Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 10:37 PM EDT

PDB ID	:	2KB4
BMRB ID	:	16039
Title	:	NMR structure of the unphosphorylated form of OdhI, OdhI.
Authors	:	Barthe, P.; Roumestand, C.; Canova, M.; Hurard, C.; Molle, V.; Cohen-Gonsaud, M.
Deposited on	:	2008-11-20

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 (i) 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 (1)) were used in the production of this report:

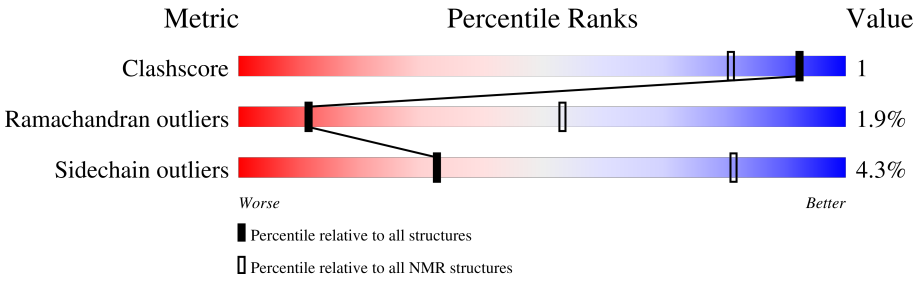
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 60%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	143	76% · 23%

2 Ensemble composition and analysis (i)

This entry contains 30 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:5-A:17 (13)	1.79	21
2	A:45-A:141 (97)	1.42	1

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

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

The models can be grouped into 6 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 6, 8, 15, 19, 20, 21, 23, 25, 26, 29
2	5, 12, 18, 27, 28
3	1, 4, 13, 16
4	3, 7, 17, 30
5	22, 24
6	9, 10
Single-model clusters	11; 14

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2134 atoms, of which 1051 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Oxoglutarate dehydrogenase inhibitor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	143	2134	666	1051	193	221	3	0

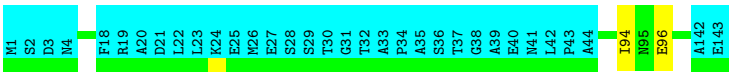
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 76% • 23%



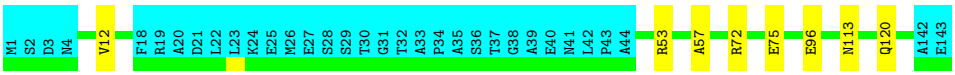
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

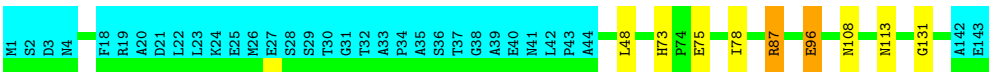
Chain A: 71% 6% 23%



4.2.2 Score per residue for model 2

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

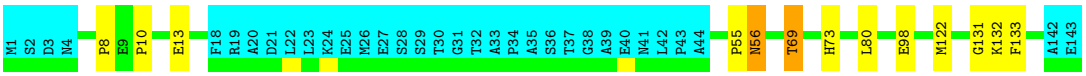
Chain A: 71% 5% • 23%



4.2.3 Score per residue for model 3

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

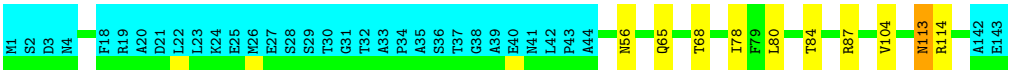
Chain A: 68% 8% • 23%



4.2.4 Score per residue for model 4

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 70% 6% • 23%



4.2.5 Score per residue for model 5

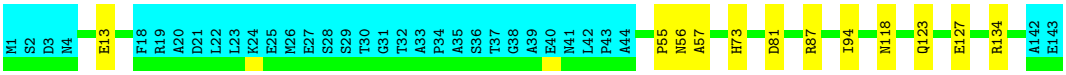
• Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 66% 10% • 23%

4.2.6 Score per residue for model 6

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

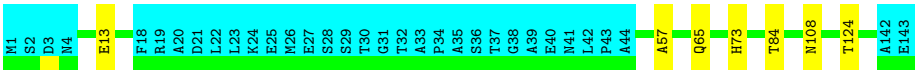
Chain A: 69% 8% 23%



4.2.7 Score per residue for model 7

• Molecule 1: Oxoglutarate dehydrogenase inhibitor

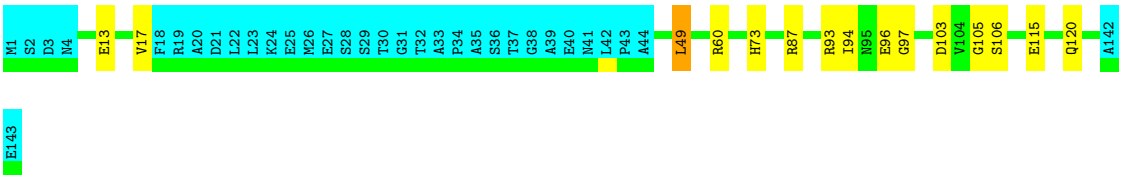
Chain A: 72% 5% 23%



4.2.8 Score per residue for model 8

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

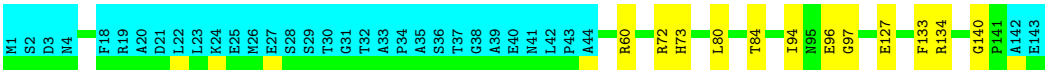
Chain A: 66% 10% • 23%



4.2.9 Score per residue for model 9

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

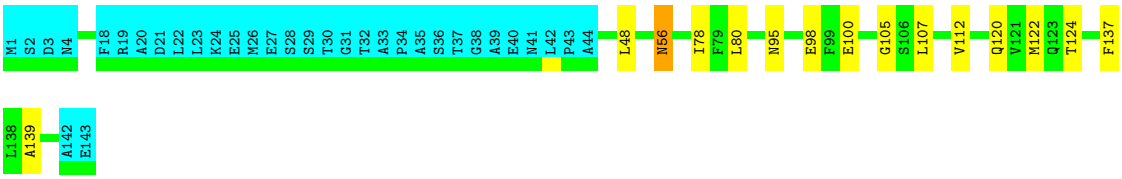
Chain A: 69% 8% 23%



4.2.10 Score per residue for model 10

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

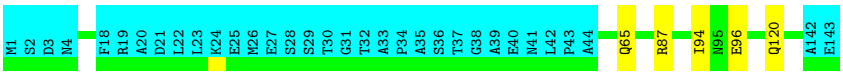
Chain A: 66% 10% • 23%



4.2.11 Score per residue for model 11

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

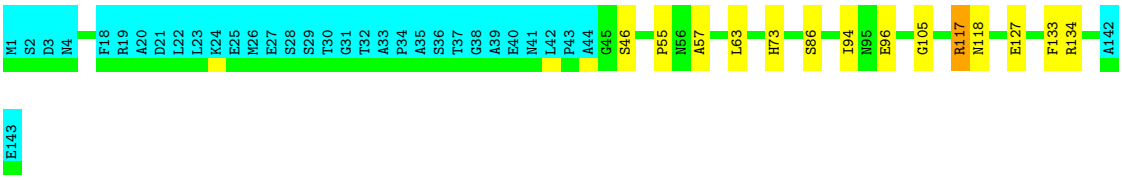
Chain A: 73% • 23%



4.2.12 Score per residue for model 12

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

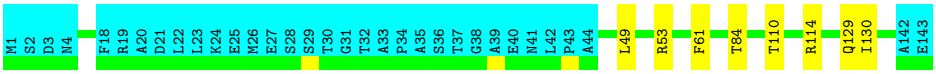
Chain A: 67% 9% • 23%



4.2.13 Score per residue for model 13

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

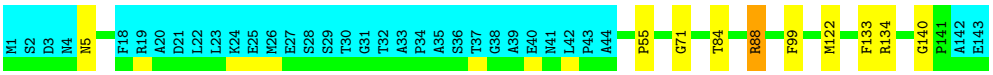
Chain A: 71% 6% 23%



4.2.14 Score per residue for model 14

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

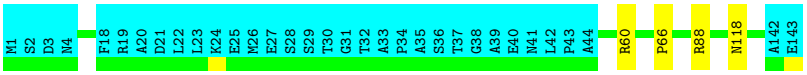
Chain A: 70% 6% • 23%



4.2.15 Score per residue for model 15

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

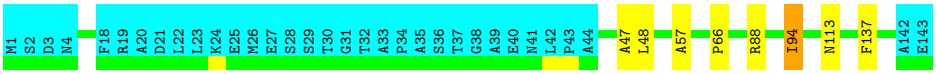
Chain A: 74% • 23%



4.2.16 Score per residue for model 16

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

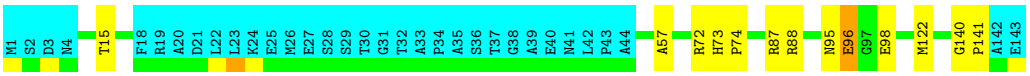
Chain A: 71% 5% • 23%



4.2.17 Score per residue for model 17

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

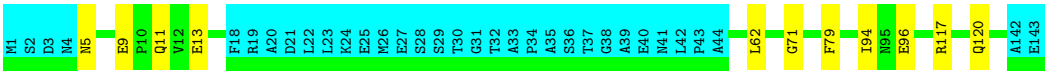
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

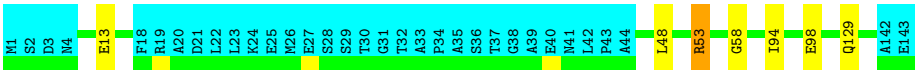
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

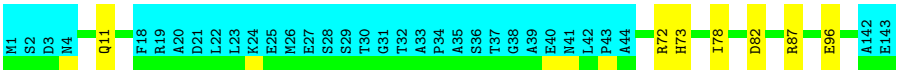
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A:



4.2.21 Score per residue for model 21

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 73% • • 23%

M1 S2 D3 N4 E9 F18 R19 A20 D21 L22 L23 K24 E25 M26 E27 S28 S29 T30 G31 T32 A33 P34 A35 S36 T37 G38 A39 E40 N41 L42 P43 A44 L48 L49 I78 F92 R93 I94 A142 E143

4.2.22 Score per residue for model 22

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 70% 6% • 23%

M1 S2 D3 N4 E9 F18 R19 A20 D21 L22 L23 K24 E25 M26 E27 S28 S29 T30 G31 T32 A33 P34 A35 S36 T37 G38 A39 E40 N41 L42 P43 A44 G45 A57 G71 R72 H73 R88 E96 G97 V101 M122 A142 E143

4.2.23 Score per residue for model 23

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 72% 5% 23%

M1 S2 D3 N4 Q11 F18 R19 A20 D21 L22 L23 K24 E25 M26 E27 S28 S29 T30 G31 T32 A33 P34 A35 S36 T37 G38 A39 E40 N41 L42 P43 A44 G54 H73 T84 I94 Q120 Q123 A142 E143

4.2.24 Score per residue for model 24

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 72% 5% 23%

M1 S2 D3 N4 F18 R19 A20 D21 L22 L23 K24 E25 M26 E27 S28 S29 T30 G31 T32 A33 P34 A35 S36 T37 G38 A39 E40 N41 L42 P43 A44 R60 R87 N95 E98 E115 P116 Q120 A142 E143

4.2.25 Score per residue for model 25

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

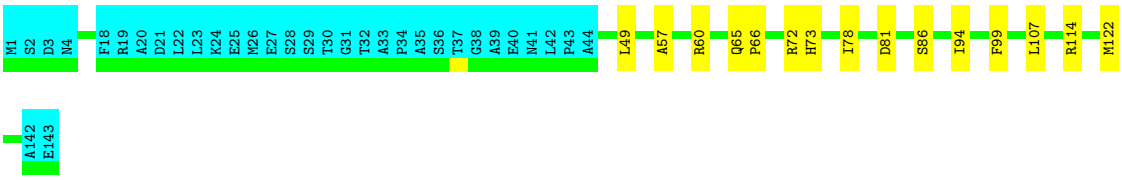
Chain A: 71% 5% • 23%

M1 S2 D3 N4 E13 F18 R19 A20 D21 L22 L23 K24 E25 M26 E27 S28 S29 T30 G31 T32 A33 P34 A35 S36 T37 G38 A39 E40 N41 L42 P43 A44 A47 N56 R60 I78 F79 L80 R88 F137 A142 E143

4.2.26 Score per residue for model 26

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

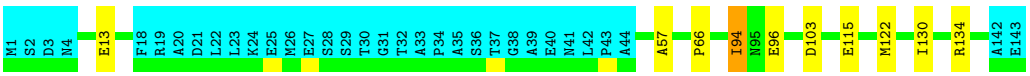
Chain A: 66% 10% 23%



4.2.27 Score per residue for model 27

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

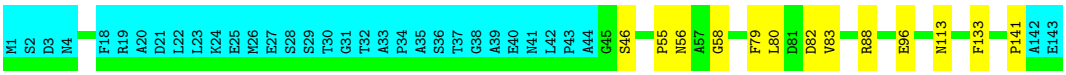
Chain A: 70% 6% • 23%



4.2.28 Score per residue for model 28

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

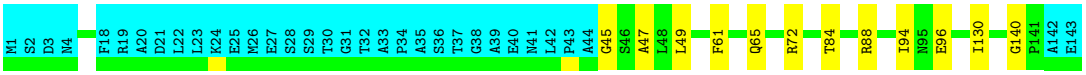
Chain A: 68% 9% 23%



4.2.29 Score per residue for model 29

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

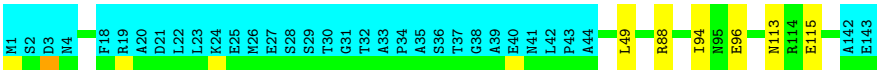
Chain A: 69% 8% 23%



4.2.30 Score per residue for model 30

- Molecule 1: Oxoglutarate dehydrogenase inhibitor

Chain A: 73% • 23%


M1
S2
D3
N4
F18
R19
A20
D21
L22
L23
K24
E25
M26
E27
S28
S29
T30
G31
T32
A33
P34
A35
S36
T37
G38
A39
E40
N41
L42
P43
A44
L49
R88
I94
N95
E96
N113
R114
E115
A142
E143

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 30 calculated structures, 30 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	refinement	1.2

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1115
Number of shifts mapped to atoms	1115
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	60%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	87	ARG	Sidechain	1
1	A	117	ARG	Sidechain	1
1	A	134	ARG	Sidechain	1

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	846	828	828	2±2
All	All	25380	24840	24840	69

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:GLY:O	1:A:88:ARG:HA	0.62	1.95	22	2
1:A:72:ARG:NH1	1:A:81:ASP:HA	0.59	2.12	26	1
1:A:112:VAL:HB	1:A:117:ARG:NE	0.59	2.12	5	1
1:A:99:PHE:HB3	1:A:122:MET:SD	0.54	2.43	14	1
1:A:72:ARG:HA	1:A:87:ARG:O	0.53	2.02	20	2
1:A:124:THR:HB	1:A:139:ALA:HB3	0.51	1.83	10	1
1:A:113:ASN:O	1:A:114:ARG:HD2	0.51	2.06	4	1
1:A:95:ASN:HB3	1:A:98:GLU:O	0.50	2.07	24	2
1:A:49:LEU:O	1:A:60:ARG:HA	0.50	2.05	8	1
1:A:103:ASP:OD2	1:A:106:SER:HB3	0.49	2.08	8	1
1:A:73:HIS:CG	1:A:74:PRO:HD2	0.49	2.42	17	1
1:A:75:GLU:OE2	1:A:87:ARG:HD2	0.48	2.08	5	1
1:A:127:GLU:OE2	1:A:134:ARG:HD3	0.47	2.09	12	1
1:A:47:ALA:HA	1:A:140:GLY:N	0.47	2.25	29	1
1:A:56:ASN:ND2	1:A:80:LEU:HB2	0.47	2.23	5	1
1:A:103:ASP:HB3	1:A:110:THR:CB	0.47	2.40	5	1
1:A:117:ARG:HD2	1:A:120:GLN:OE1	0.47	2.10	18	1
1:A:115:GLU:OE1	1:A:116:PRO:HD2	0.47	2.10	24	1
1:A:46:SER:O	1:A:141:PRO:HA	0.46	2.10	28	1
1:A:70:ALA:HB1	1:A:80:LEU:HD21	0.46	1.87	5	1
1:A:66:PRO:HA	1:A:94:ILE:O	0.46	2.11	16	1
1:A:55:PRO:HD2	1:A:133:PHE:CE1	0.45	2.46	3	3
1:A:55:PRO:HD2	1:A:133:PHE:CZ	0.45	2.47	28	2
1:A:66:PRO:HA	1:A:94:ILE:CD1	0.45	2.42	27	1
1:A:46:SER:HB3	1:A:63:LEU:O	0.45	2.10	12	1
1:A:95:ASN:ND2	1:A:96:GLU:HG2	0.45	2.27	17	1
1:A:56:ASN:CB	1:A:80:LEU:HA	0.45	2.41	4	1
1:A:56:ASN:HB2	1:A:80:LEU:HA	0.45	1.89	28	1
1:A:8:PRO:O	1:A:10:PRO:HD3	0.45	2.12	3	1
1:A:56:ASN:OD1	1:A:80:LEU:HG	0.45	2.12	10	1
1:A:108:ASN:OD1	1:A:131:GLY:HA2	0.44	2.12	2	1
1:A:56:ASN:HA	1:A:80:LEU:HA	0.44	1.89	3	1
1:A:122:MET:HB3	1:A:137:PHE:CE1	0.44	2.47	10	1
1:A:80:LEU:HD23	1:A:133:PHE:CE2	0.44	2.48	9	1
1:A:71:GLY:O	1:A:79:PHE:HA	0.44	2.13	18	1
1:A:84:THR:HB	1:A:133:PHE:CZ	0.43	2.48	14	1
1:A:56:ASN:HA	1:A:80:LEU:CB	0.43	2.43	25	1
1:A:55:PRO:HB2	1:A:81:ASP:O	0.43	2.13	6	1
1:A:92:PHE:CE2	1:A:94:ILE:HB	0.43	2.49	21	1
1:A:72:ARG:O	1:A:72:ARG:HD3	0.42	2.14	1	1
1:A:56:ASN:HA	1:A:81:ASP:N	0.42	2.29	6	1
1:A:56:ASN:HB2	1:A:79:PHE:O	0.42	2.14	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:GLU:OE1	1:A:134:ARG:HD3	0.42	2.13	6	2
1:A:53:ARG:HA	1:A:53:ARG:NE	0.42	2.29	19	1
1:A:112:VAL:HG21	1:A:120:GLN:HG3	0.42	1.92	10	1
1:A:86:SER:OG	1:A:107:LEU:HD21	0.41	2.15	26	1
1:A:115:GLU:HG2	1:A:120:GLN:NE2	0.41	2.30	8	1
1:A:114:ARG:HG2	1:A:129:GLN:OE1	0.41	2.16	13	1
1:A:11:GLN:HA	1:A:11:GLN:OE1	0.41	2.15	18	1
1:A:140:GLY:N	1:A:141:PRO:HD2	0.41	2.31	17	1
1:A:99:PHE:HB2	1:A:122:MET:HB2	0.41	1.92	26	1
1:A:69:THR:HB	1:A:73:HIS:NE2	0.41	2.30	3	1
1:A:65:GLN:OE1	1:A:68:THR:HA	0.41	2.16	4	1
1:A:84:THR:HB	1:A:108:ASN:HB2	0.41	1.93	7	1
1:A:117:ARG:NH2	1:A:128:ILE:HG12	0.40	2.31	5	1
1:A:49:LEU:HD23	1:A:61:PHE:O	0.40	2.16	13	1
1:A:47:ALA:HB3	1:A:137:PHE:CZ	0.40	2.52	16	1
1:A:94:ILE:O	1:A:94:ILE:HD12	0.40	2.16	19	1
1:A:47:ALA:HB1	1:A:137:PHE:CE1	0.40	2.51	25	1
1:A:49:LEU:HD11	1:A:61:PHE:CE1	0.40	2.51	29	1
1:A:132:LYS:HE3	1:A:133:PHE:CZ	0.40	2.52	3	1
1:A:101:VAL:HG11	1:A:122:MET:SD	0.40	2.56	22	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	110/143 (77%)	95±3 (87±3%)	12±3 (11±3%)	2±2 (2±2%)	11	53
All	All	3300/4290 (77%)	2862 (87%)	375 (11%)	63 (2%)	11	53

All 25 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	57	ALA	10
1	A	73	HIS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	113	ASN	6
1	A	96	GLU	6
1	A	122	MET	3
1	A	87	ARG	3
1	A	97	GLY	3
1	A	105	GLY	3
1	A	140	GLY	2
1	A	58	GLY	2
1	A	45	GLY	2
1	A	12	VAL	1
1	A	53	ARG	1
1	A	131	GLY	1
1	A	17	VAL	1
1	A	72	ARG	1
1	A	86	SER	1
1	A	117	ARG	1
1	A	118	ASN	1
1	A	5	ASN	1
1	A	15	THR	1
1	A	54	GLY	1
1	A	82	ASP	1
1	A	83	VAL	1
1	A	84	THR	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	92/117 (79%)	88±2 (96±2%)	4±2 (4±2%)	33 81
All	All	2760/3510 (79%)	2640 (96%)	120 (4%)	33 81

All 41 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	94	ILE	13
1	A	88	ARG	10

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Mol	Chain	Res	Type	Models (Total)
1	A	96	GLU	8
1	A	13	GLU	8
1	A	78	ILE	7
1	A	48	LEU	5
1	A	65	GLN	5
1	A	60	ARG	5
1	A	120	GLN	4
1	A	84	THR	4
1	A	49	LEU	4
1	A	87	ARG	3
1	A	98	GLU	3
1	A	130	ILE	3
1	A	9	GLU	3
1	A	75	GLU	2
1	A	56	ASN	2
1	A	134	ARG	2
1	A	118	ASN	2
1	A	123	GLN	2
1	A	53	ARG	2
1	A	11	GLN	2
1	A	73	HIS	2
1	A	115	GLU	2
1	A	69	THR	1
1	A	104	VAL	1
1	A	124	THR	1
1	A	93	ARG	1
1	A	100	GLU	1
1	A	107	LEU	1
1	A	117	ARG	1
1	A	110	THR	1
1	A	66	PRO	1
1	A	5	ASN	1
1	A	62	LEU	1
1	A	129	GLN	1
1	A	82	ASP	1
1	A	80	LEU	1
1	A	114	ARG	1
1	A	103	ASP	1
1	A	72	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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 60% for the well-defined parts and 60% 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 (i)

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

Total number of shifts	1115
Number of shifts mapped to atoms	1115
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	133	-1.13 ± 0.37	Should be applied

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 60%, i.e. 878 atoms were assigned a chemical shift out of a possible 1470. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	325/547 (59%)	223/224 (100%)	0/220 (0%)	102/103 (99%)
Sidechain	513/840 (61%)	503/543 (93%)	0/257 (0%)	10/40 (25%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	40/83 (48%)	39/42 (93%)	0/39 (0%)	1/2 (50%)
Overall	878/1470 (60%)	765/809 (95%)	0/516 (0%)	113/145 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 60%, i.e. 1114 atoms were assigned a chemical shift out of a possible 1858. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	421/710 (59%)	288/290 (99%)	0/286 (0%)	133/134 (99%)
Sidechain	648/1055 (61%)	637/683 (93%)	0/326 (0%)	11/46 (24%)
Aromatic	45/93 (48%)	44/47 (94%)	0/44 (0%)	1/2 (50%)
Overall	1114/1858 (60%)	969/1020 (95%)	0/656 (0%)	145/182 (80%)

7.1.4 Statistically unusual chemical shifts (i)

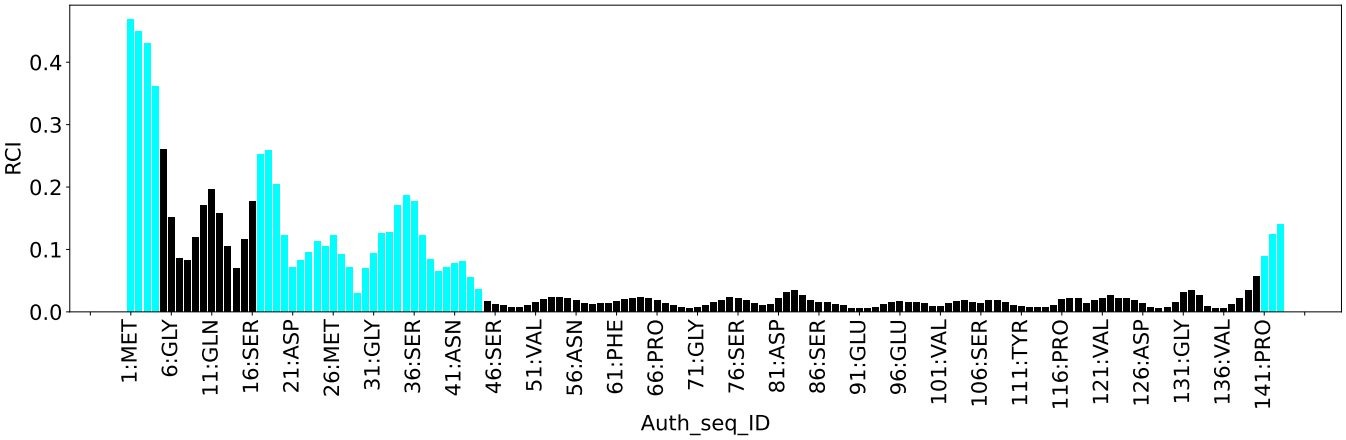
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	86	SER	H	11.38	5.45 – 11.10	5.5

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:


RCI
0.0
0.1
0.2
0.3
0.4
1:MET
6:GLY
11:GLN
16:SER
21:ASP
26:MET
31:GLY
36:SER
41:ASN
46:SER
51:VAL
56:ASN
61:PHE
66:PRO
71:GLY
76:SER
81:ASP
86:SER
91:GLU
96:GLU
101:VAL
106:SER
111:TYR
116:PRO
121:VAL
126:ASP
131:GLY
136:VAL
141:PRO
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1040
Intra-residue (|i-j|=0)	273
Sequential (|i-j|=1)	431
Medium range (|i-j|>1 and |i-j|<5)	76
Long range (|i-j|≥5)	200
Inter-chain	0
Hydrogen bond restraints	60
Disulfide bond restraints	0
Total dihedral-angle restraints	110
Number of unmapped restraints	1
Number of restraints per residue	8.0
Number of long range restraints per residue[1]	1.7

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	2.9	0.2
0.2-0.5 (Medium)	0.2	0.25
>0.5 (Large)	None	None

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)	13.1	7.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	None	None

9 Distance violation analysis (i)

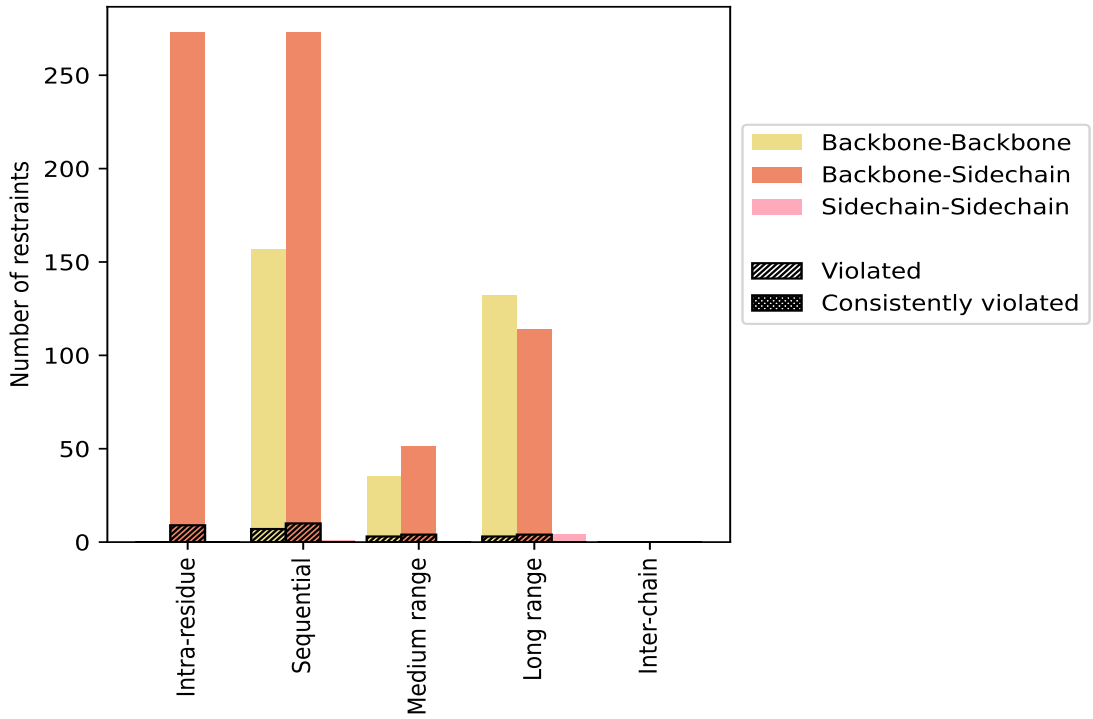
9.1 Summary of distance violations (i)

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.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	273	26.2	9	3.3	0.9	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	273	26.2	9	3.3	0.9	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	431	41.4	17	3.9	1.6	0	0.0	0.0
Backbone-Backbone	157	15.1	7	4.5	0.7	0	0.0	0.0
Backbone-Sidechain	273	26.2	10	3.7	1.0	0	0.0	0.0
Sidechain-Sidechain	1	0.1	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	76	7.3	7	9.2	0.7	0	0.0	0.0
Backbone-Backbone	25	2.4	3	12.0	0.3	0	0.0	0.0
Backbone-Sidechain	51	4.9	4	7.8	0.4	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	200	19.2	6	3.0	0.6	0	0.0	0.0
Backbone-Backbone	82	7.9	2	2.4	0.2	0	0.0	0.0
Backbone-Sidechain	114	11.0	4	3.5	0.4	0	0.0	0.0
Sidechain-Sidechain	4	0.4	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	60	5.8	1	1.7	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1040	100.0	40	3.8	3.8	0	0.0	0.0
Backbone-Backbone	324	31.2	13	4.0	1.2	0	0.0	0.0
Backbone-Sidechain	711	68.4	27	3.8	2.6	0	0.0	0.0
Sidechain-Sidechain	5	0.5	0	0.0	0.0	0	0.0	0.0

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

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



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

9.2 Distance violation statistics for each model (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	1	1	0	0	2	0.19	0.25	0.06	0.19
2	1	1	0	2	0	4	0.14	0.17	0.02	0.12
3	1	0	0	1	0	2	0.14	0.14	0.01	0.14
4	2	2	0	2	0	6	0.14	0.17	0.02	0.15
5	0	0	1	1	0	2	0.14	0.18	0.03	0.14
6	0	1	0	2	0	3	0.12	0.13	0.01	0.13
7	0	1	0	3	0	4	0.12	0.15	0.02	0.12
8	1	2	0	0	0	3	0.13	0.15	0.02	0.12
9	0	0	0	0	0	0	0.0	0.0	0.0	0.0
10	1	3	0	1	0	5	0.14	0.17	0.02	0.13
11	0	0	1	0	0	1	0.12	0.12	0.0	0.12

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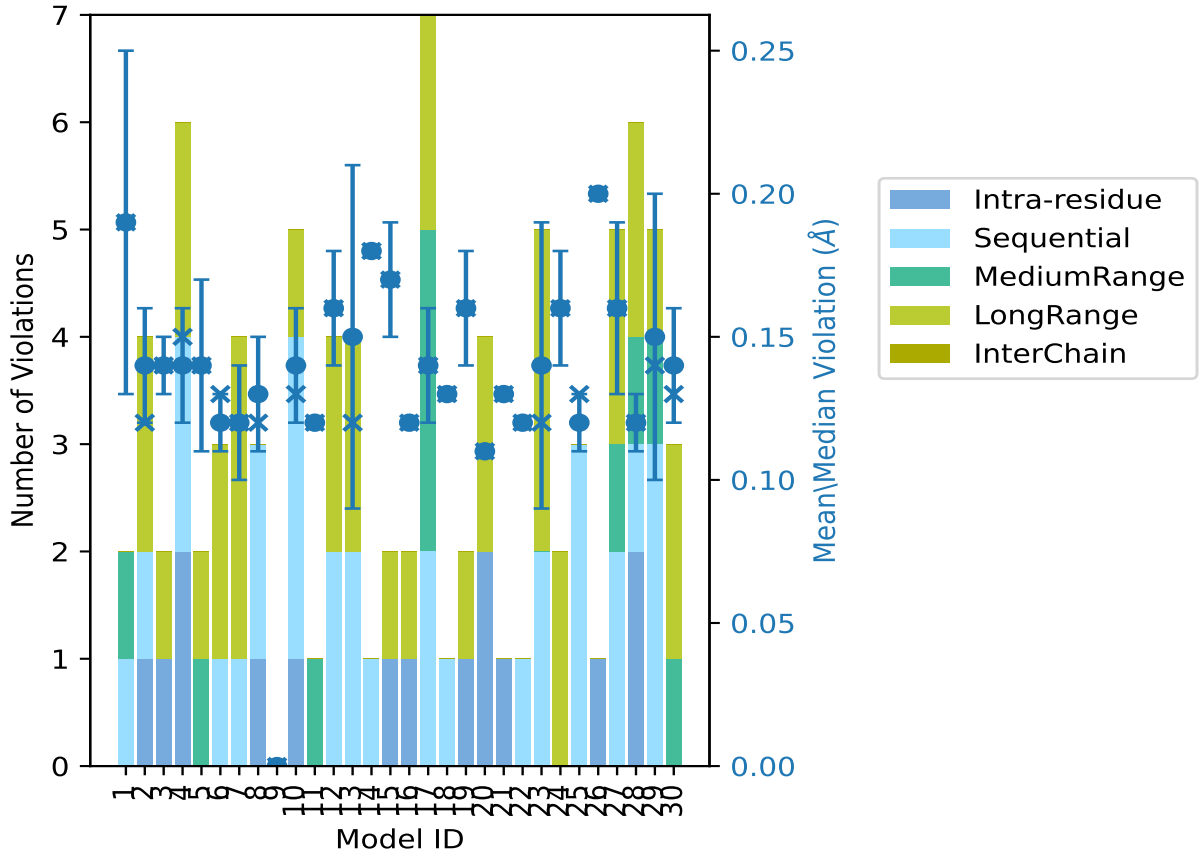
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	0	2	0	2	0	4	0.16	0.17	0.02	0.16
13	0	2	0	2	0	4	0.15	0.25	0.06	0.12
14	0	1	0	0	0	1	0.18	0.18	0.0	0.18
15	1	0	0	1	0	2	0.17	0.19	0.02	0.17
16	1	0	0	1	0	2	0.12	0.12	0.0	0.12
17	0	2	3	2	0	7	0.14	0.18	0.02	0.14
18	0	1	0	0	0	1	0.13	0.13	0.0	0.13
19	1	0	0	1	0	2	0.16	0.18	0.02	0.16
20	2	0	0	2	0	4	0.11	0.11	0.0	0.11
21	1	0	0	0	0	1	0.13	0.13	0.0	0.13
22	0	1	0	0	0	1	0.12	0.12	0.0	0.12
23	0	2	0	3	0	5	0.14	0.23	0.05	0.12
24	0	0	0	2	0	2	0.16	0.17	0.02	0.16
25	0	3	0	0	0	3	0.12	0.13	0.01	0.13
26	1	0	0	0	0	1	0.2	0.2	0.0	0.2
27	0	2	1	2	0	5	0.16	0.22	0.03	0.16
28	2	1	1	2	0	6	0.12	0.15	0.01	0.12
29	0	3	1	1	0	5	0.15	0.25	0.05	0.14
30	0	0	1	2	0	3	0.14	0.16	0.02	0.13

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 941(IR:264, SQ:414, MR:69, LR:194, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	8	5	0	0	19	1	3.3
2	6	1	1	0	10	2	6.7
0	1	1	3	0	5	3	10.0
0	2	0	0	0	2	4	13.3
1	0	0	0	0	1	5	16.7
0	0	0	0	0	0	6	20.0

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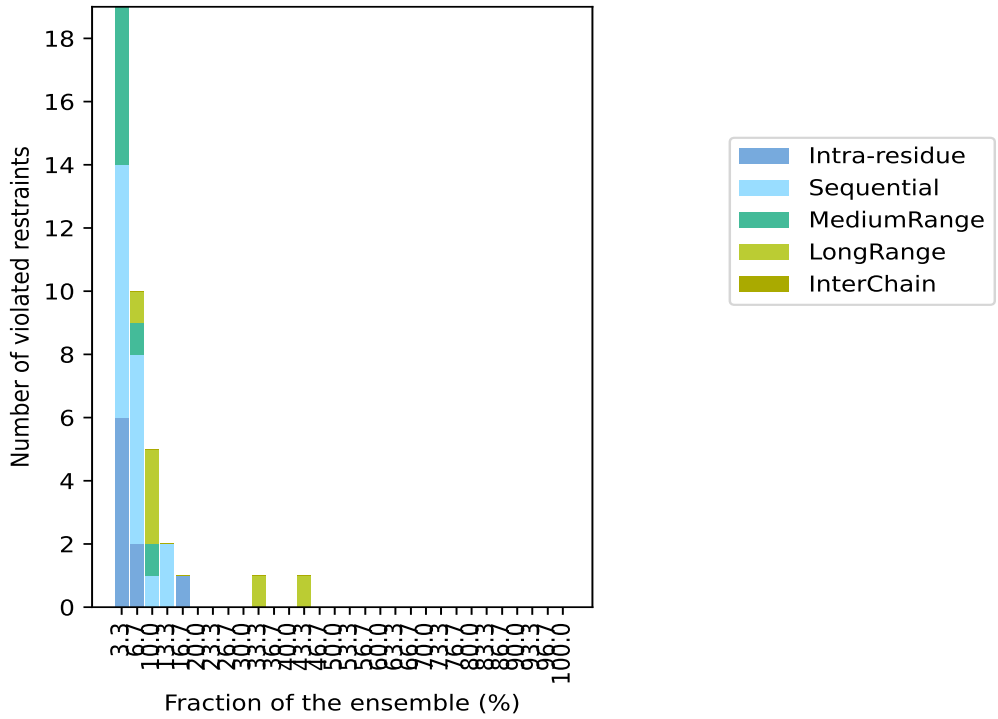
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	7	23.3
0	0	0	0	0	0	8	26.7
0	0	0	0	0	0	9	30.0
0	0	0	1	0	1	10	33.3
0	0	0	0	0	0	11	36.7
0	0	0	0	0	0	12	40.0
0	0	0	1	0	1	13	43.3
0	0	0	0	0	0	14	46.7
0	0	0	0	0	0	15	50.0
0	0	0	0	0	0	16	53.3
0	0	0	0	0	0	17	56.7
0	0	0	0	0	0	18	60.0
0	0	0	0	0	0	19	63.3
0	0	0	0	0	0	20	66.7
0	0	0	0	0	0	21	70.0
0	0	0	0	0	0	22	73.3
0	0	0	0	0	0	23	76.7
0	0	0	0	0	0	24	80.0
0	0	0	0	0	0	25	83.3
0	0	0	0	0	0	26	86.7
0	0	0	0	0	0	27	90.0
0	0	0	0	0	0	28	93.3
0	0	0	0	0	0	29	96.7
0	0	0	0	0	0	30	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

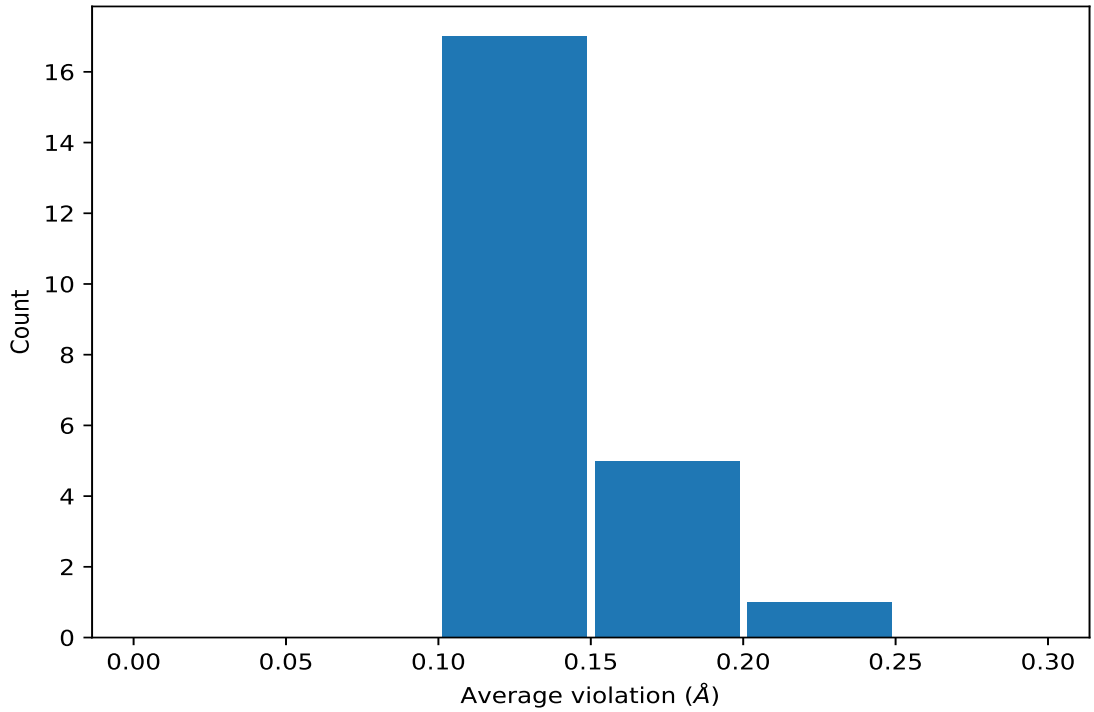
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



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)
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	13	0.14	0.02	0.14
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	10	0.14	0.03	0.13
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	5	0.15	0.03	0.13
(1,636)	1:A:100:GLU:HG2	1:A:101:VAL:H	4	0.15	0.0	0.15
(1,636)	1:A:100:GLU:HG3	1:A:101:VAL:H	4	0.15	0.0	0.15
(1,802)	1:A:120:GLN:HE21	1:A:121:VAL:H	4	0.13	0.01	0.14
(1,460)	1:A:80:LEU:HA	1:A:81:ASP:H	3	0.21	0.03	0.22
(1,674)	1:A:103:ASP:H	1:A:110:THR:HB	3	0.14	0.02	0.13
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD21	3	0.14	0.03	0.13
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD22	3	0.14	0.03	0.13
(1,240)	1:A:51:VAL:HB	1:A:58:GLY:H	3	0.13	0.02	0.12
(1,490)	1:A:82:ASP:HB2	1:A:84:THR:H	3	0.12	0.01	0.11
(1,127)	1:A:38:GLY:H	1:A:39:ALA:H	2	0.19	0.06	0.19
(1,976)	1:A:143:GLU:H	1:A:143:GLU:HB3	2	0.15	0.03	0.15
(1,411)	1:A:72:ARG:H	1:A:73:HIS:H	2	0.14	0.02	0.14
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB2	2	0.14	0.02	0.14

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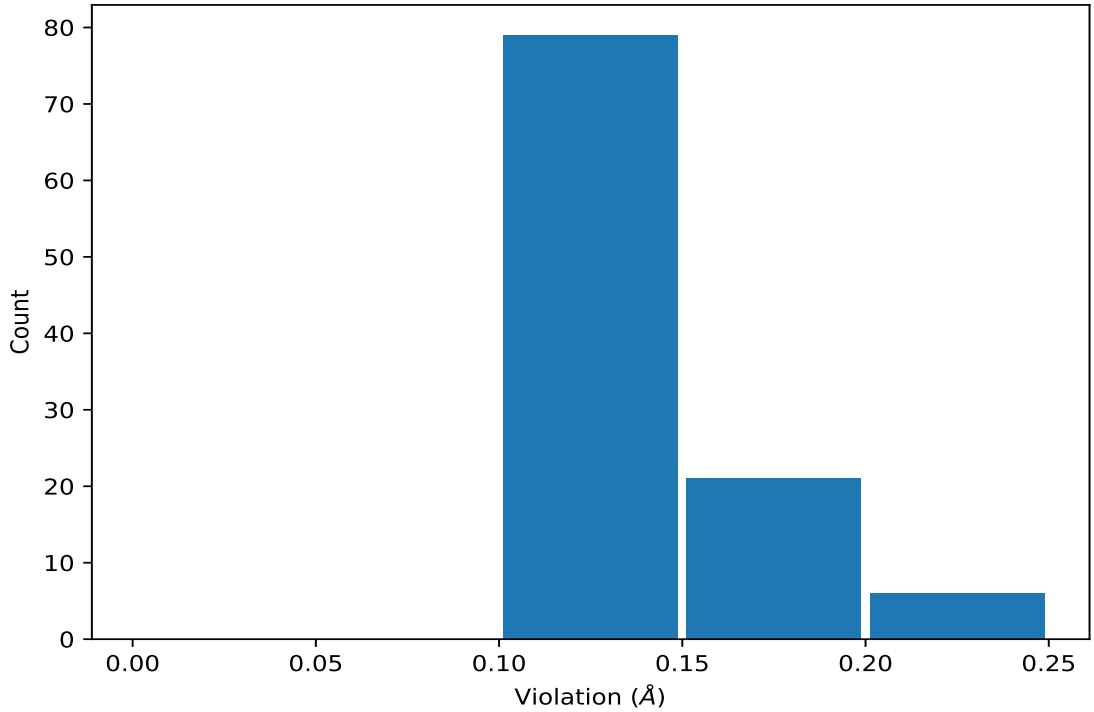
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB3	2	0.14	0.02	0.14
(1,977)	1:A:143:GLU:H	1:A:143:GLU:HB2	2	0.13	0.02	0.13
(1,138)	1:A:40:GLU:HG2	1:A:41:ASN:H	2	0.12	0.01	0.12
(1,428)	1:A:75:GLU:H	1:A:76:SER:H	2	0.12	0.01	0.12
(1,49)	1:A:15:THR:H	1:A:16:SER:H	2	0.12	0.0	0.12
(1,107)	1:A:32:THR:HB	1:A:33:ALA:H	2	0.12	0.0	0.12
(1,772)	1:A:113:ASN:HD22	1:A:127:GLU:H	2	0.12	0.0	0.12

[1]Number of violated models, [2]Standard 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)
(1,50)	1:A:16:SER:HA	1:A:17:VAL:H	29	0.25
(1,460)	1:A:80:LEU:HA	1:A:81:ASP:H	1	0.25
(1,127)	1:A:38:GLY:H	1:A:39:ALA:H	13	0.25
(1,932)	1:A:135:LEU:HG	1:A:136:VAL:H	23	0.23
(1,460)	1:A:80:LEU:HA	1:A:81:ASP:H	27	0.22
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	26	0.2
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	15	0.19
(1,901)	1:A:130:ILE:H	1:A:130:ILE:HG13	19	0.18
(1,803)	1:A:120:GLN:HE22	1:A:121:VAL:H	14	0.18
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD21	17	0.18
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD22	17	0.18
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	5	0.18
(1,976)	1:A:143:GLU:H	1:A:143:GLU:HB3	4	0.17
(1,674)	1:A:103:ASP:H	1:A:110:THR:HB	24	0.17
(1,460)	1:A:80:LEU:HA	1:A:81:ASP:H	17	0.17
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	10	0.17
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	2	0.17
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	12	0.17
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	27	0.17
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB2	27	0.16
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB3	27	0.16
(1,604)	1:A:96:GLU:HG2	1:A:97:GLY:H	12	0.16
(1,604)	1:A:96:GLU:HG3	1:A:97:GLY:H	12	0.16
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	4	0.16
(1,411)	1:A:72:ARG:H	1:A:73:HIS:H	12	0.16
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	4	0.16
(1,240)	1:A:51:VAL:HB	1:A:58:GLY:H	30	0.16
(1,977)	1:A:143:GLU:H	1:A:143:GLU:HB2	15	0.15
(1,802)	1:A:120:GLN:HE21	1:A:121:VAL:H	28	0.15
(1,636)	1:A:100:GLU:HG2	1:A:101:VAL:H	8	0.15
(1,636)	1:A:100:GLU:HG3	1:A:101:VAL:H	8	0.15
(1,636)	1:A:100:GLU:HG2	1:A:101:VAL:H	17	0.15
(1,636)	1:A:100:GLU:HG3	1:A:101:VAL:H	17	0.15
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	7	0.15
(1,802)	1:A:120:GLN:HE21	1:A:121:VAL:H	27	0.14
(1,636)	1:A:100:GLU:HG2	1:A:101:VAL:H	10	0.14
(1,636)	1:A:100:GLU:HG3	1:A:101:VAL:H	10	0.14
(1,636)	1:A:100:GLU:HG2	1:A:101:VAL:H	29	0.14
(1,636)	1:A:100:GLU:HG3	1:A:101:VAL:H	29	0.14
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	3	0.14
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	29	0.14
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	17	0.14
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	19	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	24	0.14
(1,132)	1:A:39:ALA:H	1:A:40:GLU:HG2	4	0.14
(1,132)	1:A:39:ALA:H	1:A:40:GLU:HG3	4	0.14
(1,9)	1:A:9:GLU:H	1:A:9:GLU:HG2	3	0.13
(1,9)	1:A:9:GLU:H	1:A:9:GLU:HG3	3	0.13
(1,802)	1:A:120:GLN:HE21	1:A:121:VAL:H	2	0.13
(1,774)	1:A:113:ASN:H	1:A:115:GLU:H	30	0.13
(1,674)	1:A:103:ASP:H	1:A:110:THR:HB	12	0.13
(1,588)	1:A:95:ASN:HA	1:A:97:GLY:H	17	0.13
(1,55)	1:A:17:VAL:HA	1:A:18:PHE:H	25	0.13
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD21	7	0.13
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD22	7	0.13
(1,490)	1:A:82:ASP:HB2	1:A:84:THR:H	1	0.13
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	10	0.13
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	21	0.13
(1,428)	1:A:75:GLU:H	1:A:76:SER:H	6	0.13
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	6	0.13
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	28	0.13
(1,138)	1:A:40:GLU:HG2	1:A:41:ASN:H	25	0.13
(1,127)	1:A:38:GLY:H	1:A:39:ALA:H	18	0.13
(2,15)	1:A:51:VAL:H	1:A:59:ALA:O	23	0.12
(1,976)	1:A:143:GLU:H	1:A:143:GLU:HB3	28	0.12
(1,971)	1:A:141:PRO:HB2	1:A:142:ALA:H	10	0.12
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB2	17	0.12
(1,826)	1:A:123:GLN:H	1:A:126:ASP:HB3	17	0.12
(1,772)	1:A:113:ASN:HD22	1:A:127:GLU:H	30	0.12
(1,674)	1:A:103:ASP:H	1:A:110:THR:HB	13	0.12
(1,593)	1:A:95:ASN:HB2	1:A:98:GLU:H	11	0.12
(1,49)	1:A:15:THR:H	1:A:16:SER:H	10	0.12
(1,450)	1:A:78:ILE:H	1:A:78:ILE:HG13	2	0.12
(1,411)	1:A:72:ARG:H	1:A:73:HIS:H	22	0.12
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	28	0.12
(1,240)	1:A:51:VAL:HB	1:A:58:GLY:H	2	0.12
(1,240)	1:A:51:VAL:HB	1:A:58:GLY:H	27	0.12
(1,155)	1:A:42:LEU:H	1:A:42:LEU:HB2	8	0.12
(1,154)	1:A:42:LEU:H	1:A:42:LEU:HB3	16	0.12
(1,107)	1:A:32:THR:HB	1:A:33:ALA:H	23	0.12
(1,977)	1:A:143:GLU:H	1:A:143:GLU:HB2	20	0.11
(1,802)	1:A:120:GLN:HE21	1:A:121:VAL:H	29	0.11
(1,772)	1:A:113:ASN:HD22	1:A:127:GLU:H	20	0.11
(1,745)	1:A:112:VAL:HA	1:A:114:ARG:H	28	0.11
(1,579)	1:A:94:ILE:HD11	1:A:95:ASN:H	4	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,579)	1:A:94:ILE:HD12	1:A:95:ASN:H	4	0.11
(1,579)	1:A:94:ILE:HD13	1:A:95:ASN:H	4	0.11
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD21	13	0.11
(1,504)	1:A:84:THR:HA	1:A:108:ASN:HD22	13	0.11
(1,490)	1:A:82:ASP:HB2	1:A:84:THR:H	17	0.11
(1,490)	1:A:82:ASP:HB2	1:A:84:THR:H	29	0.11
(1,49)	1:A:15:THR:H	1:A:16:SER:H	25	0.11
(1,488)	1:A:82:ASP:HB2	1:A:84:THR:H	5	0.11
(1,488)	1:A:82:ASP:HB3	1:A:84:THR:H	5	0.11
(1,482)	1:A:81:ASP:H	1:A:81:ASP:HB2	28	0.11
(1,428)	1:A:75:GLU:H	1:A:76:SER:H	7	0.11
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	4	0.11
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	6	0.11
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	20	0.11
(1,279)	1:A:56:ASN:HA	1:A:82:ASP:H	23	0.11
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	7	0.11
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	16	0.11
(1,278)	1:A:56:ASN:HA	1:A:80:LEU:H	23	0.11
(1,27)	1:A:12:VAL:H	1:A:12:VAL:HB	20	0.11
(1,138)	1:A:40:GLU:HG2	1:A:41:ASN:H	8	0.11
(1,107)	1:A:32:THR:HB	1:A:33:ALA:H	13	0.11

10 Dihedral-angle violation analysis (i)

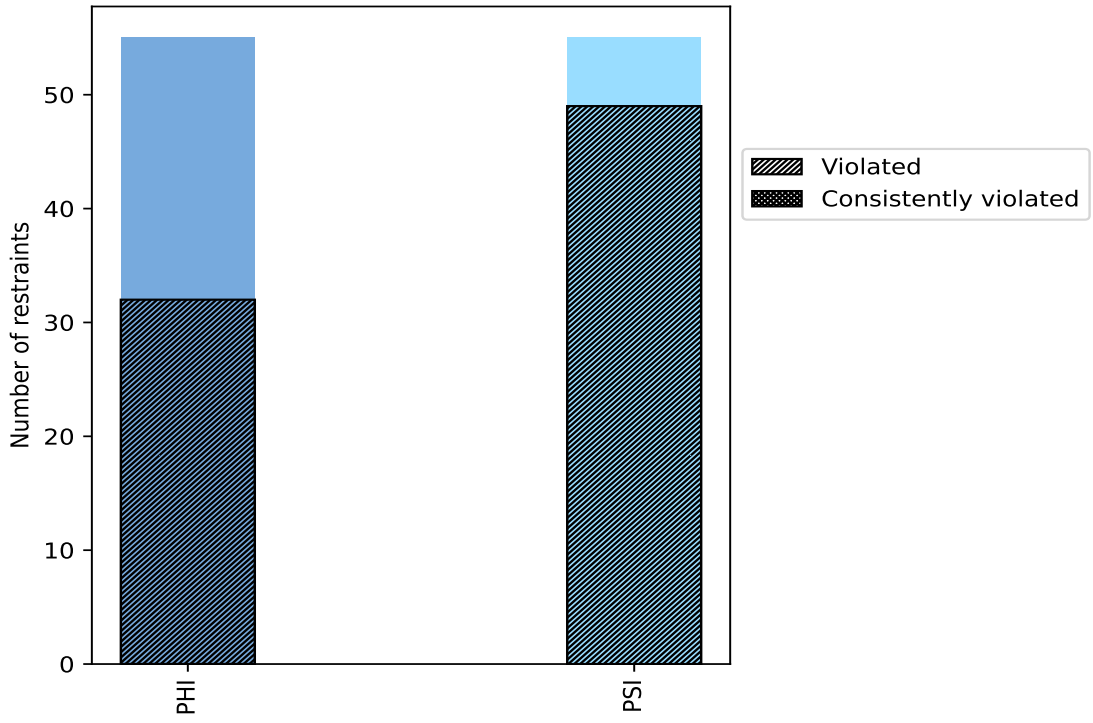
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	55	50.0	32	58.2	29.1	0	0.0	0.0
PSI	55	50.0	49	89.1	44.5	0	0.0	0.0
Total	110	100.0	81	73.6	73.6	0	0.0	0.0

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

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



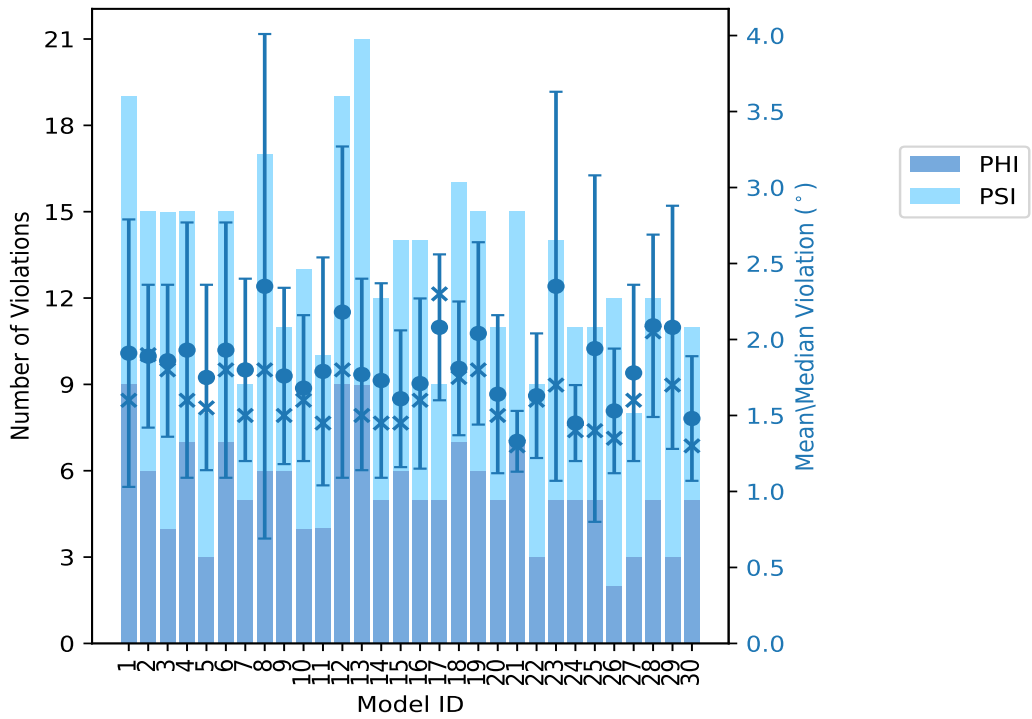
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PHI	PSI	Total				
1	9	10	19	1.91	4.4	0.88	1.6
2	6	9	15	1.89	3.0	0.47	1.9
3	4	11	15	1.86	3.0	0.5	1.8
4	7	8	15	1.93	3.7	0.84	1.6
5	3	5	8	1.75	2.8	0.61	1.55
6	7	8	15	1.93	3.9	0.84	1.8
7	5	4	9	1.8	2.9	0.6	1.5
8	6	11	17	2.35	7.0	1.66	1.8
9	6	5	11	1.76	2.7	0.58	1.5
10	4	9	13	1.68	3.1	0.48	1.6
11	4	6	10	1.79	3.8	0.75	1.45
12	9	10	19	2.18	5.7	1.09	1.8
13	9	12	21	1.77	3.0	0.63	1.5
14	5	7	12	1.73	2.9	0.64	1.45
15	6	8	14	1.61	2.9	0.45	1.45
16	5	9	14	1.71	3.2	0.56	1.6
17	5	4	9	2.08	2.7	0.48	2.3
18	7	9	16	1.81	2.8	0.44	1.75
19	6	9	15	2.04	3.4	0.6	1.8
20	5	6	11	1.64	2.7	0.52	1.5
21	7	8	15	1.33	1.7	0.2	1.3
22	3	6	9	1.63	2.6	0.41	1.6
23	5	9	14	2.35	5.4	1.28	1.7
24	5	6	11	1.45	2.1	0.25	1.4
25	5	6	11	1.94	4.7	1.14	1.4
26	2	10	12	1.53	2.3	0.41	1.35
27	3	5	8	1.78	2.8	0.58	1.6
28	5	7	12	2.09	3.0	0.6	2.05
29	3	8	11	2.08	3.4	0.8	1.7
30	5	6	11	1.48	2.6	0.41	1.3

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]	%
7	12	19	1	3.3
4	9	13	2	6.7
7	2	9	3	10.0
3	9	12	4	13.3
3	5	8	5	16.7
0	4	4	6	20.0
1	1	2	7	23.3
1	2	3	8	26.7
2	0	2	9	30.0
0	1	1	10	33.3
1	0	1	11	36.7

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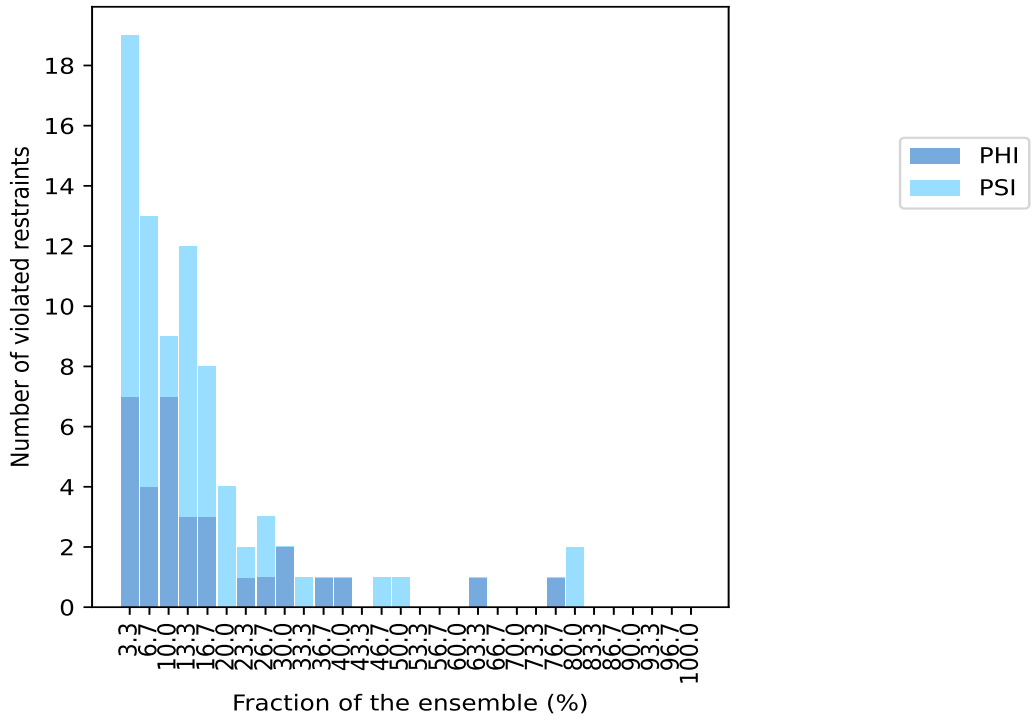
Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count[1]	%
1	0	1	12	40.0
0	0	0	13	43.3
0	1	1	14	46.7
0	1	1	15	50.0
0	0	0	16	53.3
0	0	0	17	56.7
0	0	0	18	60.0
1	0	1	19	63.3
0	0	0	20	66.7
0	0	0	21	70.0
0	0	0	22	73.3
1	0	1	23	76.7
0	2	2	24	80.0
0	0	0	25	83.3
0	0	0	26	86.7
0	0	0	27	90.0
0	0	0	28	93.3
0	0	0	29	96.7
0	0	0	30	100.0

[1] Number of models with violations

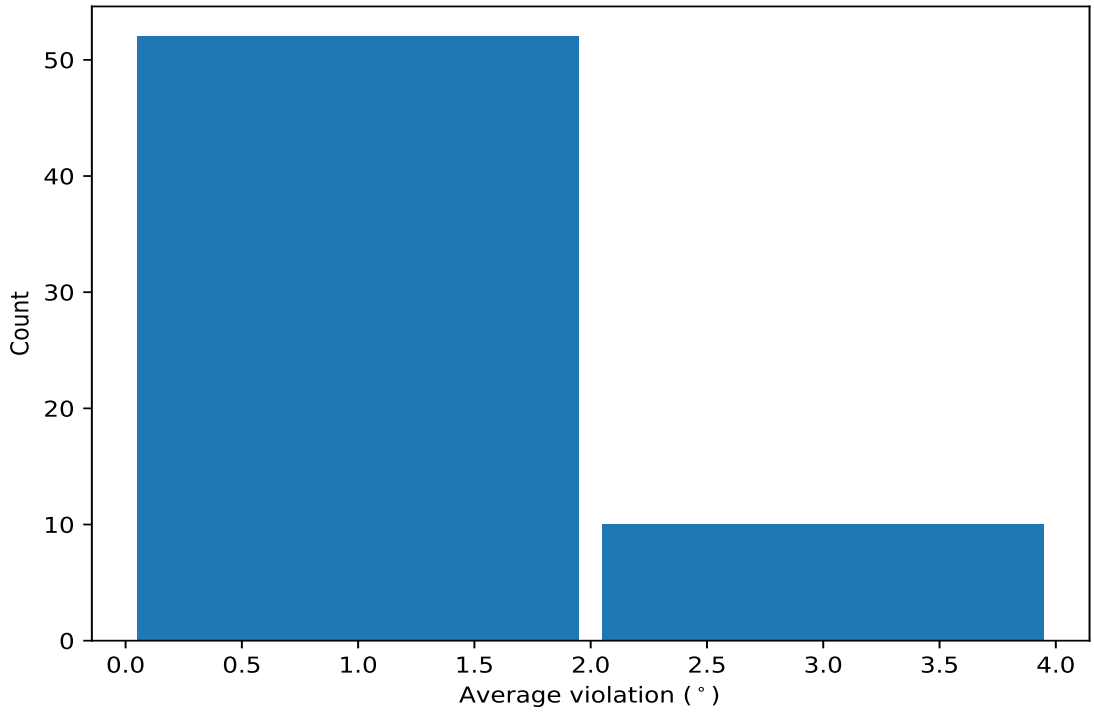
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	24	2.65	1.36	2.4
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	24	2.21	0.71	2.25
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	23	1.77	0.66	1.7
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	19	2.77	1.15	2.7
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	15	1.88	0.62	1.8
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	14	1.59	0.35	1.5
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	12	1.82	0.49	1.75
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	11	1.68	0.34	1.7
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	10	1.63	0.46	1.4
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	9	1.98	0.48	1.9
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	9	1.87	1.27	1.4
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	8	1.89	0.55	1.85
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	8	1.8	0.34	1.85
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	8	1.69	0.61	1.45
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	7	1.6	0.59	1.3
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	7	1.47	0.43	1.3
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	6	2.13	0.4	2.2
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	6	1.85	0.79	1.4
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	6	1.52	0.54	1.3
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	6	1.37	0.29	1.25
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	5	2.1	1.04	1.8

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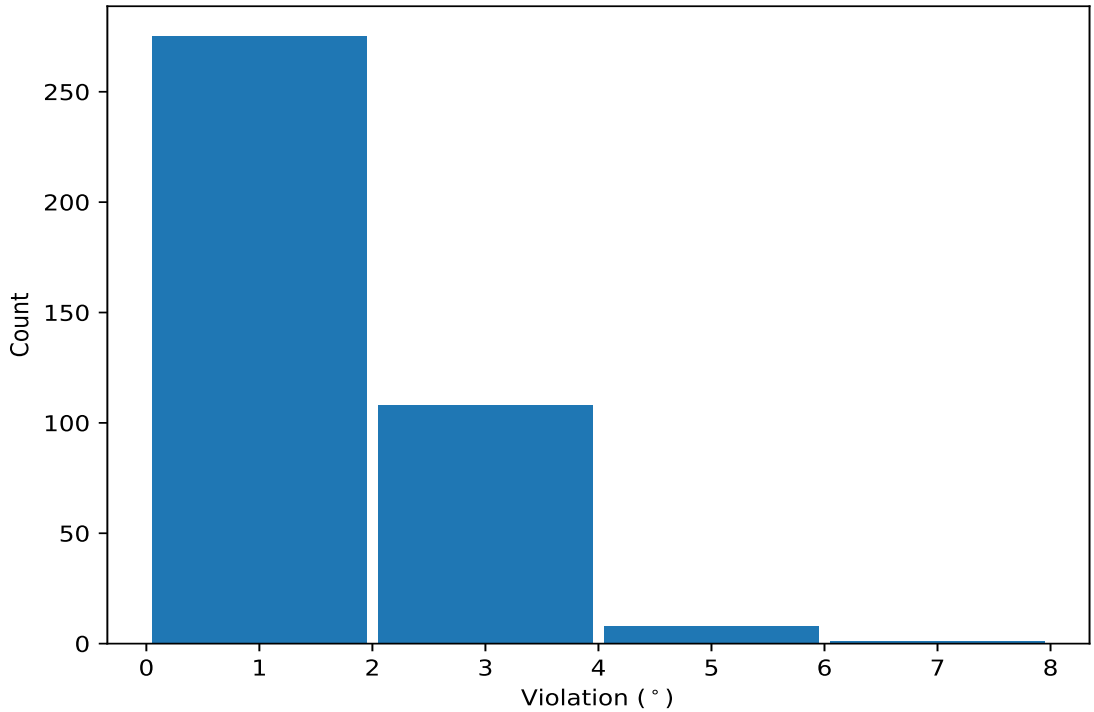
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	5	1.96	0.71	1.7
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	5	1.94	0.59	1.9
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	5	1.94	0.41	2.1
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	5	1.78	0.48	1.6
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	5	1.78	0.3	1.8
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	5	1.76	0.46	1.8
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	5	1.46	0.17	1.4
(1,31)	1:A:94:ILE:C	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	4	2.72	0.94	2.5
(1,99)	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1:A:122:MET:N	4	2.08	0.54	2.2
(1,57)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:PRO:N	4	1.8	0.27	1.85
(1,84)	1:A:93:ARG:N	1:A:93:ARG:CA	1:A:93:ARG:C	1:A:94:ILE:N	4	1.75	0.43	1.7
(1,45)	1:A:122:MET:C	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	4	1.6	0.25	1.65
(1,71)	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	1:A:52:LYS:N	4	1.55	0.36	1.55
(1,103)	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	1:A:129:GLN:N	4	1.5	0.14	1.5
(1,58)	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1:A:9:GLU:N	4	1.35	0.38	1.15
(1,1)	1:A:1:MET:C	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	4	1.32	0.08	1.35
(1,104)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:ILE:N	4	1.27	0.13	1.3
(1,90)	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1:A:103:ASP:N	4	1.23	0.08	1.25
(1,83)	1:A:92:PHE:N	1:A:92:PHE:CA	1:A:92:PHE:C	1:A:93:ARG:N	4	1.2	0.12	1.15
(1,79)	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	1:A:75:GLU:N	3	1.93	0.21	1.9
(1,36)	1:A:102:VAL:C	1:A:103:ASP:N	1:A:103:ASP:CA	1:A:103:ASP:C	3	1.67	0.66	1.3
(1,24)	1:A:73:HIS:C	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	3	1.6	0.57	1.3
(1,107)	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	1:A:136:VAL:N	3	1.53	0.33	1.6
(1,53)	1:A:135:LEU:C	1:A:136:VAL:N	1:A:136:VAL:CA	1:A:136:VAL:C	3	1.47	0.05	1.5
(1,11)	1:A:40:GLU:C	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	3	1.47	0.31	1.3
(1,13)	1:A:47:ALA:C	1:A:48:LEU:N	1:A:48:LEU:CA	1:A:48:LEU:C	3	1.43	0.17	1.5
(1,52)	1:A:134:ARG:C	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	3	1.43	0.09	1.5
(1,22)	1:A:66:PRO:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	3	1.4	0.14	1.3
(1,85)	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	1:A:95:ASN:N	2	3.4	2.3	3.4
(1,70)	1:A:50:VAL:N	1:A:50:VAL:CA	1:A:50:VAL:C	1:A:51:VAL:N	2	2.3	0.9	2.3
(1,4)	1:A:8:PRO:C	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	2	2.2	0.0	2.2
(1,32)	1:A:98:GLU:C	1:A:99:PHE:N	1:A:99:PHE:CA	1:A:99:PHE:C	2	1.5	0.1	1.5
(1,65)	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	1:A:41:ASN:N	2	1.5	0.4	1.5
(1,102)	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	1:A:128:ILE:N	2	1.5	0.2	1.5
(1,67)	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	1:A:47:ALA:N	2	1.45	0.35	1.45
(1,47)	1:A:126:ASP:C	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	2	1.45	0.05	1.45
(1,66)	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	1:A:42:LEU:N	2	1.35	0.05	1.35
(1,69)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:VAL:N	2	1.35	0.15	1.35
(1,60)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	2	1.3	0.1	1.3
(1,10)	1:A:39:ALA:C	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	2	1.25	0.05	1.25
(1,56)	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	1:A:3:ASP:N	2	1.15	0.05	1.15

[1] Number of violated models, [2]Standard 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 (°)
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	8	7.0
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	8	5.9
(1,85)	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	1:A:95:ASN:N	12	5.7
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	23	5.4
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	25	4.7
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	1	4.4
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1	4.2
(1,31)	1:A:94:ILE:C	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	12	4.1
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	23	4.1
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	6	3.9
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	6	3.9
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	23	3.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	25	3.8
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	11	3.8

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	4	3.7
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	8	3.6
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	4	3.4
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	29	3.4
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	19	3.4
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	29	3.3
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	16	3.2
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	19	3.2
(1,70)	1:A:50:VAL:N	1:A:50:VAL:CA	1:A:50:VAL:C	1:A:51:VAL:N	23	3.2
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	8	3.2
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	10	3.1
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	12	3.1
(1,31)	1:A:94:ILE:C	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	4	3.1
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	28	3.0
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	2	3.0
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	13	3.0
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	3	3.0
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	28	3.0
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	13	3.0
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	7	2.9
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	15	2.9
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	14	2.9
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	29	2.9
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	23	2.9
(1,40)	1:A:111:TYR:C	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	14	2.9
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	29	2.8
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	18	2.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	5	2.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	28	2.8
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	27	2.8
(1,99)	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1:A:122:MET:N	17	2.7
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	12	2.7
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	20	2.7
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	9	2.7
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	19	2.7
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	13	2.7
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	9	2.6
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	17	2.6
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	22	2.6
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	4	2.6
(1,48)	1:A:127:GLU:C	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	20	2.6
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	7	2.6
(1,36)	1:A:102:VAL:C	1:A:103:ASP:N	1:A:103:ASP:CA	1:A:103:ASP:C	13	2.6
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	18	2.6
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	27	2.6
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	2	2.6
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	30	2.6
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	3	2.5
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	5	2.5
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	14	2.5
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	8	2.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	19	2.4
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	28	2.4
(1,84)	1:A:93:ARG:N	1:A:93:ARG:CA	1:A:93:ARG:C	1:A:94:ILE:N	12	2.4
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	28	2.4
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	17	2.4
(1,24)	1:A:73:HIS:C	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	9	2.4
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	16	2.4
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	1	2.3
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	13	2.3
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	17	2.3
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	3	2.3
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	26	2.3
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	16	2.3
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	12	2.3
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	9	2.3
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	17	2.3
(1,99)	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1:A:122:MET:N	3	2.2
(1,99)	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1:A:122:MET:N	11	2.2
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	11	2.2
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	18	2.2
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	28	2.2
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	12	2.2
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	18	2.2
(1,79)	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	1:A:75:GLU:N	7	2.2
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	6	2.2
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	3	2.2
(1,4)	1:A:8:PRO:C	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	4	2.2
(1,4)	1:A:8:PRO:C	1:A:9:GLU:N	1:A:9:GLU:CA	1:A:9:GLU:C	26	2.2
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1	2.2
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	2	2.2
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	23	2.2
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	12	2.1
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	24	2.1
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	25	2.1
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	13	2.1
(1,57)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:PRO:N	8	2.1
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	13	2.1
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	2	2.1
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	5	2.1
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	19	2.1
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	6	2.0
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	8	2.0
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	13	2.0
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	18	2.0
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	10	2.0
(1,71)	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	1:A:52:LYS:N	19	2.0
(1,58)	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1:A:9:GLU:N	10	2.0
(1,57)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:PRO:N	15	2.0
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	2	2.0
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	1	2.0
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	6	2.0

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1	2.0
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	13	1.9
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	16	1.9
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	15	1.9
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	2	1.9
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	19	1.9
(1,79)	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	1:A:75:GLU:N	2	1.9
(1,65)	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	1:A:41:ASN:N	8	1.9
(1,45)	1:A:122:MET:C	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	28	1.9
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	2	1.9
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	3	1.9
(1,31)	1:A:94:ILE:C	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	17	1.9
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	12	1.9
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	15	1.9
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	6	1.9
(1,11)	1:A:40:GLU:C	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	2	1.9
(1,107)	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	1:A:136:VAL:N	2	1.9
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	3	1.9
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	18	1.8
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	26	1.8
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	27	1.8
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	1	1.8
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	4	1.8
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	20	1.8
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	6	1.8
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	12	1.8
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	22	1.8
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	26	1.8
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	26	1.8
(1,71)	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	1:A:52:LYS:N	18	1.8
(1,67)	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	1:A:47:ALA:N	10	1.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	3	1.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	12	1.8
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	18	1.8
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	8	1.8
(1,31)	1:A:94:ILE:C	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	14	1.8
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	17	1.8
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	29	1.8
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	27	1.8
(1,21)	1:A:62:LEU:C	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	6	1.8
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	7	1.8
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	19	1.8
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	22	1.8
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	1	1.8
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	12	1.7
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	16	1.7
(1,84)	1:A:93:ARG:N	1:A:93:ARG:CA	1:A:93:ARG:C	1:A:94:ILE:N	16	1.7
(1,84)	1:A:93:ARG:N	1:A:93:ARG:CA	1:A:93:ARG:C	1:A:94:ILE:N	19	1.7
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	23	1.7
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	28	1.7
(1,79)	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	1:A:75:GLU:N	20	1.7

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	19	1.7
(1,57)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:PRO:N	13	1.7
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	6	1.7
(1,45)	1:A:122:MET:C	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	19	1.7
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1	1.7
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	23	1.7
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	3	1.7
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	5	1.7
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	18	1.7
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	22	1.7
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	30	1.7
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	10	1.7
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	19	1.7
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	30	1.7
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	21	1.7
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	16	1.7
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	29	1.7
(1,103)	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	1:A:129:GLN:N	15	1.7
(1,102)	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	1:A:128:ILE:N	4	1.7
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	3	1.7
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	29	1.6
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	2	1.6
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	18	1.6
(1,9)	1:A:38:GLY:C	1:A:39:ALA:N	1:A:39:ALA:CA	1:A:39:ALA:C	4	1.6
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	6	1.6
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	10	1.6
(1,8)	1:A:32:THR:C	1:A:33:ALA:N	1:A:33:ALA:CA	1:A:33:ALA:C	21	1.6
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	11	1.6
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	14	1.6
(1,61)	1:A:21:ASP:N	1:A:21:ASP:CA	1:A:21:ASP:C	1:A:22:LEU:N	22	1.6
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	4	1.6
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	21	1.6
(1,45)	1:A:122:MET:C	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1	1.6
(1,33)	1:A:99:PHE:C	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	12	1.6
(1,32)	1:A:98:GLU:C	1:A:99:PHE:N	1:A:99:PHE:CA	1:A:99:PHE:C	18	1.6
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	9	1.6
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	25	1.6
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	28	1.6
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	15	1.6
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	24	1.6
(1,22)	1:A:66:PRO:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	3	1.6
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	10	1.6
(1,13)	1:A:47:ALA:C	1:A:48:LEU:N	1:A:48:LEU:CA	1:A:48:LEU:C	1	1.6
(1,109)	1:A:137:PHE:N	1:A:137:PHE:CA	1:A:137:PHE:C	1:A:138:LEU:N	10	1.6
(1,107)	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	1:A:136:VAL:N	23	1.6
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	1	1.6
(1,100)	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	1:A:124:THR:N	19	1.6
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	24	1.5
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	20	1.5
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	2	1.5
(1,93)	1:A:110:THR:N	1:A:110:THR:CA	1:A:110:THR:C	1:A:111:TYR:N	12	1.5

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,91)	1:A:103:ASP:N	1:A:103:ASP:CA	1:A:103:ASP:C	1:A:104:VAL:N	13	1.5
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	3	1.5
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	7	1.5
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	7	1.5
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	16	1.5
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	22	1.5
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	30	1.5
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	1	1.5
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	23	1.5
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	29	1.5
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	9	1.5
(1,69)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:VAL:N	30	1.5
(1,53)	1:A:135:LEU:C	1:A:136:VAL:N	1:A:136:VAL:CA	1:A:136:VAL:C	13	1.5
(1,53)	1:A:135:LEU:C	1:A:136:VAL:N	1:A:136:VAL:CA	1:A:136:VAL:C	17	1.5
(1,52)	1:A:134:ARG:C	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	8	1.5
(1,52)	1:A:134:ARG:C	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	29	1.5
(1,47)	1:A:126:ASP:C	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	14	1.5
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	18	1.5
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	11	1.5
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	15	1.5
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	20	1.5
(1,13)	1:A:47:ALA:C	1:A:48:LEU:N	1:A:48:LEU:CA	1:A:48:LEU:C	24	1.5
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	24	1.5
(1,103)	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	1:A:129:GLN:N	18	1.5
(1,103)	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	1:A:129:GLN:N	21	1.5
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	11	1.4
(1,83)	1:A:92:PHE:N	1:A:92:PHE:CA	1:A:92:PHE:C	1:A:93:ARG:N	8	1.4
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	5	1.4
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	15	1.4
(1,81)	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	1:A:86:SER:N	9	1.4
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	15	1.4
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	24	1.4
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	27	1.4
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	10	1.4
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	26	1.4
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	19	1.4
(1,73)	1:A:60:ARG:N	1:A:60:ARG:CA	1:A:60:ARG:C	1:A:61:PHE:N	21	1.4
(1,72)	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	1:A:56:ASN:N	25	1.4
(1,70)	1:A:50:VAL:N	1:A:50:VAL:CA	1:A:50:VAL:C	1:A:51:VAL:N	25	1.4
(1,66)	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	1:A:42:LEU:N	24	1.4
(1,64)	1:A:39:ALA:N	1:A:39:ALA:CA	1:A:39:ALA:C	1:A:40:GLU:N	14	1.4
(1,60)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	15	1.4
(1,57)	1:A:7:THR:N	1:A:7:THR:CA	1:A:7:THR:C	1:A:8:PRO:N	1	1.4
(1,53)	1:A:135:LEU:C	1:A:136:VAL:N	1:A:136:VAL:CA	1:A:136:VAL:C	25	1.4
(1,47)	1:A:126:ASP:C	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	27	1.4
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	16	1.4
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	8	1.4
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	25	1.4
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	21	1.4
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1	1.4
(1,32)	1:A:98:GLU:C	1:A:99:PHE:N	1:A:99:PHE:CA	1:A:99:PHE:C	11	1.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	23	1.4
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	2	1.4
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	12	1.4
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	28	1.4
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	7	1.4
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	12	1.4
(1,104)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:ILE:N	10	1.4
(1,104)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:ILE:N	28	1.4
(1,1)	1:A:1:MET:C	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	18	1.4
(1,1)	1:A:1:MET:C	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	21	1.4
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	21	1.3
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	27	1.3
(1,95)	1:A:112:VAL:N	1:A:112:VAL:CA	1:A:112:VAL:C	1:A:113:ASN:N	16	1.3
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	3	1.3
(1,90)	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1:A:103:ASP:N	6	1.3
(1,90)	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1:A:103:ASP:N	11	1.3
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	8	1.3
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	21	1.3
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	12	1.3
(1,77)	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	1:A:68:THR:N	6	1.3
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	4	1.3
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	26	1.3
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	30	1.3
(1,74)	1:A:61:PHE:N	1:A:61:PHE:CA	1:A:61:PHE:C	1:A:62:LEU:N	12	1.3
(1,71)	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	1:A:52:LYS:N	26	1.3
(1,66)	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	1:A:42:LEU:N	13	1.3
(1,55)	1:A:141:PRO:C	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	15	1.3
(1,52)	1:A:134:ARG:C	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	1	1.3
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	13	1.3
(1,36)	1:A:102:VAL:C	1:A:103:ASP:N	1:A:103:ASP:CA	1:A:103:ASP:C	10	1.3
(1,35)	1:A:101:VAL:C	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	22	1.3
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	14	1.3
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	20	1.3
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	11	1.3
(1,24)	1:A:73:HIS:C	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	16	1.3
(1,22)	1:A:66:PRO:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	9	1.3
(1,22)	1:A:66:PRO:C	1:A:67:THR:N	1:A:67:THR:CA	1:A:67:THR:C	19	1.3
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	4	1.3
(1,17)	1:A:54:GLY:C	1:A:55:PRO:N	1:A:55:PRO:CA	1:A:55:PRO:C	20	1.3
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	9	1.3
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	29	1.3
(1,11)	1:A:40:GLU:C	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	30	1.3
(1,106)	1:A:134:ARG:N	1:A:134:ARG:CA	1:A:134:ARG:C	1:A:135:LEU:N	22	1.3
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	24	1.3
(1,103)	1:A:128:ILE:N	1:A:128:ILE:CA	1:A:128:ILE:C	1:A:129:GLN:N	2	1.3
(1,102)	1:A:127:GLU:N	1:A:127:GLU:CA	1:A:127:GLU:C	1:A:128:ILE:N	14	1.3
(1,101)	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	1:A:125:GLY:N	4	1.3
(1,10)	1:A:39:ALA:C	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	28	1.3
(1,1)	1:A:1:MET:C	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	30	1.3
(1,99)	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	1:A:122:MET:N	20	1.2
(1,94)	1:A:111:TYR:N	1:A:111:TYR:CA	1:A:111:TYR:C	1:A:112:VAL:N	21	1.2

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,90)	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1:A:103:ASP:N	1	1.2
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	15	1.2
(1,88)	1:A:100:GLU:N	1:A:100:GLU:CA	1:A:100:GLU:C	1:A:101:VAL:N	24	1.2
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	5	1.2
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	30	1.2
(1,84)	1:A:93:ARG:N	1:A:93:ARG:CA	1:A:93:ARG:C	1:A:94:ILE:N	11	1.2
(1,83)	1:A:92:PHE:N	1:A:92:PHE:CA	1:A:92:PHE:C	1:A:93:ARG:N	3	1.2
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	6	1.2
(1,82)	1:A:91:GLU:N	1:A:91:GLU:CA	1:A:91:GLU:C	1:A:92:PHE:N	20	1.2
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	13	1.2
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	23	1.2
(1,78)	1:A:68:THR:N	1:A:68:THR:CA	1:A:68:THR:C	1:A:69:THR:N	1	1.2
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	10	1.2
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	14	1.2
(1,69)	1:A:49:LEU:N	1:A:49:LEU:CA	1:A:49:LEU:C	1:A:50:VAL:N	13	1.2
(1,60)	1:A:13:GLU:N	1:A:13:GLU:CA	1:A:13:GLU:C	1:A:14:THR:N	26	1.2
(1,58)	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1:A:9:GLU:N	14	1.2
(1,56)	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	1:A:3:ASP:N	18	1.2
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	7	1.2
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	20	1.2
(1,46)	1:A:123:GLN:C	1:A:124:THR:N	1:A:124:THR:CA	1:A:124:THR:C	24	1.2
(1,45)	1:A:122:MET:C	1:A:123:GLN:N	1:A:123:GLN:CA	1:A:123:GLN:C	25	1.2
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	16	1.2
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	10	1.2
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	13	1.2
(1,26)	1:A:84:THR:C	1:A:85:VAL:N	1:A:85:VAL:CA	1:A:85:VAL:C	9	1.2
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	15	1.2
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	24	1.2
(1,13)	1:A:47:ALA:C	1:A:48:LEU:N	1:A:48:LEU:CA	1:A:48:LEU:C	5	1.2
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	18	1.2
(1,12)	1:A:45:GLY:C	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	21	1.2
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	4	1.2
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	25	1.2
(1,11)	1:A:40:GLU:C	1:A:41:ASN:N	1:A:41:ASN:CA	1:A:41:ASN:C	17	1.2
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	16	1.2
(1,104)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:ILE:N	13	1.2
(1,10)	1:A:39:ALA:C	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	6	1.2
(1,1)	1:A:1:MET:C	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	12	1.2
(1,98)	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	1:A:121:VAL:N	30	1.1
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	9	1.1
(1,97)	1:A:119:ALA:N	1:A:119:ALA:CA	1:A:119:ALA:C	1:A:120:GLN:N	30	1.1
(1,92)	1:A:107:LEU:N	1:A:107:LEU:CA	1:A:107:LEU:C	1:A:108:ASN:N	26	1.1
(1,90)	1:A:102:VAL:N	1:A:102:VAL:CA	1:A:102:VAL:C	1:A:103:ASP:N	22	1.1
(1,89)	1:A:101:VAL:N	1:A:101:VAL:CA	1:A:101:VAL:C	1:A:102:VAL:N	8	1.1
(1,87)	1:A:99:PHE:N	1:A:99:PHE:CA	1:A:99:PHE:C	1:A:100:GLU:N	4	1.1
(1,86)	1:A:95:ASN:N	1:A:95:ASN:CA	1:A:95:ASN:C	1:A:96:GLU:N	23	1.1
(1,85)	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	1:A:95:ASN:N	8	1.1
(1,83)	1:A:92:PHE:N	1:A:92:PHE:CA	1:A:92:PHE:C	1:A:93:ARG:N	5	1.1
(1,83)	1:A:92:PHE:N	1:A:92:PHE:CA	1:A:92:PHE:C	1:A:93:ARG:N	29	1.1
(1,80)	1:A:79:PHE:N	1:A:79:PHE:CA	1:A:79:PHE:C	1:A:80:LEU:N	21	1.1
(1,76)	1:A:63:LEU:N	1:A:63:LEU:CA	1:A:63:LEU:C	1:A:64:ASP:N	2	1.1

Continued on next page...

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,75)	1:A:62:LEU:N	1:A:62:LEU:CA	1:A:62:LEU:C	1:A:63:LEU:N	8	1.1
(1,71)	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	1:A:52:LYS:N	21	1.1
(1,67)	1:A:46:SER:N	1:A:46:SER:CA	1:A:46:SER:C	1:A:47:ALA:N	3	1.1
(1,65)	1:A:40:GLU:N	1:A:40:GLU:CA	1:A:40:GLU:C	1:A:41:ASN:N	23	1.1
(1,58)	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1:A:9:GLU:N	1	1.1
(1,58)	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	1:A:9:GLU:N	16	1.1
(1,56)	1:A:2:SER:N	1:A:2:SER:CA	1:A:2:SER:C	1:A:3:ASP:N	21	1.1
(1,50)	1:A:129:GLN:C	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	8	1.1
(1,44)	1:A:120:GLN:C	1:A:121:VAL:N	1:A:121:VAL:CA	1:A:121:VAL:C	6	1.1
(1,43)	1:A:119:ALA:C	1:A:120:GLN:N	1:A:120:GLN:CA	1:A:120:GLN:C	26	1.1
(1,36)	1:A:102:VAL:C	1:A:103:ASP:N	1:A:103:ASP:CA	1:A:103:ASP:C	15	1.1
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	7	1.1
(1,30)	1:A:93:ARG:C	1:A:94:ILE:N	1:A:94:ILE:CA	1:A:94:ILE:C	21	1.1
(1,3)	1:A:7:THR:C	1:A:8:PRO:N	1:A:8:PRO:CA	1:A:8:PRO:C	13	1.1
(1,24)	1:A:73:HIS:C	1:A:74:PRO:N	1:A:74:PRO:CA	1:A:74:PRO:C	4	1.1
(1,16)	1:A:50:VAL:C	1:A:51:VAL:N	1:A:51:VAL:CA	1:A:51:VAL:C	13	1.1
(1,110)	1:A:142:ALA:N	1:A:142:ALA:CA	1:A:142:ALA:C	1:A:143:GLU:N	27	1.1
(1,107)	1:A:135:LEU:N	1:A:135:LEU:CA	1:A:135:LEU:C	1:A:136:VAL:N	26	1.1
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	13	1.1
(1,105)	1:A:130:ILE:N	1:A:130:ILE:CA	1:A:130:ILE:C	1:A:131:GLY:N	25	1.1
(1,104)	1:A:129:GLN:N	1:A:129:GLN:CA	1:A:129:GLN:C	1:A:130:ILE:N	14	1.1