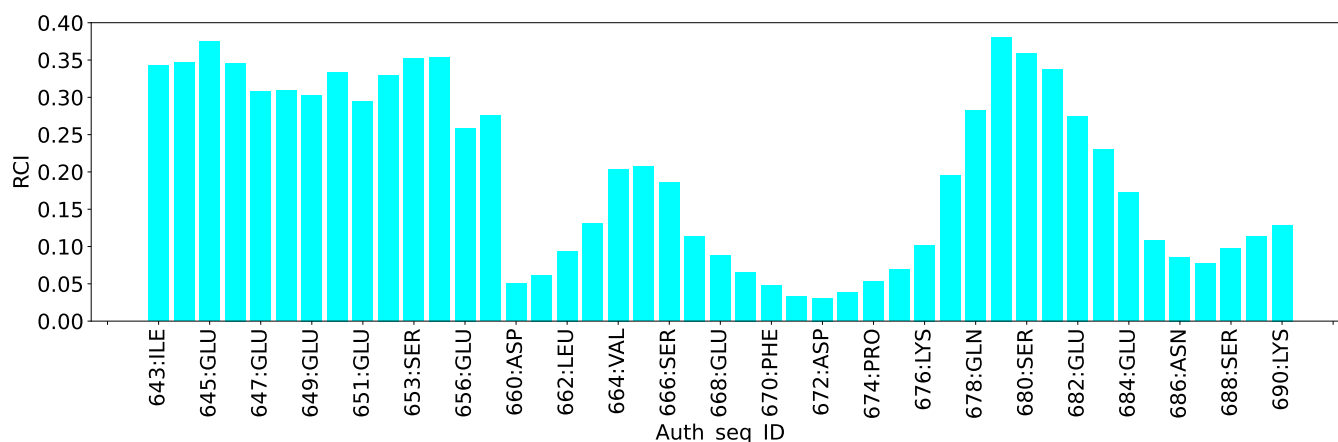
7.1.5 Random Coil Index (RCI) plots [i](#)

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:



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	1617
Intra-residue ($ i-j =0$)	377
Sequential ($ i-j =1$)	409
Medium range ($ i-j >1$ and $ i-j <5$)	240
Long range ($ i-j \geq 5$)	480
Inter-chain	75
Hydrogen bond restraints	36
Disulfide bond restraints	0
Total dihedral-angle restraints	158
Number of unmapped restraints	0
Number of restraints per residue	10.4
Number of long range restraints per residue ¹	3.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	10.2	0.2
0.2-0.5 (Medium)	1.1	0.49
>0.5 (Large)	0.8	0.86

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)	1.9	1.78
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis

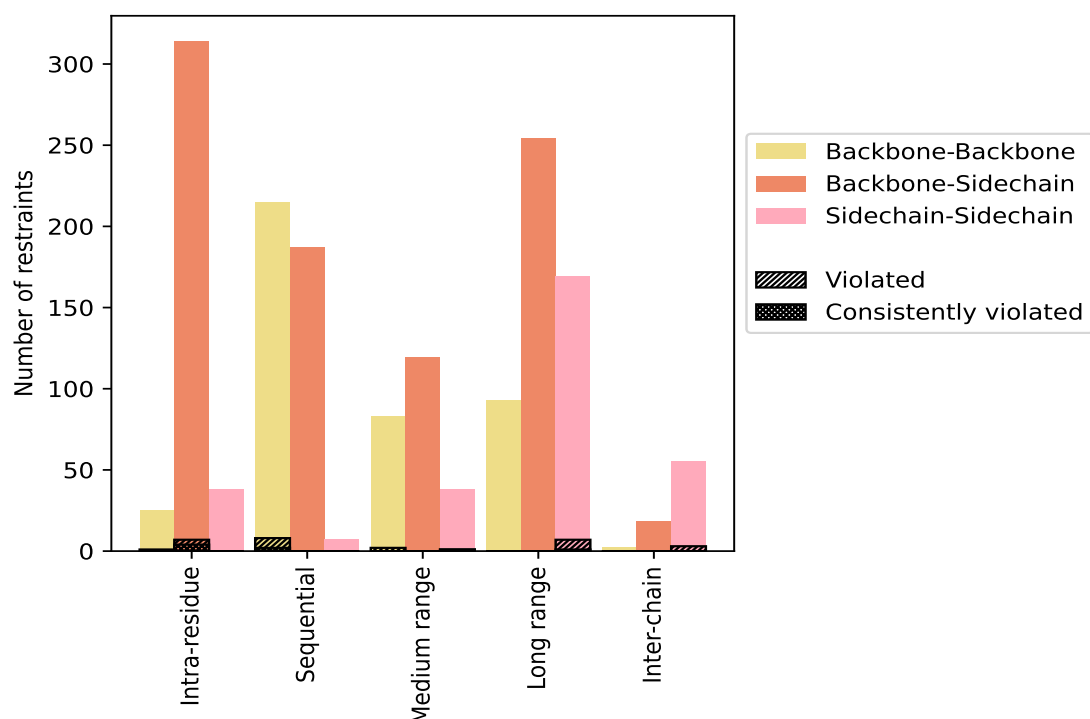
9.1 Summary of distance violations

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

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	377	23.3	8	2.1	0.5	4	1.1	0.2
Backbone-Backbone	25	1.5	1	4.0	0.1	0	0.0	0.0
Backbone-Sidechain	314	19.4	7	2.2	0.4	4	1.3	0.2
Sidechain-Sidechain	38	2.4	0	0.0	0.0	0	0.0	0.0
Sequential ($i-j =1$)	409	25.3	8	2.0	0.5	2	0.5	0.1
Backbone-Backbone	215	13.3	8	3.7	0.5	2	0.9	0.1
Backbone-Sidechain	187	11.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	7	0.4	0	0.0	0.0	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	240	14.8	3	1.2	0.2	1	0.4	0.1
Backbone-Backbone	83	5.1	2	2.4	0.1	0	0.0	0.0
Backbone-Sidechain	119	7.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	2.4	1	2.6	0.1	1	2.6	0.1
Long range ($i-j \geq 5$)	480	29.7	7	1.5	0.4	1	0.2	0.1
Backbone-Backbone	93	5.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	218	13.5	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	169	10.5	7	4.1	0.4	1	0.6	0.1
Inter-chain	75	4.6	3	4.0	0.2	0	0.0	0.0
Backbone-Backbone	2	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	1.1	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	55	3.4	3	5.5	0.2	0	0.0	0.0
Hydrogen bond	36	2.2	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	1617	100.0	29	1.8	1.8	8	0.5	0.5
Backbone-Backbone	418	25.9	11	2.6	0.7	2	0.5	0.1
Backbone-Sidechain	892	55.2	7	0.8	0.4	4	0.4	0.2
Sidechain-Sidechain	307	19.0	11	3.6	0.7	2	0.7	0.1

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	5	3	2	2	1	13	0.18	0.67	0.14	0.14
2	6	2	2	4	2	16	0.2	0.54	0.13	0.16
3	5	3	2	2	1	13	0.2	0.86	0.19	0.14
4	7	2	3	2	2	16	0.17	0.66	0.13	0.15
5	5	3	2	2	1	13	0.2	0.86	0.19	0.14
6	6	2	2	1	1	12	0.2	0.72	0.16	0.16
7	6	3	1	1	1	12	0.21	0.86	0.2	0.15
8	5	5	2	2	2	16	0.19	0.86	0.18	0.13
9	6	3	2	1	3	15	0.22	0.86	0.19	0.16
10	4	3	2	2	0	11	0.15	0.21	0.04	0.14

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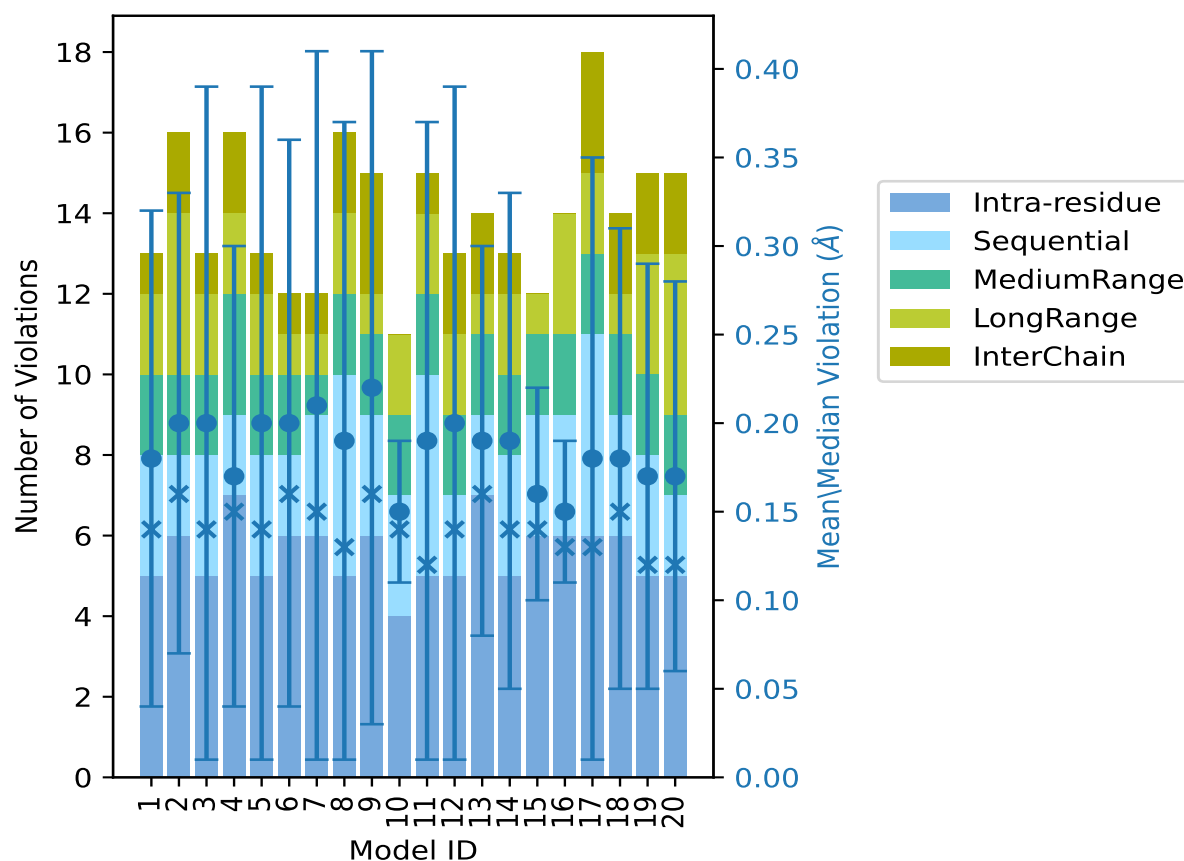
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
11	5	5	2	2	1	15	0.19	0.83	0.18	0.12
12	5	2	2	2	2	13	0.2	0.84	0.19	0.14
13	7	2	2	1	2	14	0.19	0.49	0.11	0.16
14	5	3	2	2	1	13	0.19	0.66	0.14	0.14
15	6	3	2	1	0	12	0.16	0.33	0.06	0.14
16	6	3	2	3	0	14	0.15	0.21	0.04	0.13
17	6	5	2	2	3	18	0.18	0.86	0.17	0.13
18	6	3	2	1	2	14	0.18	0.62	0.13	0.15
19	5	3	2	3	2	15	0.17	0.6	0.12	0.12
20	5	2	2	4	2	15	0.17	0.56	0.11	0.12

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

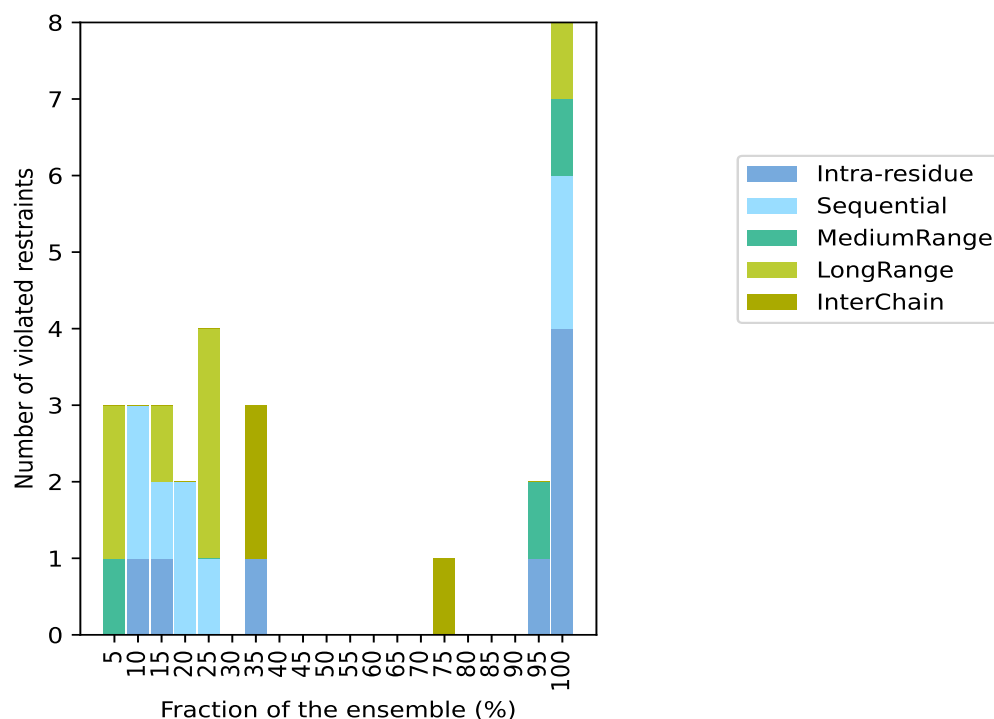
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1552(IR:369, SQ:401, MR:237, LR:473, IC:72) restraints are 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	0	1	2	0	3	1	5.0
1	2	0	0	0	3	2	10.0
1	1	0	1	0	3	3	15.0
0	2	0	0	0	2	4	20.0
0	1	0	3	0	4	5	25.0
0	0	0	0	0	0	6	30.0
1	0	0	0	2	3	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	1	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
1	0	1	0	0	2	19	95.0
4	2	1	1	0	8	20	100.0

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

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

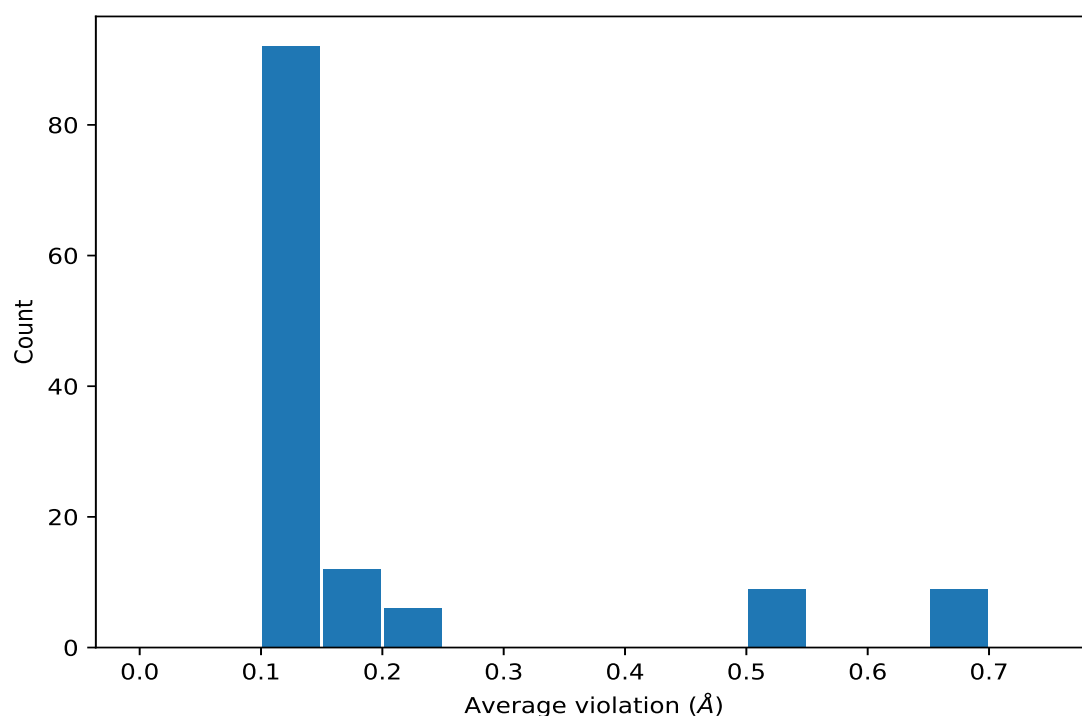
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	20	0.22	0.03	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	20	0.22	0.03	0.22
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	20	0.19	0.01	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	20	0.19	0.0	0.19
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	20	0.18	0.0	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	20	0.18	0.01	0.18

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	20	0.18	0.01	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	20	0.18	0.01	0.18
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	20	0.14	0.0	0.14
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	20	0.12	0.0	0.12
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	20	0.11	0.0	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	19	0.11	0.01	0.11
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	19	0.1	0.0	0.1
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	15	0.69	0.16	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	15	0.69	0.16	0.66
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	7	0.53	0.26	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	7	0.53	0.26	0.51
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	7	0.14	0.0	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	7	0.13	0.01	0.13

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	7	0.13	0.01	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	7	0.13	0.01	0.13
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	5	0.12	0.02	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	5	0.12	0.02	0.11
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	5	0.11	0.01	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	5	0.11	0.01	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	5	0.11	0.01	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	5	0.1	0.0	0.1

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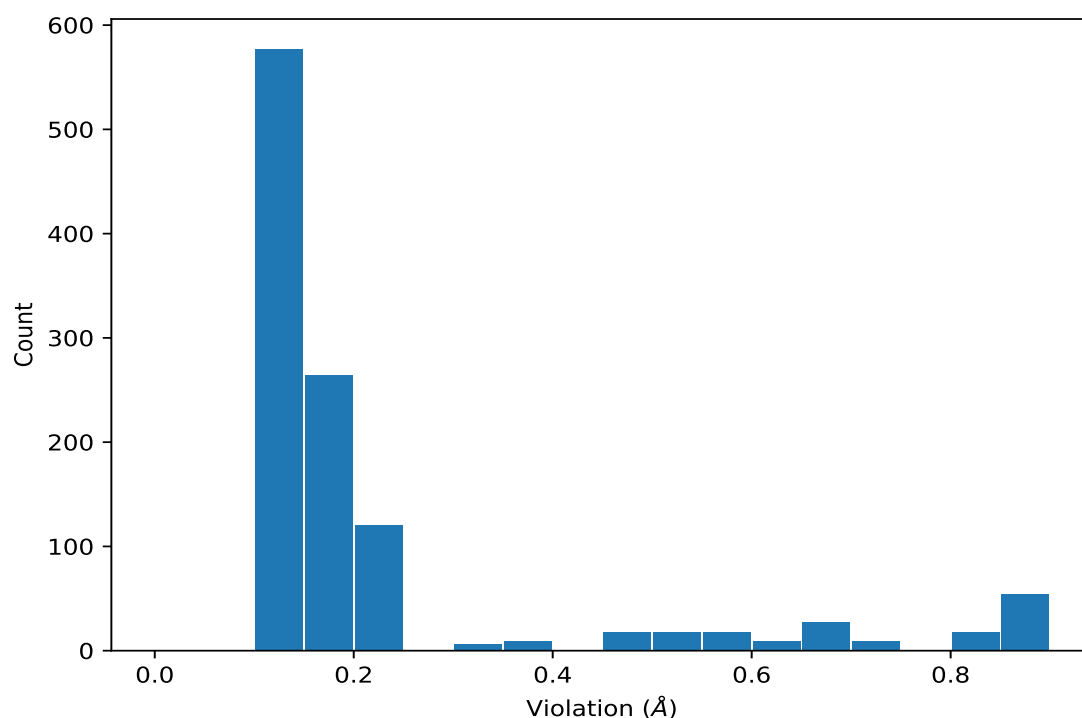
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	5	0.1	0.0	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	5	0.1	0.0	0.1
(1,1465)	2:667:B:GLU:H	2:666:B:SER:HA	4	0.11	0.01	0.11
(1,1278)	1:79:A:GLU:HA	1:78:A:ASN:HA	4	0.11	0.0	0.11
(1,603)	1:81:A:VAL:H	1:81:A:VAL:HB	3	0.15	0.0	0.15
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD2	3	0.12	0.02	0.13
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD3	3	0.12	0.02	0.13
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD2	3	0.12	0.02	0.13
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD3	3	0.12	0.02	0.13
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD2	3	0.12	0.02	0.13
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD3	3	0.12	0.02	0.13
(1,1)	1:2:A:SER:H	1:1:A:PRO:HA	3	0.12	0.0	0.12
(1,1466)	2:669:B:LEU:H	2:668:B:GLU:HA	2	0.12	0.0	0.12
(1,1463)	2:678:B:GLN:H	2:677:B:SER:HA	2	0.11	0.0	0.11
(1,345)	1:42:A:LEU:H	1:42:A:LEU:HG	2	0.1	0.0	0.1

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	9	0.86
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	9	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	3	0.86

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	3	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	3	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	5	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	5	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	7	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	7	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	8	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	8	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	8	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	17	0.86
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	17	0.86
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	12	0.84
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	12	0.84
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	12	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	12	0.84
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	12	0.84
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	11	0.83
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	11	0.83
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	6	0.72
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	6	0.72
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	1	0.67
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	1	0.67
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	1	0.67
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	1	0.67
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	1	0.67
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	1	0.67
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	1	0.67
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	1	0.67
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	1	0.67
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	4	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	4	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	4	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	4	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	4	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	4	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	4	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	4	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	4	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	14	0.66

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	14	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	14	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	14	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	14	0.66
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	14	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	14	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	14	0.66
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	14	0.66
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	18	0.62
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	18	0.62
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	18	0.62
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	18	0.62
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	18	0.62
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	18	0.62
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	18	0.62
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	18	0.62
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	18	0.62
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	19	0.6
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	19	0.6
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	19	0.6
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	19	0.6
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	19	0.6
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	19	0.6
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	19	0.6
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	19	0.6
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	19	0.6
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	20	0.56
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	20	0.56
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	20	0.56
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	20	0.56
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	20	0.56
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	20	0.56
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	20	0.56
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	20	0.56
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	20	0.56
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	2	0.54
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	2	0.54
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	2	0.54
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	2	0.54
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	2	0.54
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	2	0.54
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	2	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	2	0.54
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	2	0.54
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	2	0.51
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	2	0.51
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	2	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	2	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	2	0.51
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	2	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	2	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	2	0.51
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	2	0.51
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	13	0.49
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	13	0.49
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	13	0.49
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	13	0.49
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	13	0.49
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	13	0.49
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	13	0.49
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	13	0.49
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	13	0.49
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	9	0.46
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	9	0.46
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	9	0.46
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	9	0.46
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	9	0.46
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	9	0.46
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	9	0.46
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	9	0.46
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	9	0.46
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD11	13	0.39
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD12	13	0.39
(1,1500)	1:59:A:MET:HE1	2:665:B:LEU:HD13	13	0.39
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD11	13	0.39
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD12	13	0.39
(1,1500)	1:59:A:MET:HE2	2:665:B:LEU:HD13	13	0.39
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD11	13	0.39
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD12	13	0.39
(1,1500)	1:59:A:MET:HE3	2:665:B:LEU:HD13	13	0.39
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	15	0.33
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	15	0.33
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	15	0.33
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	15	0.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	15	0.33
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	15	0.33
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	6	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	6	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	6	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	6	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	6	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	6	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	7	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	7	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	7	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	7	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	7	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	7	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	9	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	9	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	9	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	9	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	9	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	9	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	18	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	18	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	18	0.23
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	18	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	18	0.23
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	18	0.23
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	2	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	2	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	2	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	2	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	2	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	2	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	3	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	3	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	3	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	3	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	3	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	3	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	8	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	8	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	8	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	8	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	8	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	8	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	13	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	13	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	13	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	13	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	13	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	13	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	20	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	20	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	20	0.22
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	20	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	20	0.22
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	20	0.22
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	1	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	1	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	1	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	1	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	1	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	1	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	5	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	5	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	5	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	5	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	5	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	5	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	10	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	10	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	10	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	10	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	10	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	10	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	11	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	11	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	11	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	11	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	11	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	11	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	12	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	12	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	12	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	12	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	12	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	12	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	16	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	16	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	16	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	16	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	16	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	16	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	17	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	17	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	17	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	17	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	17	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	17	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	19	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	19	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	19	0.21
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	19	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	19	0.21
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	19	0.21
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	6	0.21
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	4	0.2
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	4	0.2
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	4	0.2
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	4	0.2
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	4	0.2
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	4	0.2
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE1	14	0.2
(1,1409)	1:107:A:ILE:HG21	1:111:A:TYR:HE2	14	0.2
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE1	14	0.2
(1,1409)	1:107:A:ILE:HG22	1:111:A:TYR:HE2	14	0.2
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE1	14	0.2
(1,1409)	1:107:A:ILE:HG23	1:111:A:TYR:HE2	14	0.2
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	2	0.2
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	3	0.2
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	5	0.2
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	11	0.2
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	20	0.2
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	17	0.19
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	17	0.19
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	17	0.19
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	17	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	17	0.19
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	17	0.19
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	17	0.19
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	17	0.19
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	17	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	1	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	2	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	4	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	5	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	7	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	9	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	10	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	11	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	12	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	13	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	14	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	15	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	16	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	17	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	18	0.19
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	20	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	2	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	2	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	2	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	2	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	2	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	2	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	2	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	2	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	2	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	3	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	3	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	3	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	3	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	3	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	3	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	3	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	3	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	3	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	8	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	8	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	8	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	8	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	8	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	8	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	8	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	8	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	8	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	13	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	13	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	13	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	13	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	13	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	13	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	13	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	13	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	13	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	16	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	16	0.19
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	16	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	16	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	16	0.19
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	16	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	16	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	16	0.19
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	16	0.19
(1,1072)	1:29:A:TRP:HD1	1:16:A:ILE:HG12	2	0.19
(1,1072)	1:29:A:TRP:HD1	1:16:A:ILE:HG13	2	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	7	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	8	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	9	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	10	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	13	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	15	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	16	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	17	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	18	0.19
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	19	0.19
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD21	8	0.18
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD22	8	0.18
(1,1501)	1:59:A:MET:HE1	2:665:B:LEU:HD23	8	0.18
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD21	8	0.18
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD22	8	0.18
(1,1501)	1:59:A:MET:HE2	2:665:B:LEU:HD23	8	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD21	8	0.18
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD22	8	0.18
(1,1501)	1:59:A:MET:HE3	2:665:B:LEU:HD23	8	0.18
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	3	0.18
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	6	0.18
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	8	0.18
(1,1467)	2:668:B:GLU:H	2:667:B:GLU:HA	19	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	1	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	2	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	3	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	4	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	5	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	6	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	8	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	9	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	10	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	11	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	12	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	13	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	14	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	15	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	16	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	17	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	18	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	19	0.18
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	20	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	6	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	6	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	6	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	6	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	6	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	6	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	6	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	6	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	6	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	9	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	9	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	9	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	9	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	9	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	9	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	9	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	9	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	11	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	11	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	11	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	11	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	11	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	11	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	11	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	11	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	11	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	12	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	12	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	12	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	12	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	12	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	12	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	12	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	12	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	12	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	14	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	14	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	14	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	14	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	14	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	14	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	14	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	14	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	14	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	17	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	17	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	17	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	17	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	17	0.18
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	17	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	17	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	17	0.18
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	17	0.18
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	1	0.18
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	12	0.18
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	1	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	1	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	1	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	1	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	1	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	1	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	1	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	1	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	1	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	4	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	4	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	4	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	4	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	4	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	4	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	4	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	4	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	4	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	5	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	5	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	5	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	5	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	5	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	5	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	5	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	5	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	5	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	10	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	10	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	10	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	10	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	10	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	10	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	10	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	10	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	10	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	15	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	15	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	15	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	15	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	15	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	15	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	15	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	15	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	15	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	18	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	18	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	18	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	18	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	18	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	18	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	18	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	18	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	18	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	19	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	19	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	19	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	19	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	19	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	19	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	19	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	19	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	19	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	20	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	20	0.17
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	20	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	20	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	20	0.17
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	20	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	20	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	20	0.17
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	20	0.17
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	4	0.17
(1,231)	1:29:A:TRP:H	1:29:A:TRP:HD1	14	0.17
(1,1282)	1:80:A:VAL:HA	1:80:A:VAL:HB	7	0.16
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB1	7	0.16
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB2	7	0.16
(1,1206)	1:60:A:LEU:HD21	1:50:A:ALA:HB3	7	0.16
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB1	7	0.16
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB2	7	0.16
(1,1206)	1:60:A:LEU:HD22	1:50:A:ALA:HB3	7	0.16
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB1	7	0.16
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB2	7	0.16
(1,1206)	1:60:A:LEU:HD23	1:50:A:ALA:HB3	7	0.16
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	4	0.16
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	4	0.16
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	4	0.16
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	4	0.16
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	4	0.16
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	4	0.16
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	4	0.16
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	4	0.16
(1,603)	1:81:A:VAL:H	1:81:A:VAL:HB	9	0.16
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	9	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	9	0.15
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	9	0.15
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	9	0.15
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	9	0.15
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	9	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	9	0.15
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	9	0.15
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	4	0.15
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	16	0.15
(1,603)	1:81:A:VAL:H	1:81:A:VAL:HB	13	0.15
(1,603)	1:81:A:VAL:H	1:81:A:VAL:HB	18	0.15
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	9	0.15
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	11	0.15
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	18	0.15
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	4	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	4	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	4	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	4	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	4	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	12	0.14
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	12	0.14
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD2	14	0.14
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD3	14	0.14
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD2	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD3	14	0.14
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD2	14	0.14
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD3	14	0.14
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	2	0.14
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	6	0.14
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	13	0.14
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	15	0.14
(1,701)	1:95:A:THR:H	1:95:A:THR:HB	17	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	1	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	2	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	3	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	4	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	5	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	6	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	7	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	8	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	10	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	12	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	13	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	14	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	15	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	16	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	17	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	19	0.14
(1,365)	1:44:A:THR:H	1:44:A:THR:HB	20	0.14
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	18	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	18	0.13
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	18	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	18	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	18	0.13
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	18	0.13
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	18	0.13
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	18	0.13
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD2	3	0.13
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD3	3	0.13
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD2	3	0.13
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD3	3	0.13
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD2	3	0.13
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD3	3	0.13
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	12	0.13
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	12	0.13
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	12	0.13
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	12	0.13
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	12	0.13
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	12	0.13
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	12	0.13
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	12	0.13
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	12	0.13
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	19	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	19	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	20	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	20	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	20	0.12
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	20	0.12
(1,1466)	2:669:B:LEU:H	2:668:B:GLU:HA	8	0.12
(1,1466)	2:669:B:LEU:H	2:668:B:GLU:HA	11	0.12
(1,1465)	2:667:B:GLU:H	2:666:B:SER:HA	8	0.12
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	11	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	10	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	10	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	10	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	10	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	10	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	10	0.12
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	10	0.12
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	10	0.12
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	10	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	20	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	20	0.12
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	20	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	20	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	20	0.12
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	20	0.12
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	20	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	20	0.12
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	20	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	1	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	2	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	5	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	6	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	7	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	9	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	10	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	14	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	15	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	16	0.12
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	18	0.12
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	7	0.12
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	10	0.12
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	16	0.12
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	2	0.12
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	6	0.12
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	16	0.12
(1,1)	1:2:A:SER:H	1:1:A:PRO:HA	1	0.12
(1,1)	1:2:A:SER:H	1:1:A:PRO:HA	14	0.12
(1,1)	1:2:A:SER:H	1:1:A:PRO:HA	17	0.12
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG12	17	0.11
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD11	2:673:B:VAL:HG23	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG12	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD12	2:673:B:VAL:HG23	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG12	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD13	2:673:B:VAL:HG23	17	0.11
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG12	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD21	2:673:B:VAL:HG23	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG12	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD22	2:673:B:VAL:HG23	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG11	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG12	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG13	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG21	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG22	17	0.11
(1,1573)	1:48:A:LEU:HD23	2:673:B:VAL:HG23	17	0.11
(1,1465)	2:667:B:GLU:H	2:666:B:SER:HA	9	0.11
(1,1465)	2:667:B:GLU:H	2:666:B:SER:HA	11	0.11
(1,1463)	2:678:B:GLN:H	2:677:B:SER:HA	11	0.11
(1,1463)	2:678:B:GLN:H	2:677:B:SER:HA	18	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	1	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	2	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	4	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	5	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	6	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	7	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	8	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	9	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	10	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	12	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	13	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	14	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	15	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	16	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	17	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	18	0.11
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	19	0.11
(1,1278)	1:79:A:GLU:HA	1:78:A:ASN:HA	3	0.11
(1,1278)	1:79:A:GLU:HA	1:78:A:ASN:HA	5	0.11
(1,1278)	1:79:A:GLU:HA	1:78:A:ASN:HA	19	0.11
(1,1211)	1:62:A:LEU:HB2	1:45:A:ILE:HD11	1	0.11
(1,1211)	1:62:A:LEU:HB2	1:45:A:ILE:HD12	1	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1211)	1:62:A:LEU:HB2	1:45:A:ILE:HD13	1	0.11
(1,1211)	1:62:A:LEU:HB3	1:45:A:ILE:HD11	1	0.11
(1,1211)	1:62:A:LEU:HB3	1:45:A:ILE:HD12	1	0.11
(1,1211)	1:62:A:LEU:HB3	1:45:A:ILE:HD13	1	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	16	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	16	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	16	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	16	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	16	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	16	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	16	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	16	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	16	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	17	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	17	0.11
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	17	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	17	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	17	0.11
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	17	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	17	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	17	0.11
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	17	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	19	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	19	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	19	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	20	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	20	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	20	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	20	0.11
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	20	0.11
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	20	0.11
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	20	0.11
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	8	0.11
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	8	0.11
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	8	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	8	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	8	0.11
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	8	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	8	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	8	0.11
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	8	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	3	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	4	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	8	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	11	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	12	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	13	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	17	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	19	0.11
(1,828)	1:109:A:SER:H	1:108:A:ILE:HA	20	0.11
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	8	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	3	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	4	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	5	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	8	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	9	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	10	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	11	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	13	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	14	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	15	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	17	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	18	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	19	0.11
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	20	0.11
(1,1465)	2:667:B:GLU:H	2:666:B:SER:HA	15	0.1
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	3	0.1
(1,1345)	1:95:A:THR:HB	1:95:A:THR:HA	20	0.1
(1,1278)	1:79:A:GLU:HA	1:78:A:ASN:HA	17	0.1
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD2	20	0.1
(1,1172)	1:50:A:ALA:HB1	1:101:A:LYS:HD3	20	0.1
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD2	20	0.1
(1,1172)	1:50:A:ALA:HB2	1:101:A:LYS:HD3	20	0.1
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD2	20	0.1
(1,1172)	1:50:A:ALA:HB3	1:101:A:LYS:HD3	20	0.1
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD21	2	0.1
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD22	2	0.1
(1,1122)	1:42:A:LEU:HD11	1:104:A:LEU:HD23	2	0.1
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD21	2	0.1
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD22	2	0.1
(1,1122)	1:42:A:LEU:HD12	1:104:A:LEU:HD23	2	0.1
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD21	2	0.1
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD22	2	0.1
(1,1122)	1:42:A:LEU:HD13	1:104:A:LEU:HD23	2	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	5	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	5	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	5	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	5	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	5	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	5	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	5	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	5	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	11	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	11	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	11	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG11	16	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG12	16	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG13	16	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG21	16	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG22	16	0.1
(1,1066)	1:28:A:THR:HG21	1:37:A:VAL:HG23	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG11	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG12	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG13	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG21	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG22	16	0.1
(1,1066)	1:28:A:THR:HG22	1:37:A:VAL:HG23	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG11	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG12	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG13	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG21	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG22	16	0.1
(1,1066)	1:28:A:THR:HG23	1:37:A:VAL:HG23	16	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	2	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	2	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	2	0.1
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	2	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	2	0.1
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	2	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	2	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	2	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	2	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD11	19	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD12	19	0.1
(1,1060)	1:27:A:LEU:HD21	1:62:A:LEU:HD13	19	0.1
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD11	19	0.1
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD12	19	0.1
(1,1060)	1:27:A:LEU:HD22	1:62:A:LEU:HD13	19	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD11	19	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD12	19	0.1
(1,1060)	1:27:A:LEU:HD23	1:62:A:LEU:HD13	19	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	1	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	2	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	3	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	4	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	5	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	6	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	7	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	8	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	9	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	11	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	12	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	13	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	14	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	15	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	16	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	17	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	18	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	19	0.1
(1,891)	1:114:A:ALA:H	1:114:A:ALA:HA	20	0.1
(1,564)	1:75:A:ASN:H	1:74:A:ASP:HA	17	0.1
(1,444)	1:57:A:LYS:H	1:55:A:SER:HA	4	0.1
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	1	0.1
(1,371)	1:45:A:ILE:H	1:43:A:SER:H	12	0.1
(1,345)	1:42:A:LEU:H	1:42:A:LEU:HG	4	0.1
(1,345)	1:42:A:LEU:H	1:42:A:LEU:HG	7	0.1

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

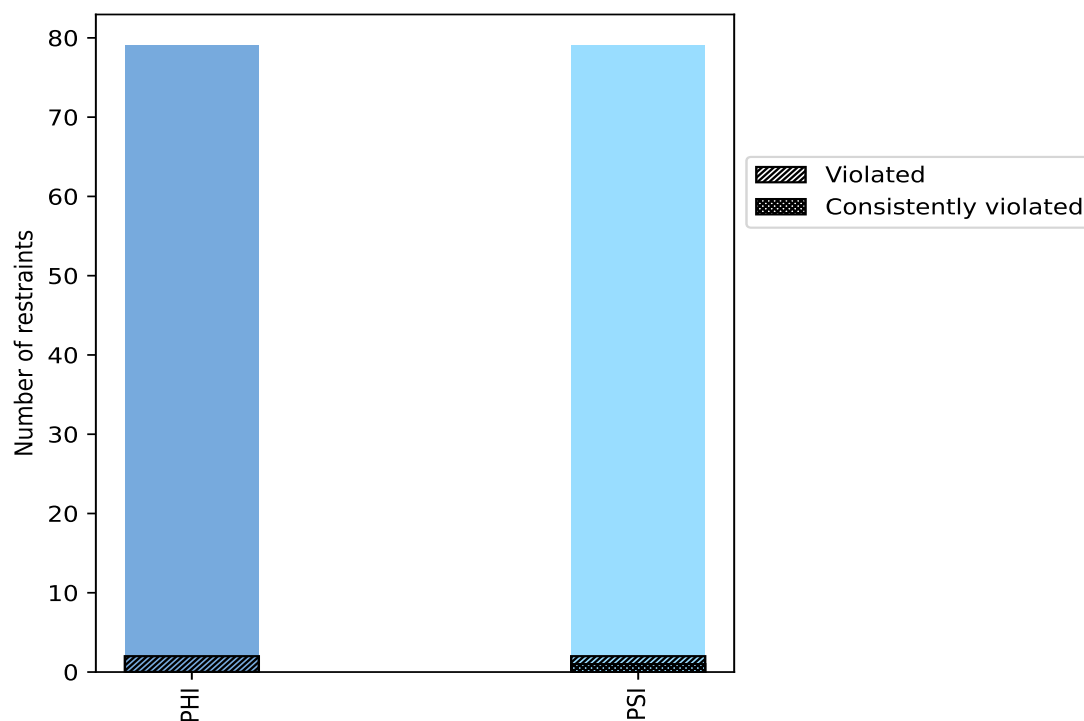
10.1 Summary of dihedral-angle violations [i](#)

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

Angle type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
PHI	79	50.0	2	2.5	1.3	0	0.0	0.0
PSI	79	50.0	2	2.5	1.3	1	1.3	0.6
Total	158	100.0	4	2.5	2.5	1	0.6	0.6

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

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



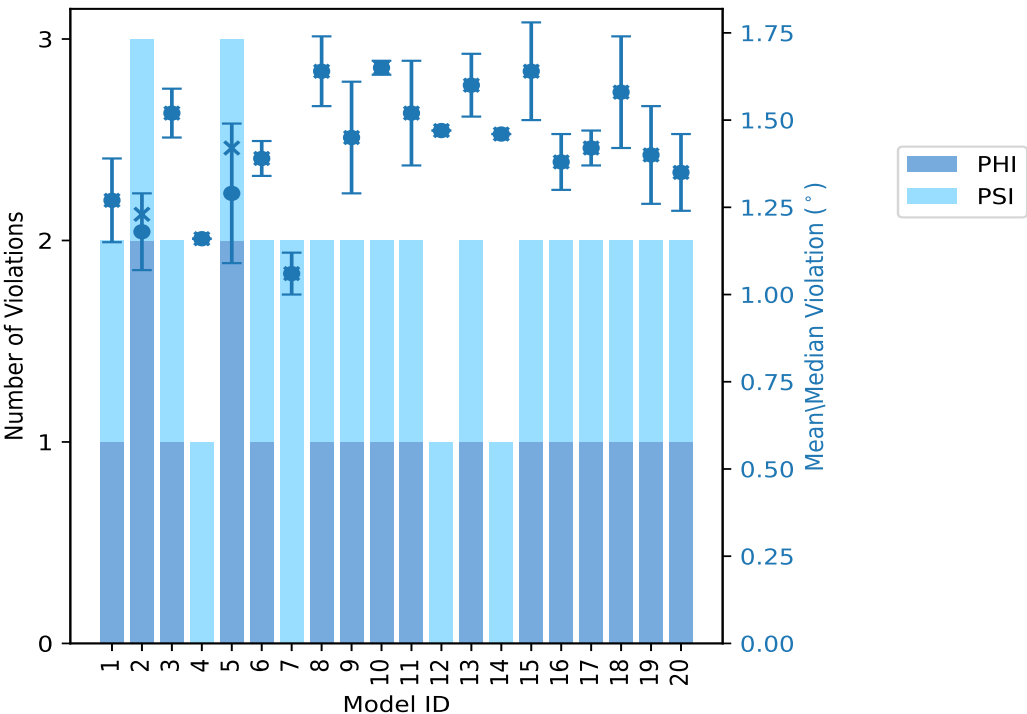
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	1	1	2	1.27	1.39	0.12	1.27
2	2	1	3	1.18	1.28	0.11	1.23
3	1	1	2	1.52	1.59	0.07	1.52
4	0	1	1	1.16	1.16	0.0	1.16
5	2	1	3	1.29	1.45	0.2	1.42
6	1	1	2	1.39	1.44	0.05	1.39
7	0	2	2	1.06	1.12	0.06	1.06
8	1	1	2	1.64	1.74	0.1	1.64
9	1	1	2	1.45	1.61	0.16	1.45
10	1	1	2	1.65	1.67	0.02	1.65
11	1	1	2	1.52	1.68	0.15	1.52
12	0	1	1	1.47	1.47	0.0	1.47
13	1	1	2	1.6	1.69	0.09	1.6
14	0	1	1	1.46	1.46	0.0	1.46
15	1	1	2	1.64	1.78	0.14	1.64
16	1	1	2	1.38	1.47	0.08	1.38
17	1	1	2	1.42	1.47	0.05	1.42
18	1	1	2	1.58	1.74	0.16	1.58
19	1	1	2	1.4	1.54	0.14	1.4
20	1	1	2	1.35	1.46	0.11	1.35

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



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

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

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

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

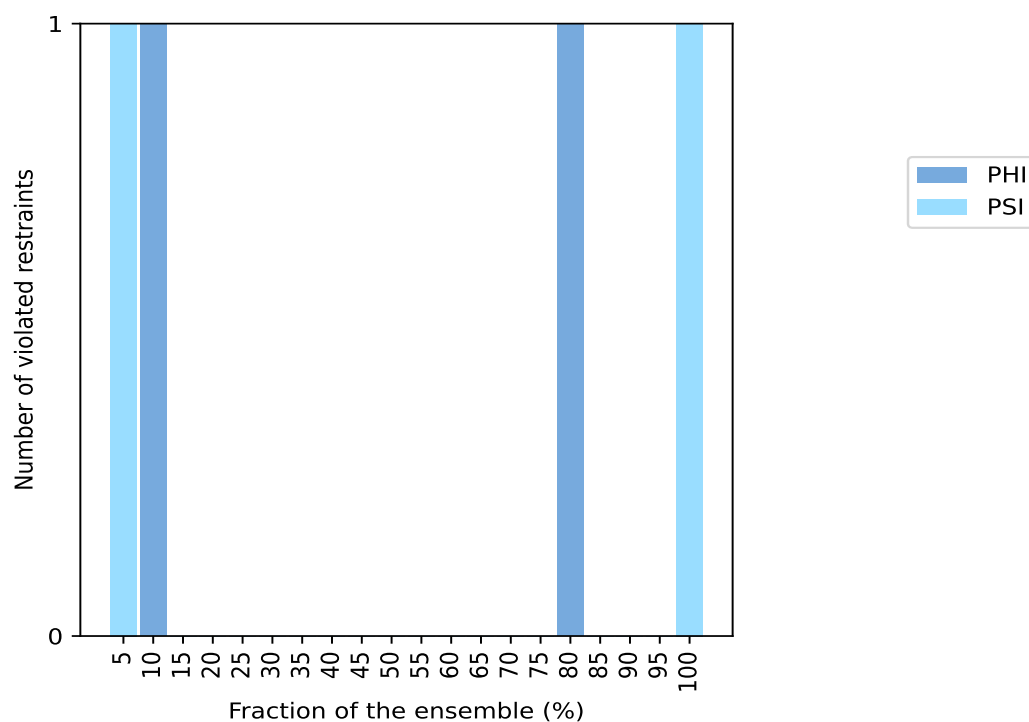
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Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
0	0	0	12	60.0
0	0	0	13	65.0
0	0	0	14	70.0
0	0	0	15	75.0
1	0	1	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	1	1	20	100.0

¹ Number of models with violations

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

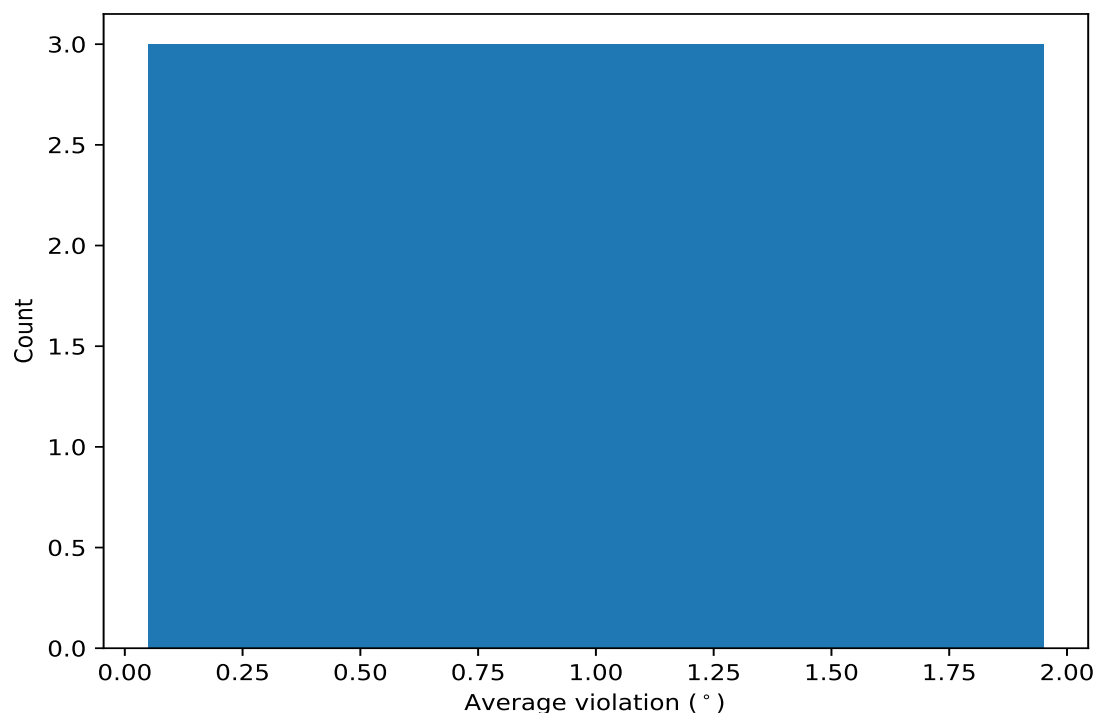


10.4 Most violated dihedral-angle restraints in the ensemble [i](#)

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

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

in the ensemble



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

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

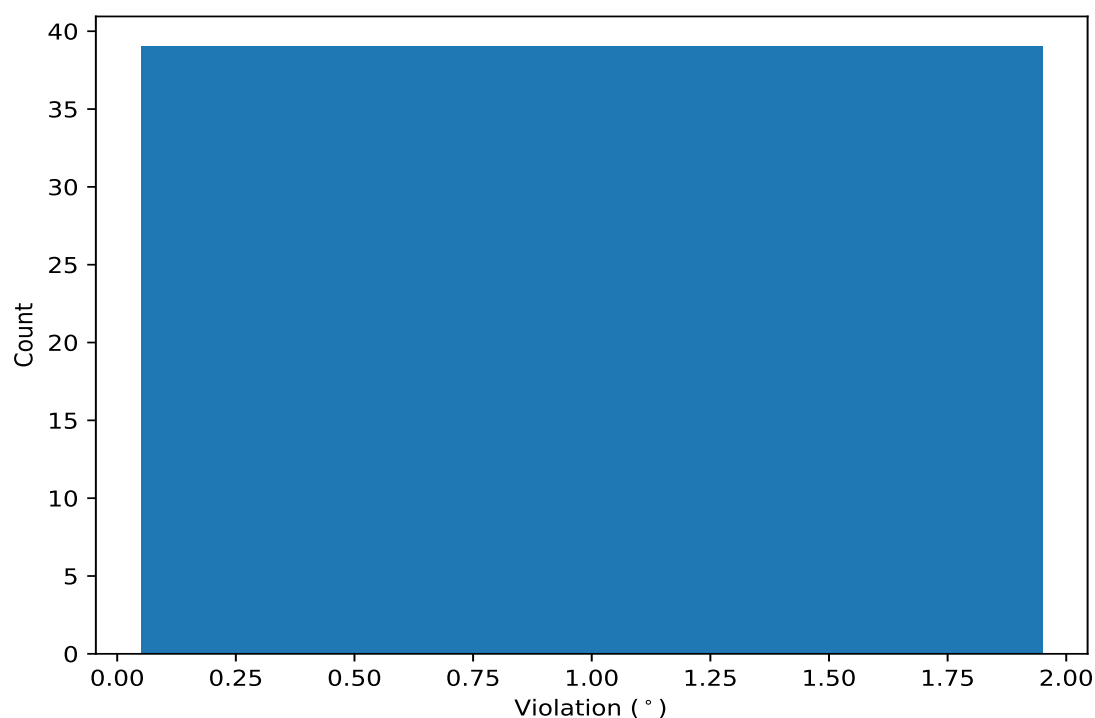
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	20	1.46	0.15	1.46
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	16	1.44	0.19	1.37
(1,33)	1:28:A:THR:C	1:29:A:TRP:N	1:29:A:TRP:CA	1:29:A:TRP:C	2	1.02	0.01	1.02

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 (°)
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	15	1.78
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	8	1.74
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	18	1.74
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	13	1.69
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	11	1.68
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	10	1.67
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	10	1.63
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	9	1.61
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	3	1.59
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	19	1.54
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	8	1.53
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	15	1.51
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	13	1.5
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	12	1.47
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	16	1.47
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	17	1.47
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	3	1.46
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	14	1.46
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	20	1.46
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	5	1.45
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	6	1.44

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	18	1.42
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	5	1.42
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	1	1.39
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	11	1.37
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	17	1.36
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	6	1.34
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	16	1.3
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	9	1.29
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	2	1.28
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	19	1.26
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	20	1.24
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	2	1.23
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	4	1.16
(1,19)	1:15:A:ILE:C	1:16:A:ILE:N	1:16:A:ILE:CA	1:16:A:ILE:C	1	1.16
(1,140)	2:667:B:GLU:N	2:667:B:GLU:CA	2:667:B:GLU:C	2:668:B:GLU:N	7	1.12
(1,33)	1:28:A:THR:C	1:29:A:TRP:N	1:29:A:TRP:CA	1:29:A:TRP:C	2	1.03
(1,33)	1:28:A:THR:C	1:29:A:TRP:N	1:29:A:TRP:CA	1:29:A:TRP:C	5	1.01
(1,6)	1:7:A:ALA:N	1:7:A:ALA:CA	1:7:A:ALA:C	1:8:A:ILE:N	7	1.0