



wwPDB NMR Structure Validation Summary Report ⓘ

Aug 10, 2026 – 10:26 AM EDT

PDB ID : 9Q2X / pdb_00009q2x
BMRB ID : 52073
Title : Solution Structure of G12D mutant GppNHp-bound T35S KRAS4b
Authors : Sharma, A.K.; Maciag, A.E.
Deposited on : 2025-08-15

This is a wwPDB NMR Structure Validation Summary 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
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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 : v1.2.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

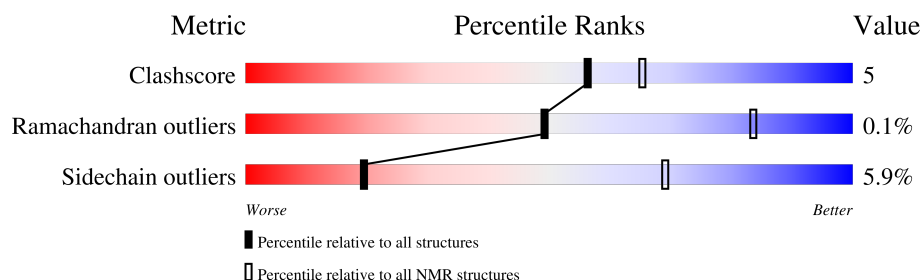
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 58%.

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	170	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 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 & target function*.

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:1-A:57, A:68-A:166 (156)	0.64	11

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

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

The models can be grouped into 3 clusters and 1 single-model cluster was found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2735 atoms, of which 1348 are hydrogens and 0 are deuteriums.

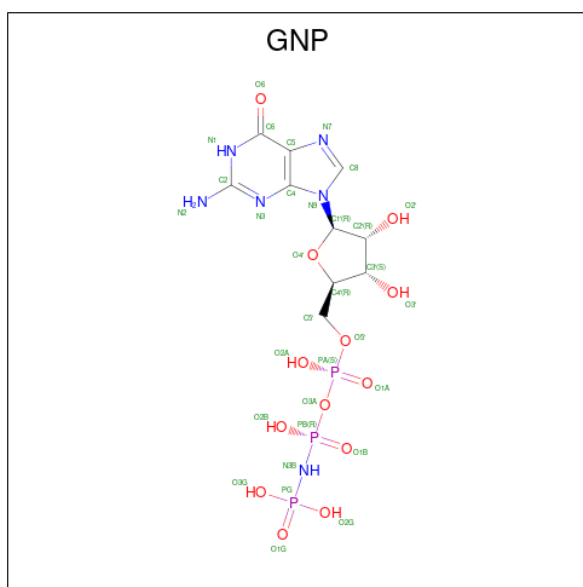
- Molecule 1 is a protein called Isoform 2B of GTPase KRas.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	169	2689	846	1335	232	270	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P01116
A	12	ASP	GLY	engineered mutation	UNP P01116
A	35	SER	THR	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
2	A	1	45	10	13	6	13	3

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

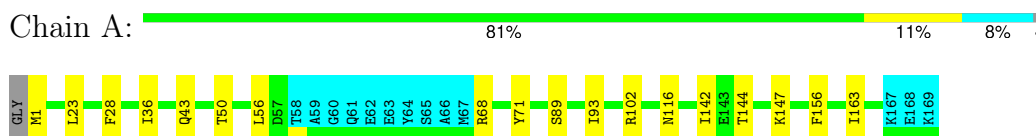
Mol	Chain	Residues	Atoms	
3	A	1	Total	Mg
			1	1

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.

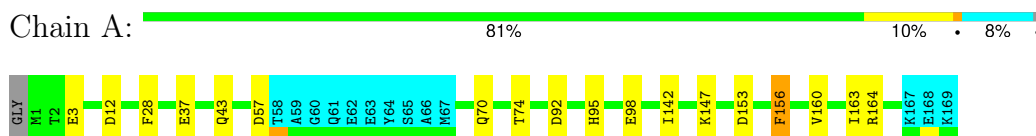
- Molecule 1: Isoform 2B of GTPase KRas



4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 11. Colouring as in section 4.1 above.

- Molecule 1: Isoform 2B of GTPase KRas



5 Refinement protocol and experimental data overview

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

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

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

Software name	Classification	Version
CYANA	structure calculation	
CNS	refinement	1.3

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2114
Number of shifts mapped to atoms	2108
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	58%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, MG

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	1252	1240	1238	12±4
2	A	32	13	13	1±1
All	All	25700	25060	25020	248

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

5 of 99 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:116:ASN:HA	1:A:144:THR:O	0.72	1.85	17	14
1:A:160:VAL:HA	1:A:163:ILE:HD12	0.72	1.62	9	7
1:A:68:ARG:HA	1:A:71:TYR:CE2	0.68	2.24	4	11
1:A:68:ARG:HA	1:A:71:TYR:CZ	0.66	2.26	7	5
1:A:69:ASP:O	1:A:73:ARG:HB2	0.63	1.93	5	7

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	155/170 (91%)	150±2 (96±1%)	5±2 (3±1%)	0±0 (0±0%)	49	83
All	All	3100/3400 (91%)	2990 (96%)	108 (3%)	2 (0%)	49	83

All 2 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	36	ILE	1
1	A	38	ASP	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	140/150 (93%)	132±2 (94±2%)	8±2 (6±2%)	19	69
All	All	2800/3000 (93%)	2634 (94%)	166 (6%)	19	69

5 of 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	43	GLN	18
1	A	142	ILE	16
1	A	36	ILE	14
1	A	56	LEU	12
1	A	102	ARG	10

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	GNP	A	201	3	34,34,34	2.16±0.02	5±1 (13±1%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	GNP	A	201	3	47,54,54	1.94±0.01	13±1 (27±2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	A	201	3	-	0±0,18,38,38	0±0,3,3,3

5 of 6 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	GNP	PG-O1G	10.22	1.61	1.46	5	20
2	A	201	GNP	PB-O2B	3.38	1.47	1.56	17	20
2	A	201	GNP	PG-O3G	3.30	1.48	1.56	7	20
2	A	201	GNP	C5-N7	3.04	1.33	1.39	18	20
2	A	201	GNP	C8-N9	2.16	1.32	1.37	1	10

5 of 16 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

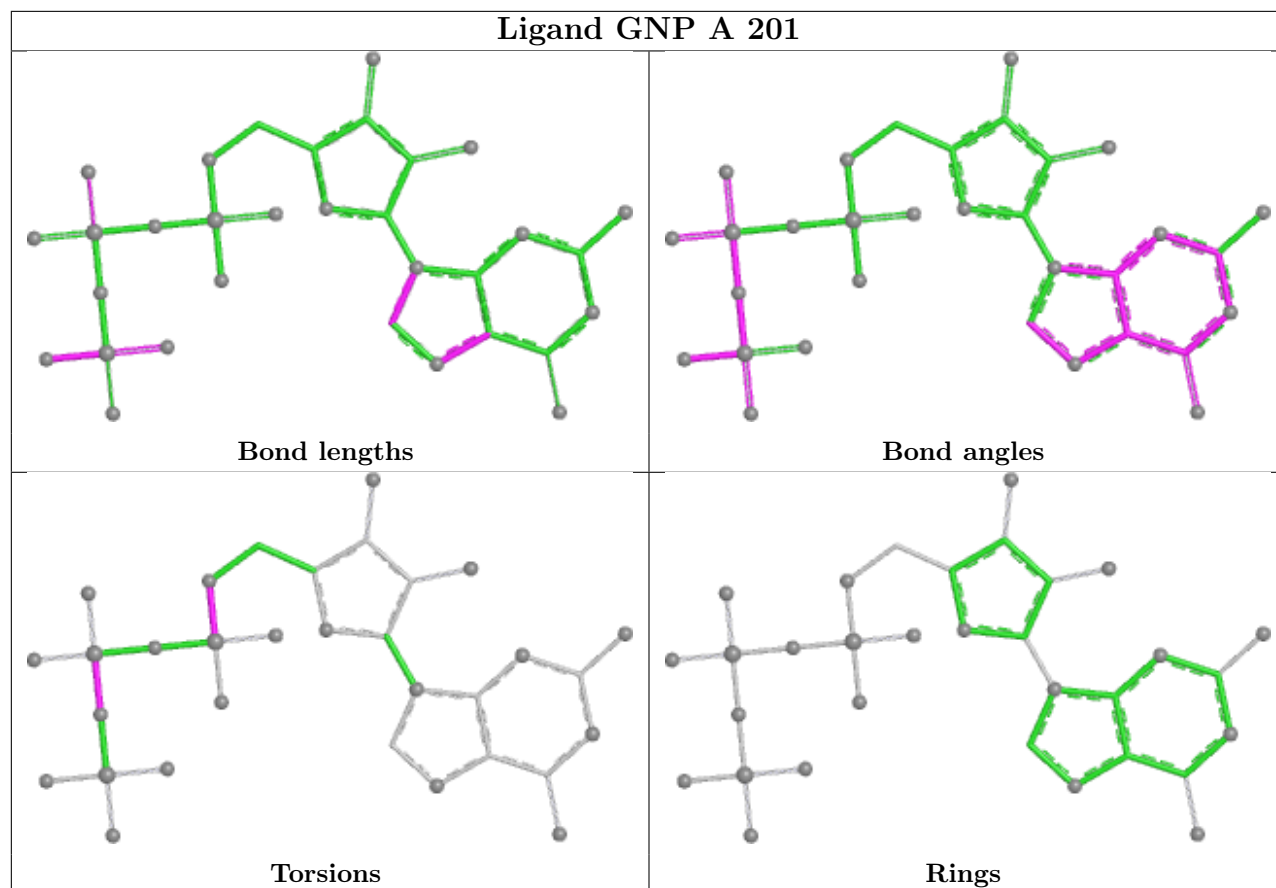
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	201	GNP	C2-N3-C4	5.41	121.61	112.30	3	20
2	A	201	GNP	C5-C4-N3	4.90	120.59	128.39	16	20
2	A	201	GNP	O2B-PB-O1B	4.31	119.11	109.87	8	20
2	A	201	GNP	O1G-PG-N3B	4.17	105.63	111.77	13	20
2	A	201	GNP	C2-N1-C6	3.42	118.91	125.11	4	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 58% for the well-defined parts and 59% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	2114
Number of shifts mapped to atoms	2108
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

- Can not parse the chemical shift value. First 5 (of 743) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	HB2	1.891	0.003	.
1	A	1	MET	HB3	1.946	0.005	.
1	A	1	MET	HG2	2.347	0.002	.
1	A	1	MET	HG3	2.389	0.005	.
1	A	3	GLU	HB2	1.861	0.000	.
1	A	3	GLU	HB3	1.777	0.000	.
1	A	3	GLU	HG2	2.012	0.011	.
1	A	3	GLU	HG3	2.187	0.000	.
1	A	4	TYR	HB2	2.646	0.000	.
1	A	4	TYR	HB3	2.646	0.000	.
1	A	4	TYR	HD1	6.889	0.001	.
1	A	4	TYR	HD2	6.889	0.001	.
1	A	4	TYR	HE1	6.634	0.003	.
1	A	4	TYR	HE2	6.634	0.003	.
1	A	4	TYR	CD1	132.967	0.012	.
1	A	4	TYR	CE1	118.118	0.014	.
1	A	5	LYS	HB2	1.784	0.011	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	5	LYS	HB3	1.913	0.013	.
1	A	5	LYS	HD2	1.606	0.007	.
1	A	5	LYS	HD3	1.606	0.000	.
1	A	5	LYS	HE2	2.889	0.002	.
1	A	5	LYS	HE3	2.889	0.000	.
1	A	5	LYS	HG2	1.408	0.000	.
1	A	5	LYS	HG3	1.464	0.000	.
1	A	6	LEU	HB2	1.886	0.013	.
1	A	6	LEU	HB3	1.178	0.000	.
1	A	6	LEU	HD11	0.667	0.001	.
1	A	6	LEU	HD12	0.667	0.001	.
1	A	6	LEU	HD13	0.667	0.001	.
1	A	6	LEU	HD21	0.948	0.002	.
1	A	6	LEU	HD22	0.948	0.002	.
1	A	6	LEU	HD23	0.948	0.002	.
1	A	6	LEU	CD1	24.391	0.028	.
1	A	6	LEU	CD2	26.578	0.063	.
1	A	7	VAL	HG11	0.714	0.000	.
1	A	7	VAL	HG12	0.714	0.000	.
1	A	7	VAL	HG13	0.714	0.000	.
1	A	7	VAL	HG21	0.992	0.000	.
1	A	7	VAL	HG22	0.992	0.000	.
1	A	7	VAL	HG23	0.992	0.000	.
1	A	7	VAL	CG1	22.010	0.000	.
1	A	7	VAL	CG2	22.260	0.000	.
1	A	8	VAL	HG11	0.944	0.001	.
1	A	8	VAL	HG12	0.944	0.001	.
1	A	8	VAL	HG13	0.944	0.001	.
1	A	8	VAL	HG21	0.934	0.000	.
1	A	8	VAL	HG22	0.934	0.000	.
1	A	8	VAL	HG23	0.934	0.000	.
1	A	8	VAL	CG1	20.516	0.029	.
1	A	8	VAL	CG2	22.350	0.000	.
1	A	9	VAL	HG11	0.856	0.014	.
1	A	9	VAL	HG12	0.856	0.014	.
1	A	9	VAL	HG13	0.856	0.014	.
1	A	9	VAL	HG21	1.001	0.000	.
1	A	9	VAL	HG22	1.001	0.000	.
1	A	9	VAL	HG23	1.001	0.000	.
1	A	9	VAL	CG1	20.925	0.080	.
1	A	9	VAL	CG2	22.277	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	10	GLY	HA2	2.941	0.006	.
1	A	10	GLY	HA3	4.641	0.014	.
1	A	12	GLY	HA2	3.706	0.004	.
1	A	12	GLY	HA3	4.798	0.000	.
1	A	13	GLY	HA2	3.915	0.010	.
1	A	13	GLY	HA3	4.201	0.000	.
1	A	14	VAL	HG11	0.961	0.000	.
1	A	14	VAL	HG12	0.961	0.000	.
1	A	14	VAL	HG13	0.961	0.000	.
1	A	14	VAL	HG21	1.164	0.000	.
1	A	14	VAL	HG22	1.164	0.000	.
1	A	14	VAL	HG23	1.164	0.000	.
1	A	14	VAL	CG1	17.725	0.000	.
1	A	14	VAL	CG2	22.108	0.000	.
1	A	15	GLY	HA2	4.608	0.011	.
1	A	15	GLY	HA3	4.301	0.004	.
1	A	16	LYS	HB2	2.457	0.000	.
1	A	16	LYS	HB3	1.662	0.000	.
1	A	17	SER	HB2	3.705	0.006	.
1	A	17	SER	HB3	3.705	0.006	.
1	A	19	LEU	HB2	1.313	0.003	.
1	A	19	LEU	HB3	2.227	0.005	.
1	A	19	LEU	HD11	0.631	0.006	.
1	A	19	LEU	HD12	0.631	0.006	.
1	A	19	LEU	HD13	0.631	0.006	.
1	A	19	LEU	HD21	0.795	0.000	.
1	A	19	LEU	HD22	0.795	0.000	.
1	A	19	LEU	HD23	0.795	0.000	.
1	A	19	LEU	CD1	26.821	0.064	.
1	A	19	LEU	CD2	24.568	0.000	.
1	A	21	ILE	HG12	1.086	0.005	.
1	A	21	ILE	HG13	1.327	0.000	.
1	A	22	GLN	HB2	2.020	0.000	.
1	A	22	GLN	HB3	2.359	0.004	.
1	A	22	GLN	HE21	6.624	0.042	.
1	A	22	GLN	HE22	7.754	0.001	.
1	A	22	GLN	HG2	2.376	0.000	.
1	A	22	GLN	HG3	2.602	0.000	.
1	A	23	LEU	HB2	0.972	0.006	.
1	A	23	LEU	HB3	1.570	0.004	.
1	A	23	LEU	HD11	-0.230	0.001	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	23	LEU	HD12	-0.230	0.001	.
1	A	23	LEU	HD13	-0.230	0.001	.
1	A	23	LEU	HD21	0.622	0.005	.
1	A	23	LEU	HD22	0.622	0.005	.
1	A	23	LEU	HD23	0.622	0.005	.
1	A	23	LEU	CD1	24.064	0.016	.
1	A	23	LEU	CD2	22.756	0.128	.
1	A	24	ILE	HG12	1.540	0.006	.
1	A	24	ILE	HG13	1.106	0.008	.
1	A	25	GLN	HB2	2.171	0.000	.
1	A	25	GLN	HB3	1.823	0.000	.
1	A	25	GLN	HE21	6.945	0.002	.
1	A	25	GLN	HE22	7.491	0.000	.
1	A	25	GLN	HG2	2.243	0.015	.
1	A	25	GLN	HG3	2.421	0.007	.
1	A	26	ASN	HB2	2.775	0.002	.
1	A	26	ASN	HB3	3.071	0.001	.
1	A	26	ASN	HD21	6.733	0.002	.
1	A	26	ASN	HD22	7.461	0.004	.
1	A	27	HIS	HB2	3.004	0.010	.
1	A	27	HIS	HB3	3.121	0.003	.
1	A	28	PHE	HB2	3.065	0.003	.
1	A	28	PHE	HB3	2.828	0.000	.
1	A	28	PHE	HD1	7.029	0.001	.
1	A	28	PHE	HD2	7.029	0.001	.
1	A	28	PHE	HE1	6.581	0.030	.
1	A	28	PHE	HE2	6.581	0.030	.
1	A	28	PHE	CD2	131.943	0.057	.
1	A	29	VAL	HG11	0.622	0.001	.
1	A	29	VAL	HG12	0.622	0.001	.
1	A	29	VAL	HG13	0.622	0.001	.
1	A	29	VAL	HG21	0.709	0.002	.
1	A	29	VAL	HG22	0.709	0.002	.
1	A	29	VAL	HG23	0.709	0.002	.
1	A	29	VAL	CG1	19.700	0.013	.
1	A	29	VAL	CG2	21.429	0.083	.
1	A	30	ASP	HB2	2.588	0.000	.
1	A	30	ASP	HB3	2.510	0.004	.
1	A	31	GLU	HB2	1.873	0.000	.
1	A	31	GLU	HB3	1.956	0.008	.
1	A	31	GLU	HG2	2.111	0.006	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	31	GLU	HG3	2.111	0.006	.
1	A	32	TYR	HB2	2.882	0.006	.
1	A	32	TYR	HB3	2.882	0.006	.
1	A	32	TYR	HD1	7.059	0.002	.
1	A	32	TYR	HD2	7.059	0.002	.
1	A	32	TYR	HE1	6.777	0.000	.
1	A	32	TYR	HE2	6.777	0.000	.
1	A	32	TYR	CD1	132.933	0.039	.
1	A	32	TYR	CE1	118.227	0.000	.
1	A	33	ASP	HB2	2.462	0.000	.
1	A	33	ASP	HB3	2.720	0.000	.
1	A	34	PRO	HB2	2.282	0.003	.
1	A	34	PRO	HB3	1.997	0.009	.
1	A	34	PRO	HD2	3.549	0.003	.
1	A	34	PRO	HD3	3.746	0.002	.
1	A	34	PRO	HG2	1.967	0.010	.
1	A	34	PRO	HG3	1.967	0.010	.
1	A	35	SER	HB2	3.855	0.006	.
1	A	35	SER	HB3	3.893	0.002	.
1	A	36	ILE	HG12	1.154	0.001	.
1	A	36	ILE	HG13	1.420	0.009	.
1	A	37	GLU	HB2	1.792	0.006	.
1	A	37	GLU	HB3	1.979	0.008	.
1	A	37	GLU	HG2	2.184	0.000	.
1	A	37	GLU	HG3	1.184	0.000	.
1	A	38	ASP	HB2	2.544	0.005	.
1	A	38	ASP	HB3	2.704	0.003	.
1	A	39	SER	HB2	3.640	0.002	.
1	A	39	SER	HB3	3.640	0.020	.
1	A	40	TYR	HB2	2.712	0.000	.
1	A	40	TYR	HB3	2.910	0.000	.
1	A	40	TYR	HD1	6.995	0.001	.
1	A	40	TYR	HD2	6.995	0.001	.
1	A	40	TYR	HE1	6.760	0.002	.
1	A	40	TYR	HE2	6.760	0.002	.
1	A	40	TYR	CD2	133.242	0.019	.
1	A	40	TYR	CE2	117.917	0.035	.
1	A	41	ARG	HB2	1.678	0.003	.
1	A	41	ARG	HB3	1.678	0.003	.
1	A	41	ARG	HD2	3.082	0.003	.
1	A	41	ARG	HD3	3.121	0.007	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	ARG	HG2	1.564	0.003	.
1	A	41	ARG	HG3	1.541	0.007	.
1	A	42	LYS	HB2	1.474	0.003	.
1	A	42	LYS	HB3	1.679	0.004	.
1	A	42	LYS	HD2	1.397	0.002	.
1	A	42	LYS	HD3	1.731	0.006	.
1	A	42	LYS	HE2	3.057	0.000	.
1	A	42	LYS	HE3	3.057	0.000	.
1	A	42	LYS	HG2	1.255	0.004	.
1	A	42	LYS	HG3	1.471	0.000	.
1	A	43	GLN	HB2	1.942	0.003	.
1	A	43	GLN	HB3	1.942	0.003	.
1	A	43	GLN	HE21	7.260	0.001	.
1	A	43	GLN	HE22	6.783	0.001	.
1	A	43	GLN	HG2	2.123	0.001	.
1	A	43	GLN	HG3	2.231	0.001	.
1	A	44	VAL	HG11	0.706	0.001	.
1	A	44	VAL	HG12	0.706	0.001	.
1	A	44	VAL	HG13	0.706	0.001	.
1	A	44	VAL	HG21	0.849	0.003	.
1	A	44	VAL	HG22	0.849	0.003	.
1	A	44	VAL	HG23	0.849	0.003	.
1	A	44	VAL	CG1	19.966	0.045	.
1	A	44	VAL	CG2	21.677	0.045	.
1	A	45	VAL	HG11	0.636	0.001	.
1	A	45	VAL	HG12	0.636	0.001	.
1	A	45	VAL	HG13	0.636	0.001	.
1	A	45	VAL	HG21	0.880	0.001	.
1	A	45	VAL	HG22	0.880	0.001	.
1	A	45	VAL	HG23	0.880	0.001	.
1	A	45	VAL	CG1	20.866	0.019	.
1	A	45	VAL	CG2	20.964	0.009	.
1	A	46	ILE	HG12	-0.322	0.002	.
1	A	46	ILE	HG13	0.910	0.000	.
1	A	47	ASP	HB2	2.784	0.004	.
1	A	47	ASP	HB3	2.884	0.004	.
1	A	48	GLY	HA2	4.140	0.005	.
1	A	48	GLY	HA3	3.452	0.007	.
1	A	49	GLU	HB2	1.816	0.000	.
1	A	49	GLU	HB3	2.049	0.000	.
1	A	49	GLU	HG2	2.269	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	49	GLU	HG3	2.098	0.000	.
1	A	51	CYS	HB2	2.840	0.005	.
1	A	51	CYS	HB3	2.903	0.010	.
1	A	52	LEU	HB2	1.461	0.004	.
1	A	52	LEU	HB3	1.554	0.002	.
1	A	52	LEU	HD11	0.782	0.000	.
1	A	52	LEU	HD12	0.782	0.000	.
1	A	52	LEU	HD13	0.782	0.000	.
1	A	52	LEU	CD1	24.588	0.000	.
1	A	53	LEU	HB2	1.930	0.000	.
1	A	53	LEU	HB3	1.172	0.003	.
1	A	53	LEU	HD11	0.774	0.001	.
1	A	53	LEU	HD12	0.774	0.001	.
1	A	53	LEU	HD13	0.774	0.001	.
1	A	53	LEU	HD21	0.783	0.000	.
1	A	53	LEU	HD22	0.783	0.000	.
1	A	53	LEU	HD23	0.783	0.000	.
1	A	53	LEU	CD1	25.418	0.057	.
1	A	53	LEU	CD2	24.190	0.000	.
1	A	54	ASP	HB2	2.438	0.000	.
1	A	54	ASP	HB3	2.789	0.000	.
1	A	55	ILE	HG12	1.034	0.000	.
1	A	55	ILE	HG13	1.314	0.000	.
1	A	56	LEU	HB2	1.369	0.000	.
1	A	56	LEU	HB3	1.369	0.000	.
1	A	56	LEU	HD11	0.526	0.001	.
1	A	56	LEU	HD12	0.526	0.001	.
1	A	56	LEU	HD13	0.526	0.001	.
1	A	56	LEU	HD21	0.604	0.001	.
1	A	56	LEU	HD22	0.604	0.001	.
1	A	56	LEU	HD23	0.604	0.001	.
1	A	56	LEU	CD1	25.009	0.017	.
1	A	56	LEU	CD2	23.924	0.033	.
1	A	57	ASP	HB2	2.889	0.000	.
1	A	57	ASP	HB3	2.553	0.000	.
1	A	60	GLY	HA2	3.825	0.004	.
1	A	60	GLY	HA3	4.326	0.012	.
1	A	61	GLN	HB2	2.088	0.000	.
1	A	61	GLN	HB3	2.229	0.008	.
1	A	61	GLN	HE21	7.631	0.002	.
1	A	61	GLN	HE22	7.062	0.001	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	61	GLN	HG2	2.428	0.001	.
1	A	61	GLN	HG3	2.428	0.001	.
1	A	62	GLU	HB2	2.081	0.002	.
1	A	62	GLU	HB3	2.008	0.000	.
1	A	62	GLU	HG2	2.321	0.000	.
1	A	62	GLU	HG3	2.321	0.000	.
1	A	63	GLU	HB2	1.889	0.003	.
1	A	63	GLU	HB3	1.889	0.003	.
1	A	63	GLU	HG2	2.098	0.000	.
1	A	63	GLU	HG3	2.125	0.000	.
1	A	64	TYR	HB2	2.940	0.006	.
1	A	64	TYR	HB3	3.087	0.002	.
1	A	64	TYR	HD1	7.085	0.001	.
1	A	64	TYR	HD2	7.085	0.001	.
1	A	64	TYR	HE1	6.784	0.000	.
1	A	64	TYR	HE2	6.784	0.000	.
1	A	64	TYR	CD1	133.008	0.057	.
1	A	64	TYR	CE1	118.257	0.000	.
1	A	65	SER	HB2	3.781	0.002	.
1	A	65	SER	HB3	3.968	0.003	.
1	A	67	MET	HB2	1.902	0.003	.
1	A	67	MET	HB3	1.979	0.005	.
1	A	67	MET	HG2	2.436	0.005	.
1	A	67	MET	HG3	2.521	0.002	.
1	A	68	ARG	HB2	1.947	0.009	.
1	A	68	ARG	HB3	1.947	0.009	.
1	A	68	ARG	HD2	3.360	0.007	.
1	A	68	ARG	HD3	3.360	0.007	.
1	A	68	ARG	HG2	1.689	0.000	.
1	A	68	ARG	HG3	1.733	0.010	.
1	A	69	ASP	HB2	2.632	0.002	.
1	A	69	ASP	HB3	2.759	0.009	.
1	A	70	GLN	HB2	2.120	0.008	.
1	A	70	GLN	HB3	2.168	0.006	.
1	A	70	GLN	HE21	6.886	0.001	.
1	A	70	GLN	HE22	7.442	0.002	.
1	A	70	GLN	HG2	2.360	0.006	.
1	A	70	GLN	HG3	2.360	0.006	.
1	A	71	TYR	HB2	2.990	0.005	.
1	A	71	TYR	HB3	3.209	0.006	.
1	A	71	TYR	HD1	7.014	0.002	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	71	TYR	HD2	7.014	0.002	.
1	A	71	TYR	HE1	6.818	0.002	.
1	A	71	TYR	HE2	6.818	0.002	.
1	A	71	TYR	CD2	132.485	0.073	.
1	A	71	TYR	CE2	118.358	0.017	.
1	A	72	MET	HB2	1.958	0.008	.
1	A	72	MET	HB3	2.365	0.008	.
1	A	72	MET	HG2	2.961	0.001	.
1	A	72	MET	HG3	2.469	0.004	.
1	A	73	ARG	HB2	1.948	0.000	.
1	A	73	ARG	HB3	1.948	0.000	.
1	A	73	ARG	HD2	3.201	0.008	.
1	A	73	ARG	HD3	3.284	0.000	.
1	A	73	ARG	HG2	1.682	0.000	.
1	A	73	ARG	HG3	1.794	0.010	.
1	A	75	GLY	HA2	3.510	0.005	.
1	A	75	GLY	HA3	3.223	0.005	.
1	A	76	GLU	HB2	2.154	0.000	.
1	A	76	GLU	HB3	2.374	0.012	.
1	A	76	GLU	HG2	2.396	0.001	.
1	A	76	GLU	HG3	2.482	0.007	.
1	A	77	GLY	HA2	4.914	0.018	.
1	A	77	GLY	HA3	3.155	0.004	.
1	A	78	PHE	HB2	2.746	0.000	.
1	A	78	PHE	HB3	2.746	0.000	.
1	A	78	PHE	HD1	7.085	0.003	.
1	A	78	PHE	HD2	7.085	0.003	.
1	A	78	PHE	HE1	7.066	0.001	.
1	A	78	PHE	HE2	7.066	0.001	.
1	A	78	PHE	CD2	132.699	0.074	.
1	A	78	PHE	CE2	130.582	0.045	.
1	A	79	LEU	HB2	1.184	0.000	.
1	A	79	LEU	HB3	1.623	0.004	.
1	A	79	LEU	HD11	0.113	0.001	.
1	A	79	LEU	HD12	0.113	0.001	.
1	A	79	LEU	HD13	0.113	0.001	.
1	A	79	LEU	HD21	0.161	0.001	.
1	A	79	LEU	HD22	0.161	0.001	.
1	A	79	LEU	HD23	0.161	0.001	.
1	A	79	LEU	CD1	25.027	0.029	.
1	A	79	LEU	CD2	25.609	0.012	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	80	CYS	HB2	2.665	0.001	.
1	A	80	CYS	HB3	2.957	0.002	.
1	A	81	VAL	HG11	0.556	0.000	.
1	A	81	VAL	HG12	0.556	0.000	.
1	A	81	VAL	HG13	0.556	0.000	.
1	A	81	VAL	HG21	0.663	0.010	.
1	A	81	VAL	HG22	0.663	0.010	.
1	A	81	VAL	HG23	0.663	0.010	.
1	A	81	VAL	CG1	22.779	0.000	.
1	A	81	VAL	CG2	22.090	0.010	.
1	A	82	PHE	HB2	2.932	0.000	.
1	A	82	PHE	HB3	3.683	0.000	.
1	A	84	ILE	HG12	1.267	0.000	.
1	A	84	ILE	HG13	1.028	0.000	.
1	A	85	ASN	HB2	3.308	0.000	.
1	A	85	ASN	HB3	2.394	0.000	.
1	A	85	ASN	HD21	6.848	0.001	.
1	A	85	ASN	HD22	7.773	0.000	.
1	A	86	ASN	HB2	2.488	0.000	.
1	A	86	ASN	HB3	3.201	0.000	.
1	A	86	ASN	HD21	7.187	0.000	.
1	A	86	ASN	HD22	8.059	0.000	.
1	A	88	LYS	HB2	1.958	0.000	.
1	A	88	LYS	HB3	2.054	0.000	.
1	A	88	LYS	HD2	1.821	0.000	.
1	A	88	LYS	HD3	1.691	0.000	.
1	A	88	LYS	HE2	3.076	0.000	.
1	A	88	LYS	HE3	3.076	0.000	.
1	A	88	LYS	HG2	1.545	0.000	.
1	A	88	LYS	HG3	1.545	0.000	.
1	A	89	SER	HB2	4.064	0.000	.
1	A	89	SER	HB3	4.495	0.000	.
1	A	90	PHE	HB2	2.720	0.000	.
1	A	90	PHE	HB3	3.263	0.000	.
1	A	90	PHE	HD1	6.000	0.001	.
1	A	90	PHE	HD2	6.000	0.001	.
1	A	90	PHE	HE1	6.779	0.000	.
1	A	90	PHE	HE2	6.779	0.000	.
1	A	90	PHE	CD1	131.544	0.020	.
1	A	90	PHE	CE1	130.381	0.000	.
1	A	91	GLU	HB2	2.120	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	91	GLU	HB3	2.248	0.000	.
1	A	91	GLU	HG2	2.546	0.000	.
1	A	91	GLU	HG3	2.325	0.000	.
1	A	92	ASP	HB2	2.899	0.000	.
1	A	92	ASP	HB3	2.899	0.000	.
1	A	93	ILE	HG12	2.231	0.000	.
1	A	93	ILE	HG13	1.392	0.000	.
1	A	94	HIS	HB2	3.132	0.003	.
1	A	94	HIS	HB3	3.255	0.007	.
1	A	95	HIS	HB2	3.034	0.004	.
1	A	95	HIS	HB3	3.034	0.004	.
1	A	96	TYR	HB2	2.882	0.000	.
1	A	96	TYR	HB3	2.882	0.000	.
1	A	96	TYR	HD1	7.078	0.000	.
1	A	96	TYR	HD2	7.078	0.000	.
1	A	96	TYR	HE1	6.887	0.001	.
1	A	96	TYR	HE2	6.887	0.001	.
1	A	96	TYR	CD1	132.479	0.000	.
1	A	96	TYR	CE1	118.581	0.018	.
1	A	97	ARG	HB2	1.381	0.000	.
1	A	97	ARG	HB3	1.774	0.000	.
1	A	97	ARG	HD2	2.024	0.000	.
1	A	97	ARG	HD3	2.231	0.000	.
1	A	97	ARG	HG2	1.095	0.000	.
1	A	97	ARG	HG3	1.145	0.000	.
1	A	98	GLU	HB2	2.012	0.000	.
1	A	98	GLU	HB3	2.012	0.000	.
1	A	98	GLU	HG2	2.246	0.000	.
1	A	98	GLU	HG3	2.205	0.000	.
1	A	99	GLN	HB2	2.005	0.000	.
1	A	99	GLN	HB3	2.005	0.000	.
1	A	99	GLN	HE21	7.223	0.001	.
1	A	99	GLN	HE22	6.673	0.000	.
1	A	99	GLN	HG2	2.168	0.000	.
1	A	99	GLN	HG3	2.278	0.000	.
1	A	100	ILE	HG12	-0.110	0.004	.
1	A	100	ILE	HG13	1.571	0.000	.
1	A	101	LYS	HB2	1.685	0.000	.
1	A	101	LYS	HB3	1.773	0.000	.
1	A	101	LYS	HD2	1.525	0.000	.
1	A	101	LYS	HD3	1.549	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	LYS	HE2	2.831	0.000	.
1	A	101	LYS	HE3	2.831	0.000	.
1	A	101	LYS	HG2	1.346	0.000	.
1	A	101	LYS	HG3	1.346	0.000	.
1	A	102	ARG	HB2	1.937	0.000	.
1	A	102	ARG	HB3	1.877	0.000	.
1	A	102	ARG	HD2	3.175	0.000	.
1	A	102	ARG	HD3	3.241	0.000	.
1	A	102	ARG	HG2	1.545	0.000	.
1	A	102	ARG	HG3	1.663	0.000	.
1	A	103	VAL	HG11	1.040	0.000	.
1	A	103	VAL	HG12	1.040	0.000	.
1	A	103	VAL	HG13	1.040	0.000	.
1	A	103	VAL	HG21	0.940	0.000	.
1	A	103	VAL	HG22	0.940	0.000	.
1	A	103	VAL	HG23	0.940	0.000	.
1	A	103	VAL	CG1	22.349	0.000	.
1	A	103	VAL	CG2	21.641	0.000	.
1	A	104	LYS	HB2	1.861	0.000	.
1	A	104	LYS	HB3	1.861	0.000	.
1	A	104	LYS	HD2	1.917	0.000	.
1	A	104	LYS	HD3	1.835	0.000	.
1	A	104	LYS	HE2	3.220	0.000	.
1	A	104	LYS	HE3	3.265	0.000	.
1	A	104	LYS	HG2	1.589	0.000	.
1	A	104	LYS	HG3	1.422	0.000	.
1	A	105	ASP	HB2	3.113	0.000	.
1	A	105	ASP	HB3	2.360	0.000	.
1	A	106	SER	HB2	3.233	0.005	.
1	A	106	SER	HB3	3.802	0.002	.
1	A	107	GLU	HB2	1.886	0.000	.
1	A	107	GLU	HB3	2.169	0.000	.
1	A	107	GLU	HG2	2.208	0.000	.
1	A	107	GLU	HG3	2.325	0.000	.
1	A	108	ASP	HB2	2.537	0.000	.
1	A	108	ASP	HB3	2.760	0.000	.
1	A	109	VAL	HG11	0.743	0.000	.
1	A	109	VAL	HG12	0.743	0.000	.
1	A	109	VAL	HG13	0.743	0.000	.
1	A	109	VAL	HG21	0.956	0.000	.
1	A	109	VAL	HG22	0.956	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	109	VAL	HG23	0.956	0.000	.
1	A	109	VAL	CG1	21.599	0.000	.
1	A	109	VAL	CG2	21.202	0.000	.
1	A	110	PRO	HB2	1.826	0.000	.
1	A	110	PRO	HB3	2.125	0.000	.
1	A	110	PRO	HD2	3.572	0.002	.
1	A	110	PRO	HD3	3.781	0.004	.
1	A	110	PRO	HG2	2.228	0.000	.
1	A	110	PRO	HG3	1.506	0.000	.
1	A	111	MET	HB2	2.099	0.003	.
1	A	111	MET	HB3	2.119	0.000	.
1	A	111	MET	HG2	2.607	0.006	.
1	A	111	MET	HG3	2.695	0.015	.
1	A	112	VAL	HG11	0.748	0.000	.
1	A	112	VAL	HG12	0.748	0.000	.
1	A	112	VAL	HG13	0.748	0.000	.
1	A	112	VAL	HG21	0.783	0.000	.
1	A	112	VAL	HG22	0.783	0.000	.
1	A	112	VAL	HG23	0.783	0.000	.
1	A	112	VAL	CG1	21.177	0.000	.
1	A	112	VAL	CG2	22.706	0.000	.
1	A	113	LEU	HB2	2.491	0.000	.
1	A	113	LEU	HB3	1.476	0.000	.
1	A	113	LEU	HD11	1.339	0.000	.
1	A	113	LEU	HD12	1.339	0.000	.
1	A	113	LEU	HD13	1.339	0.000	.
1	A	113	LEU	HD21	1.068	0.000	.
1	A	113	LEU	HD22	1.068	0.000	.
1	A	113	LEU	HD23	1.068	0.000	.
1	A	113	LEU	CD1	25.402	0.000	.
1	A	113	LEU	CD2	27.262	0.000	.
1	A	114	VAL	HG11	0.609	0.000	.
1	A	114	VAL	HG12	0.609	0.000	.
1	A	114	VAL	HG13	0.609	0.000	.
1	A	114	VAL	HG21	0.699	0.000	.
1	A	114	VAL	HG22	0.699	0.000	.
1	A	114	VAL	HG23	0.699	0.000	.
1	A	114	VAL	CG1	23.073	0.000	.
1	A	114	VAL	CG2	23.404	0.000	.
1	A	115	GLY	HA2	2.414	0.003	.
1	A	115	GLY	HA3	2.899	0.001	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	116	ASN	HB2	2.182	0.000	.
1	A	116	ASN	HB3	2.543	0.000	.
1	A	116	ASN	HD21	8.842	0.002	.
1	A	116	ASN	HD22	7.454	0.001	.
1	A	117	LYS	HB2	1.647	0.000	.
1	A	117	LYS	HB3	2.395	0.000	.
1	A	118	SER	HB2	3.653	0.000	.
1	A	118	SER	HB3	3.881	0.000	.
1	A	119	ASP	HB2	2.592	0.000	.
1	A	119	ASP	HB3	2.592	0.000	.
1	A	120	LEU	HB2	1.948	0.000	.
1	A	120	LEU	HB3	1.431	0.000	.
1	A	120	LEU	HD11	0.892	0.000	.
1	A	120	LEU	HD12	0.892	0.000	.
1	A	120	LEU	HD13	0.892	0.000	.
1	A	120	LEU	HD21	0.923	0.000	.
1	A	120	LEU	HD22	0.923	0.000	.
1	A	120	LEU	HD23	0.923	0.000	.
1	A	120	LEU	CD1	27.211	0.000	.
1	A	120	LEU	CD2	22.390	0.000	.
1	A	121	PRO	HB2	2.115	0.000	.
1	A	121	PRO	HB3	2.264	0.000	.
1	A	121	PRO	HD2	3.833	0.002	.
1	A	121	PRO	HD3	3.894	0.010	.
1	A	121	PRO	HG2	2.129	0.000	.
1	A	121	PRO	HG3	1.985	0.000	.
1	A	122	SER	HB2	3.806	0.000	.
1	A	122	SER	HB3	3.988	0.000	.
1	A	123	ARG	HB2	1.659	0.000	.
1	A	123	ARG	HB3	1.890	0.000	.
1	A	123	ARG	HD2	3.120	0.000	.
1	A	123	ARG	HD3	3.468	0.000	.
1	A	123	ARG	HG2	1.468	0.000	.
1	A	123	ARG	HG3	1.435	0.000	.
1	A	125	VAL	HG11	-0.125	0.001	.
1	A	125	VAL	HG12	-0.125	0.001	.
1	A	125	VAL	HG13	-0.125	0.001	.
1	A	125	VAL	HG21	0.703	0.000	.
1	A	125	VAL	HG22	0.703	0.000	.
1	A	125	VAL	HG23	0.703	0.000	.
1	A	125	VAL	CG1	19.346	0.013	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	125	VAL	CG2	20.295	0.000	.
1	A	126	ASP	HB2	2.664	0.000	.
1	A	126	ASP	HB3	2.664	0.000	.
1	A	128	LYS	HB2	1.805	0.000	.
1	A	128	LYS	HB3	1.805	0.000	.
1	A	128	LYS	HD2	1.620	0.000	.
1	A	128	LYS	HD3	1.708	0.000	.
1	A	128	LYS	HE2	3.006	0.000	.
1	A	128	LYS	HE3	3.006	0.000	.
1	A	128	LYS	HG2	1.396	0.000	.
1	A	128	LYS	HG3	1.434	0.000	.
1	A	129	GLN	HB2	1.918	0.000	.
1	A	129	GLN	HB3	2.034	0.000	.
1	A	129	GLN	HE21	6.911	0.001	.
1	A	129	GLN	HE22	7.574	0.001	.
1	A	129	GLN	HG2	2.293	0.000	.
1	A	129	GLN	HG3	2.368	0.000	.
1	A	131	GLN	HB2	2.233	0.000	.
1	A	131	GLN	HB3	2.018	0.000	.
1	A	131	GLN	HE21	7.552	0.002	.
1	A	131	GLN	HE22	6.960	0.001	.
1	A	131	GLN	HG2	2.518	0.000	.
1	A	131	GLN	HG3	2.518	0.000	.
1	A	132	ASP	HB2	2.562	0.000	.
1	A	132	ASP	HB3	2.751	0.000	.
1	A	133	LEU	HB2	1.753	0.000	.
1	A	133	LEU	HB3	1.449	0.000	.
1	A	133	LEU	HD11	0.424	0.001	.
1	A	133	LEU	HD12	0.424	0.001	.
1	A	133	LEU	HD13	0.424	0.001	.
1	A	133	LEU	HD21	0.463	0.000	.
1	A	133	LEU	HD22	0.463	0.000	.
1	A	133	LEU	HD23	0.463	0.000	.
1	A	133	LEU	CD1	26.185	0.024	.
1	A	133	LEU	CD2	22.873	0.000	.
1	A	135	ARG	HB2	1.957	0.000	.
1	A	135	ARG	HB3	2.016	0.000	.
1	A	135	ARG	HD2	3.271	0.000	.
1	A	135	ARG	HD3	3.271	0.000	.
1	A	135	ARG	HG2	1.660	0.000	.
1	A	135	ARG	HG3	1.803	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	136	SER	HB2	3.925	0.000	.
1	A	136	SER	HB3	3.925	0.000	.
1	A	137	TYR	HB2	3.076	0.000	.
1	A	137	TYR	HB3	3.269	0.000	.
1	A	137	TYR	HD1	6.801	0.000	.
1	A	137	TYR	HD2	6.801	0.000	.
1	A	137	TYR	HE1	6.593	0.002	.
1	A	137	TYR	HE2	6.593	0.002	.
1	A	137	TYR	CD1	130.255	0.000	.
1	A	137	TYR	CE1	118.153	0.019	.
1	A	138	GLY	HA2	4.175	0.013	.
1	A	138	GLY	HA3	4.014	0.004	.
1	A	139	ILE	HG12	1.413	0.000	.
1	A	139	ILE	HG13	1.691	0.000	.
1	A	140	PRO	HB2	2.533	0.000	.
1	A	140	PRO	HB3	1.669	0.000	.
1	A	140	PRO	HD2	3.974	0.003	.
1	A	140	PRO	HD3	4.068	0.004	.
1	A	140	PRO	HG2	1.957	0.000	.
1	A	140	PRO	HG3	1.783	0.000	.
1	A	141	PHE	HB2	2.788	0.000	.
1	A	141	PHE	HB3	3.099	0.000	.
1	A	141	PHE	HD1	7.168	0.001	.
1	A	141	PHE	HD2	7.168	0.001	.
1	A	141	PHE	HE1	7.287	0.003	.
1	A	141	PHE	HE2	7.287	0.003	.
1	A	141	PHE	CD1	131.842	0.021	.
1	A	141	PHE	CE1	131.193	0.075	.
1	A	142	ILE	HG12	1.024	0.000	.
1	A	142	ILE	HG13	1.253	0.000	.
1	A	143	GLU	HB2	1.744	0.000	.
1	A	143	GLU	HB3	1.873	0.000	.
1	A	143	GLU	HG2	2.123	0.000	.
1	A	143	GLU	HG3	2.280	0.000	.
1	A	145	SER	HB2	3.995	0.000	.
1	A	145	SER	HB3	3.995	0.000	.
1	A	147	LYS	HB2	0.391	0.007	.
1	A	147	LYS	HB3	1.071	0.011	.
1	A	147	LYS	HD2	1.210	0.000	.
1	A	147	LYS	HD3	1.338	0.000	.
1	A	147	LYS	HE2	2.733	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	147	LYS	HE3	2.785	0.000	.
1	A	147	LYS	HG2	0.434	0.000	.
1	A	147	LYS	HG3	0.676	0.000	.
1	A	149	ARG	HB2	1.671	0.000	.
1	A	149	ARG	HB3	2.218	0.000	.
1	A	149	ARG	HD2	3.118	0.000	.
1	A	149	ARG	HD3	3.118	0.000	.
1	A	149	ARG	HG2	1.166	0.005	.
1	A	149	ARG	HG3	1.935	0.000	.
1	A	150	GLN	HB2	1.929	0.000	.
1	A	150	GLN	HB3	1.752	0.000	.
1	A	150	GLN	HE21	7.342	0.002	.
1	A	150	GLN	HE22	6.927	0.001	.
1	A	150	GLN	HG2	2.192	0.000	.
1	A	150	GLN	HG3	2.306	0.000	.
1	A	151	GLY	HA2	3.804	0.009	.
1	A	151	GLY	HA3	4.058	0.007	.
1	A	152	VAL	HG11	0.929	0.000	.
1	A	152	VAL	HG12	0.929	0.000	.
1	A	152	VAL	HG13	0.929	0.000	.
1	A	152	VAL	HG21	0.766	0.000	.
1	A	152	VAL	HG22	0.766	0.000	.
1	A	152	VAL	HG23	0.766	0.000	.
1	A	152	VAL	CG1	20.933	0.000	.
1	A	152	VAL	CG2	24.145	0.000	.
1	A	153	ASP	HB2	1.846	0.000	.
1	A	153	ASP	HB3	2.204	0.000	.
1	A	154	ASP	HB2	2.428	0.000	.
1	A	154	ASP	HB3	2.481	0.000	.
1	A	156	PHE	HB2	2.652	0.000	.
1	A	156	PHE	HB3	2.845	0.000	.
1	A	156	PHE	HD1	7.377	0.003	.
1	A	156	PHE	HD2	7.377	0.003	.
1	A	156	PHE	HE1	6.931	0.000	.
1	A	156	PHE	HE2	6.931	0.000	.
1	A	156	PHE	CD2	132.363	0.048	.
1	A	156	PHE	CE2	131.174	0.000	.
1	A	157	TYR	HB2	2.931	0.000	.
1	A	157	TYR	HB3	3.286	0.000	.
1	A	157	TYR	HD1	6.910	0.000	.
1	A	157	TYR	HD2	6.910	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	TYR	HE1	6.676	0.001	.
1	A	157	TYR	HE2	6.676	0.001	.
1	A	157	TYR	CD1	131.155	0.000	.
1	A	157	TYR	CE1	117.546	0.036	.
1	A	159	LEU	HB2	1.241	0.000	.
1	A	159	LEU	HB3	2.131	0.000	.
1	A	159	LEU	HD11	0.691	0.000	.
1	A	159	LEU	HD12	0.691	0.000	.
1	A	159	LEU	HD13	0.691	0.000	.
1	A	159	LEU	HD21	0.826	0.000	.
1	A	159	LEU	HD22	0.826	0.000	.
1	A	159	LEU	HD23	0.826	0.000	.
1	A	159	LEU	CD1	27.425	0.000	.
1	A	159	LEU	CD2	21.665	0.000	.
1	A	160	VAL	HG11	0.078	0.001	.
1	A	160	VAL	HG12	0.078	0.001	.
1	A	160	VAL	HG13	0.078	0.001	.
1	A	160	VAL	HG21	0.704	0.000	.
1	A	160	VAL	HG22	0.704	0.000	.
1	A	160	VAL	HG23	0.704	0.000	.
1	A	160	VAL	CG1	19.849	0.006	.
1	A	160	VAL	CG2	23.950	0.000	.
1	A	161	ARG	HB2	1.869	0.000	.
1	A	161	ARG	HB3	2.069	0.000	.
1	A	161	ARG	HD2	3.142	0.000	.
1	A	161	ARG	HD3	3.142	0.000	.
1	A	161	ARG	HG2	1.551	0.000	.
1	A	161	ARG	HG3	1.793	0.000	.
1	A	162	GLU	HB2	2.428	0.000	.
1	A	162	GLU	HB3	2.242	0.000	.
1	A	162	GLU	HG2	2.160	0.000	.
1	A	162	GLU	HG3	2.506	0.000	.
1	A	163	ILE	HG12	0.851	0.000	.
1	A	163	ILE	HG13	1.825	0.000	.
1	A	164	ARG	HB2	1.991	0.000	.
1	A	164	ARG	HB3	1.936	0.000	.
1	A	164	ARG	HD2	3.116	0.000	.
1	A	164	ARG	HD3	3.051	0.000	.
1	A	164	ARG	HG2	1.845	0.000	.
1	A	164	ARG	HG3	1.845	0.000	.
1	A	165	LYS	HB2	1.897	0.000	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	165	LYS	HB3	1.931	0.000	.
1	A	165	LYS	HD2	1.708	0.000	.
1	A	165	LYS	HD3	1.708	0.000	.
1	A	165	LYS	HE2	2.923	0.000	.
1	A	165	LYS	HE3	2.923	0.000	.
1	A	165	LYS	HG2	1.590	0.000	.
1	A	165	LYS	HG3	1.590	0.000	.
1	A	166	HIS	HB2	3.617	0.005	.
1	A	166	HIS	HB3	3.313	0.007	.
1	A	167	LYS	HB2	1.956	0.000	.
1	A	167	LYS	HB3	2.002	0.000	.
1	A	167	LYS	HD2	1.782	0.000	.
1	A	167	LYS	HD3	1.749	0.000	.
1	A	167	LYS	HE2	2.999	0.000	.
1	A	167	LYS	HE3	2.999	0.000	.
1	A	167	LYS	HG2	1.736	0.000	.
1	A	167	LYS	HG3	1.568	0.000	.
1	A	168	GLU	HB2	2.020	0.000	.
1	A	168	GLU	HB3	2.154	0.000	.
1	A	168	GLU	HG2	2.436	0.000	.
1	A	168	GLU	HG3	2.333	0.000	.
1	A	169	LYS	HB2	1.762	0.000	.
1	A	169	LYS	HB3	1.846	0.000	.
1	A	169	LYS	HD2	1.446	0.000	.
1	A	169	LYS	HD3	1.691	0.000	.
1	A	169	LYS	HE2	3.004	0.000	.
1	A	169	LYS	HE3	3.004	0.000	.
1	A	169	LYS	HG2	1.445	0.000	.
1	A	169	LYS	HG3	1.445	0.000	.

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

- No matching atom found in the structure. First 5 (of 6) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	GLY	H	8.674	0.005	1
1	A	12	GLY	HA2	3.706	0.004	.
1	A	12	GLY	HA3	4.798	0.000	.
1	A	12	GLY	C	176.836	0.045	1
1	A	12	GLY	CA	46.522	0.046	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	12	GLY	N	106.217	0.036	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	169	-0.30 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	158	0.32 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	169	0.10 ± 0.07	None needed (< 0.5 ppm)
^{15}N	165	0.03 ± 0.23	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 58%, i.e. 1264 atoms were assigned a chemical shift out of a possible 2162. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	758/781 (97%)	297/317 (94%)	310/312 (99%)	151/152 (99%)
Sidechain	481/1226 (39%)	183/791 (23%)	276/383 (72%)	22/52 (42%)
Aromatic	25/155 (16%)	13/74 (18%)	12/73 (16%)	0/8 (0%)
Overall	1264/2162 (58%)	493/1182 (42%)	598/768 (78%)	173/212 (82%)

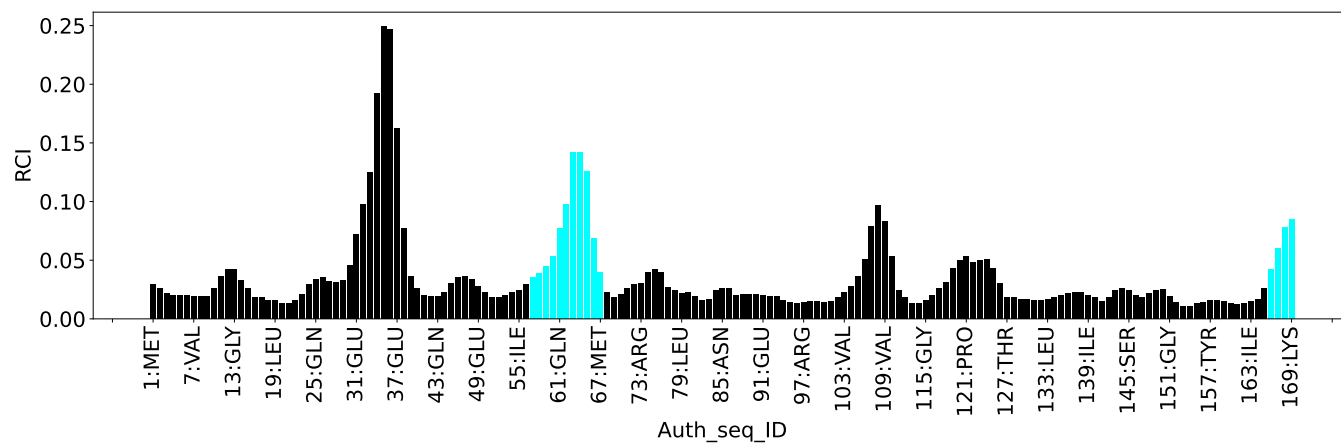
7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

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

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	3341
Intra-residue ($ i-j =0$)	795
Sequential ($ i-j =1$)	859
Medium range ($ i-j >1$ and $ i-j <5$)	583
Long range ($ i-j \geq 5$)	1063
Inter-chain	35
Hydrogen bond restraints	3
Disulfide bond restraints	0
Total dihedral-angle restraints	268
Number of unmapped restraints	16
Number of restraints per residue	21.0
Number of long range restraints per residue ¹	6.2

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	79.5	0.2
0.2-0.5 (Medium)	173.2	0.5
>0.5 (Large)	262.1	6.01

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)	7.2	9.68
10.0-20.0 (Medium)	0.7	17.07
>20.0 (Large)	1.9	150.82

9 Distance violation analysis ⓘ

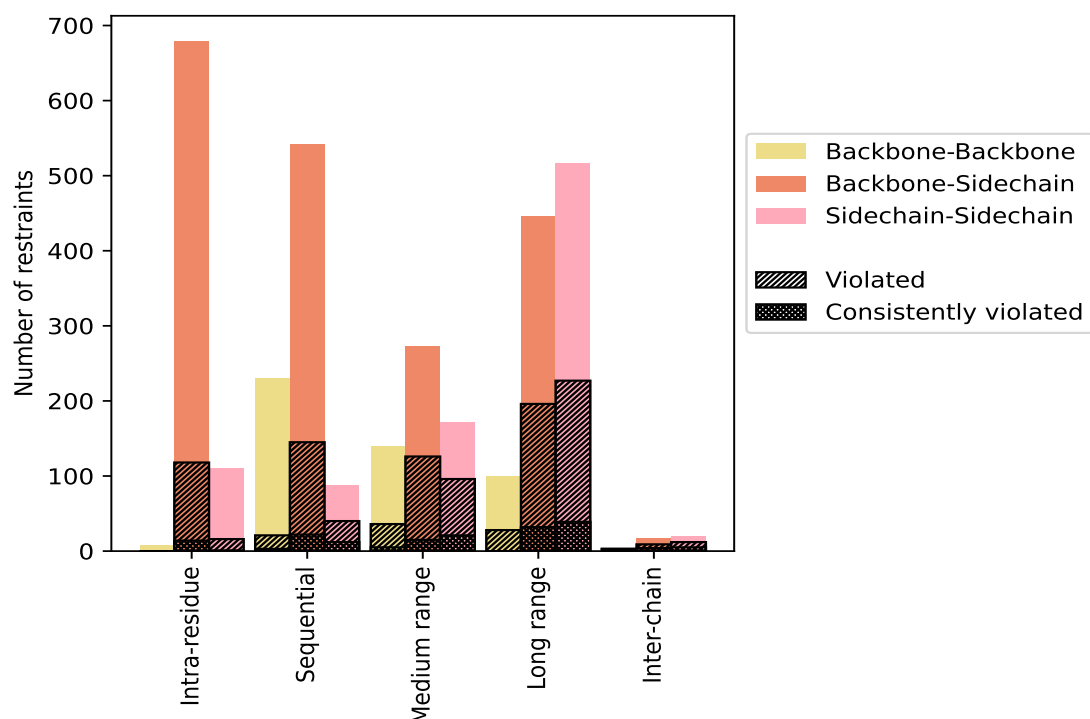
9.1 Summary of distance violations ⓘ

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 ($i-j =0$)	795	23.8	134	16.9	4.0	15	1.9	0.4
Backbone-Backbone	7	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	679	20.3	118	17.4	3.5	14	2.1	0.4
Sidechain-Sidechain	109	3.3	16	14.7	0.5	1	0.9	0.0
Sequential ($i-j =1$)	859	25.7	206	24.0	6.2	37	4.3	1.1
Backbone-Backbone	230	6.9	21	9.1	0.6	3	1.3	0.1
Backbone-Sidechain	542	16.2	145	26.8	4.3	22	4.1	0.7
Sidechain-Sidechain	87	2.6	40	46.0	1.2	12	13.8	0.4
Medium range ($i-j >1$ & $i-j <5$)	583	17.4	258	44.3	7.7	41	7.0	1.2
Backbone-Backbone	139	4.2	36	25.9	1.1	5	3.6	0.1
Backbone-Sidechain	273	8.2	126	46.2	3.8	15	5.5	0.4
Sidechain-Sidechain	171	5.1	96	56.1	2.9	21	12.3	0.6
Long range ($i-j \geq 5$)	1063	31.8	451	42.4	13.5	71	6.7	2.1
Backbone-Backbone	100	3.0	28	28.0	0.8	0	0.0	0.0
Backbone-Sidechain	446	13.3	196	43.9	5.9	32	7.2	1.0
Sidechain-Sidechain	517	15.5	227	43.9	6.8	39	7.5	1.2
Inter-chain	35	1.0	22	62.9	0.7	12	34.3	0.4
Backbone-Backbone	4	0.1	3	75.0	0.1	3	75.0	0.1
Backbone-Sidechain	17	0.5	9	52.9	0.3	4	23.5	0.1
Sidechain-Sidechain	14	0.4	10	71.4	0.3	5	35.7	0.1
Hydrogen bond	3	0.1	1	33.3	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3341	100.0	1073	32.1	32.1	176	5.3	5.3
Backbone-Backbone	480	14.4	88	18.3	2.6	11	2.3	0.3
Backbone-Sidechain	1957	58.6	594	30.4	17.8	87	4.4	2.6
Sidechain-Sidechain	904	27.1	391	43.3	11.7	78	8.6	2.3

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

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



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

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

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total				
1	55	115	111	223	20	524	0.82	5.11	0.82	0.53
2	66	121	125	230	15	557	0.8	5.93	0.83	0.51
3	51	111	116	219	15	512	0.79	5.43	0.81	0.52
4	55	129	120	230	19	553	0.76	4.89	0.77	0.51
5	59	115	122	228	18	542	0.81	5.43	0.82	0.54
6	53	103	107	237	14	514	0.83	5.44	0.84	0.52
7	54	113	109	211	15	502	0.76	5.1	0.78	0.49
8	62	120	109	211	17	519	0.79	6.01	0.85	0.49
9	60	112	116	211	19	518	0.8	5.44	0.81	0.52
10	62	125	120	203	15	525	0.78	5.43	0.79	0.49

Continued on next page...

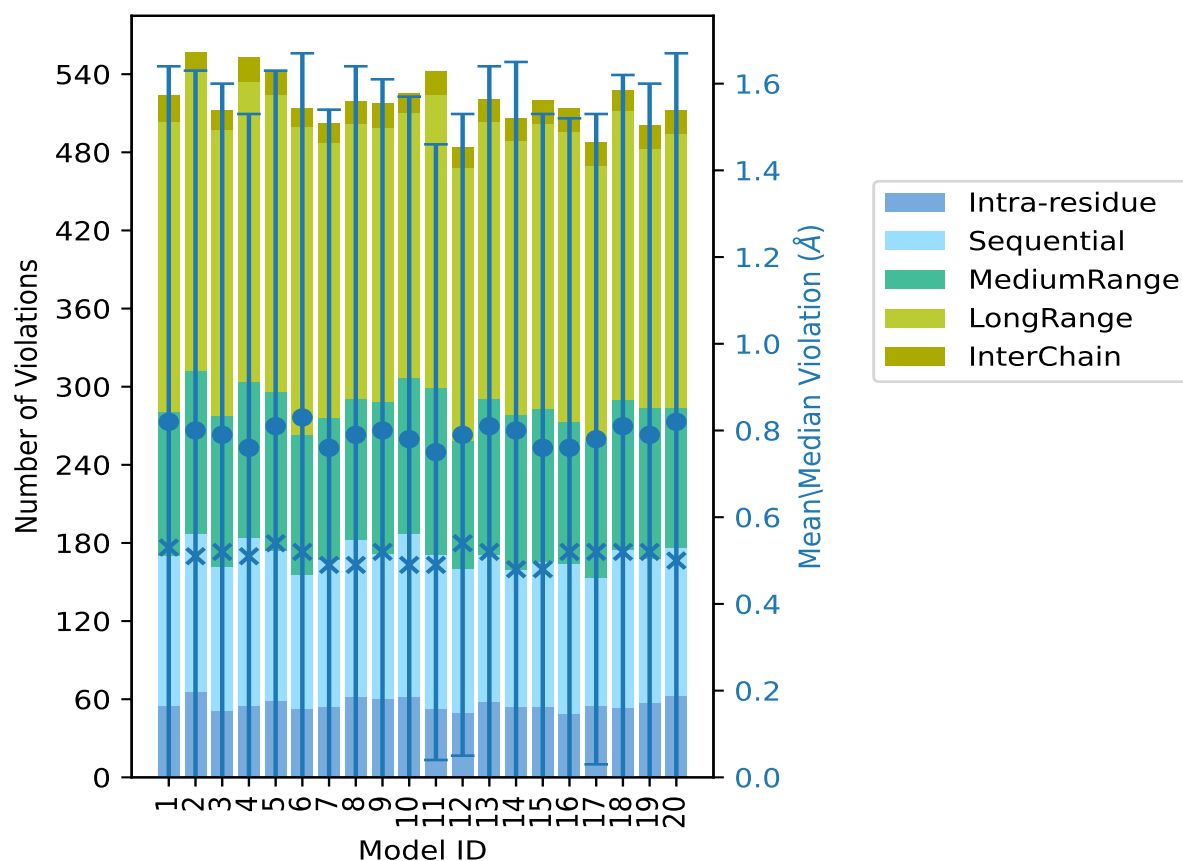
Continued from previous page...

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	53	118	128	225	18	542	0.75	4.31	0.71	0.49
12	50	110	99	209	16	484	0.79	4.43	0.74	0.54
13	58	113	120	213	17	521	0.81	5.51	0.83	0.52
14	54	105	119	211	17	506	0.8	5.66	0.85	0.48
15	54	112	117	219	18	520	0.76	5.13	0.77	0.48
16	49	115	109	223	18	514	0.76	5.36	0.76	0.52
17	55	98	105	212	18	488	0.78	4.49	0.75	0.52
18	53	122	115	222	16	528	0.81	5.38	0.81	0.52
19	57	111	116	199	18	501	0.79	5.68	0.81	0.52
20	63	113	108	210	18	512	0.82	5.51	0.85	0.5

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

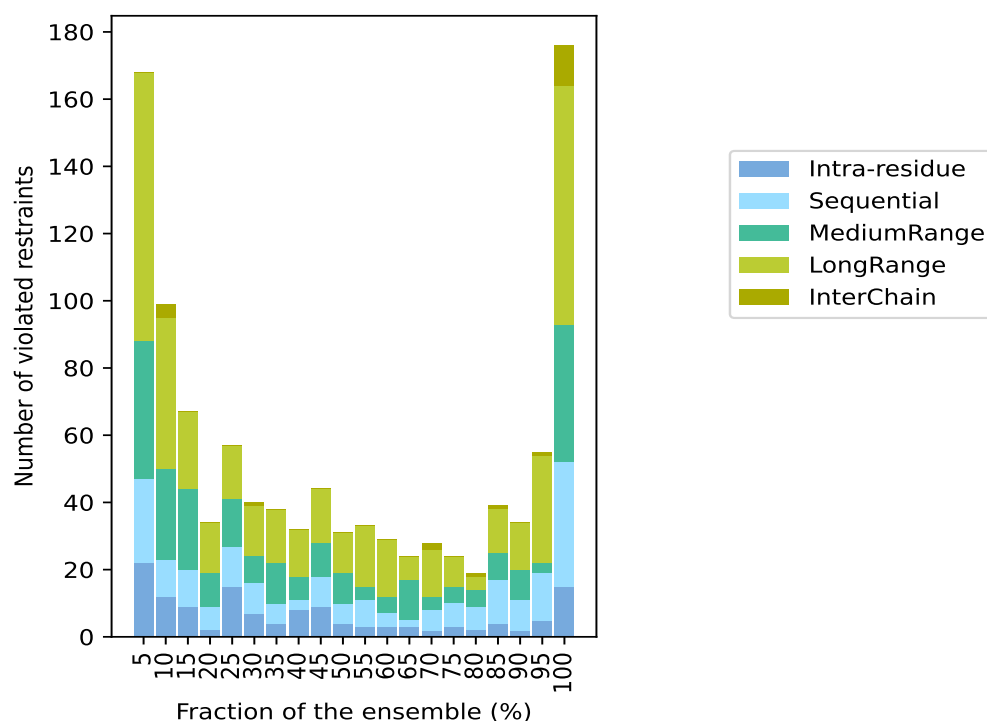
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2264(IR:661, SQ:653, MR:325, LR:612, IC:13) restraints are 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	%
22	25	41	80	0	168	1	5.0
12	11	27	45	4	99	2	10.0
9	11	24	23	0	67	3	15.0
2	7	10	15	0	34	4	20.0
15	12	14	16	0	57	5	25.0
7	9	8	15	1	40	6	30.0
4	6	12	16	0	38	7	35.0
8	3	7	14	0	32	8	40.0
9	9	10	16	0	44	9	45.0
4	6	9	12	0	31	10	50.0
3	8	4	18	0	33	11	55.0
3	4	5	17	0	29	12	60.0
3	2	12	7	0	24	13	65.0
2	6	4	14	2	28	14	70.0
3	7	5	9	0	24	15	75.0
2	7	5	4	1	19	16	80.0
4	13	8	13	1	39	17	85.0
2	9	9	14	0	34	18	90.0
5	14	3	32	1	55	19	95.0
15	37	41	71	12	176	20	100.0

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

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

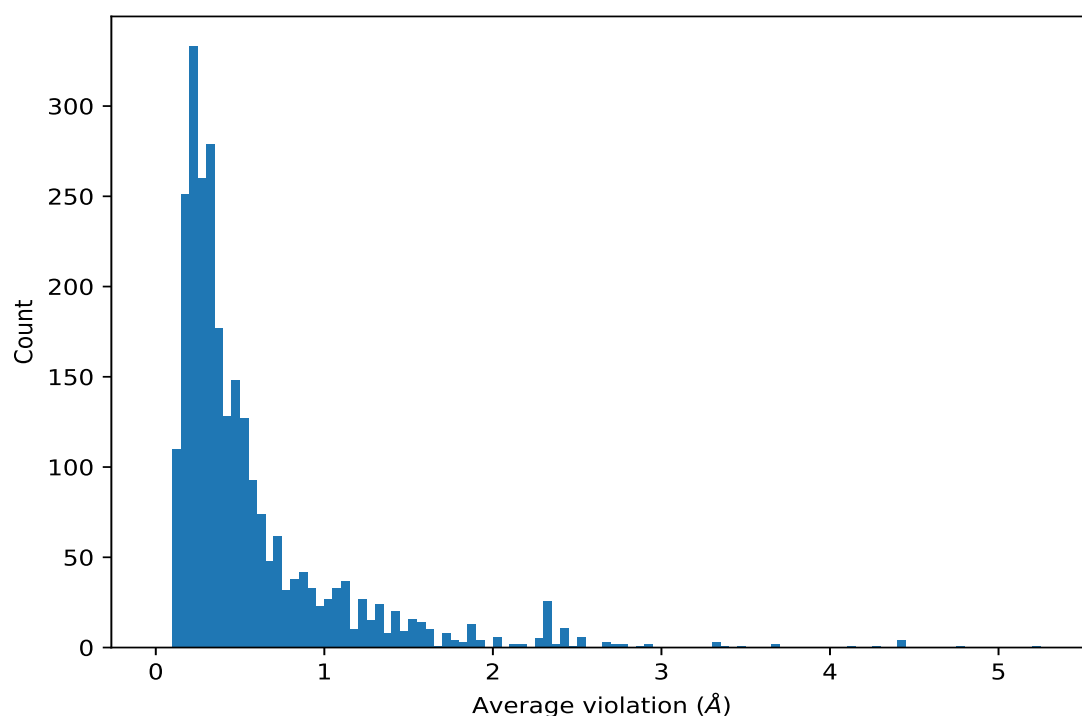
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation 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.

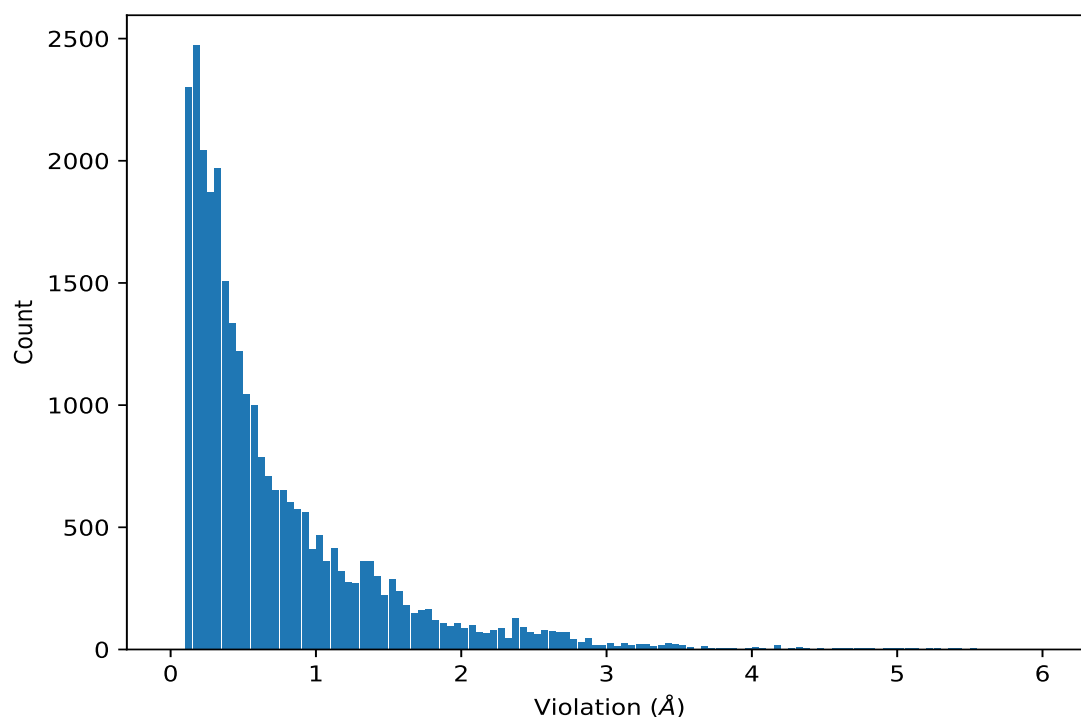
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	20	5.23	0.39	5.4
(1,567)	1:19:A:LEU:H	1:156:A:PHE:HZ	20	4.78	0.62	4.97
(1,1966)	1:19:A:LEU:HB2	1:156:A:PHE:HZ	20	4.41	0.61	4.61
(1,1171)	1:55:A:ILE:HG21	1:156:A:PHE:HZ	20	4.4	0.69	4.46
(1,1171)	1:55:A:ILE:HG22	1:156:A:PHE:HZ	20	4.4	0.69	4.46
(1,1171)	1:55:A:ILE:HG23	1:156:A:PHE:HZ	20	4.4	0.69	4.46
(1,1979)	1:55:A:ILE:HB	1:156:A:PHE:HZ	20	4.25	0.44	4.15
(1,547)	1:20:A:THR:H	1:156:A:PHE:HZ	20	4.12	0.51	4.31
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE21	20	3.67	1.18	3.6
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE22	20	3.67	1.18	3.6
(1,1160)	1:55:A:ILE:HG13	1:156:A:PHE:HZ	20	3.46	0.41	3.4
(1,1102)	1:26:A:ASN:HB2	1:27:A:HIS:HD2	20	3.36	0.25	3.38
(1,1381)	1:71:A:TYR:HB3	1:74:A:THR:HG21	20	3.31	0.41	3.31

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 provides the 10 worst performing restraints, sorted by the violation 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)
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE21	8	6.01
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE22	8	6.01
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE21	2	5.93
(1,670)	1:65:A:SER:HA	1:99:A:GLN:HE22	2	5.93
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	2	5.72
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	19	5.68
(1,567)	1:19:A:LEU:H	1:156:A:PHE:HZ	14	5.66
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	14	5.54
(1,1171)	1:55:A:ILE:HG21	1:156:A:PHE:HZ	13	5.51
(1,1171)	1:55:A:ILE:HG22	1:156:A:PHE:HZ	13	5.51
(1,1171)	1:55:A:ILE:HG23	1:156:A:PHE:HZ	13	5.51

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	20	5.51
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	6	5.44
(1,226)	1:20:A:THR:HB	1:156:A:PHE:HZ	9	5.44

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

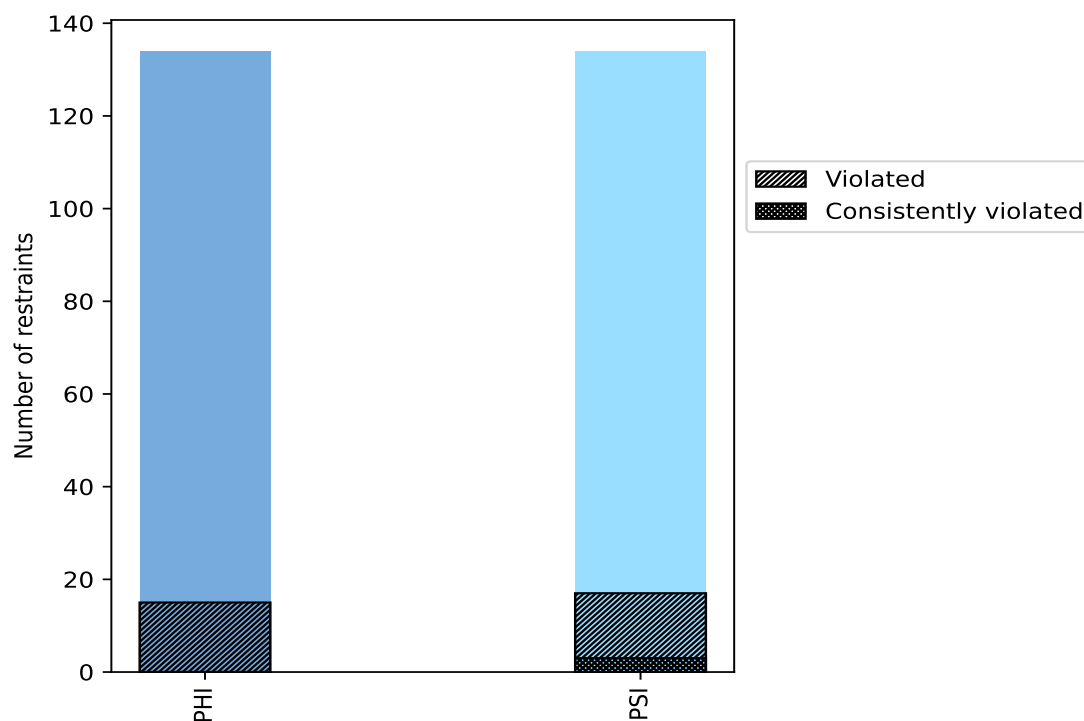
10.1 Summary of dihedral-angle violations [i](#)

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	134	50.0	15	11.2	5.6	0	0.0	0.0
PSI	134	50.0	17	12.7	6.3	3	2.2	1.1
Total	268	100.0	32	11.9	11.9	3	1.1	1.1

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](#)



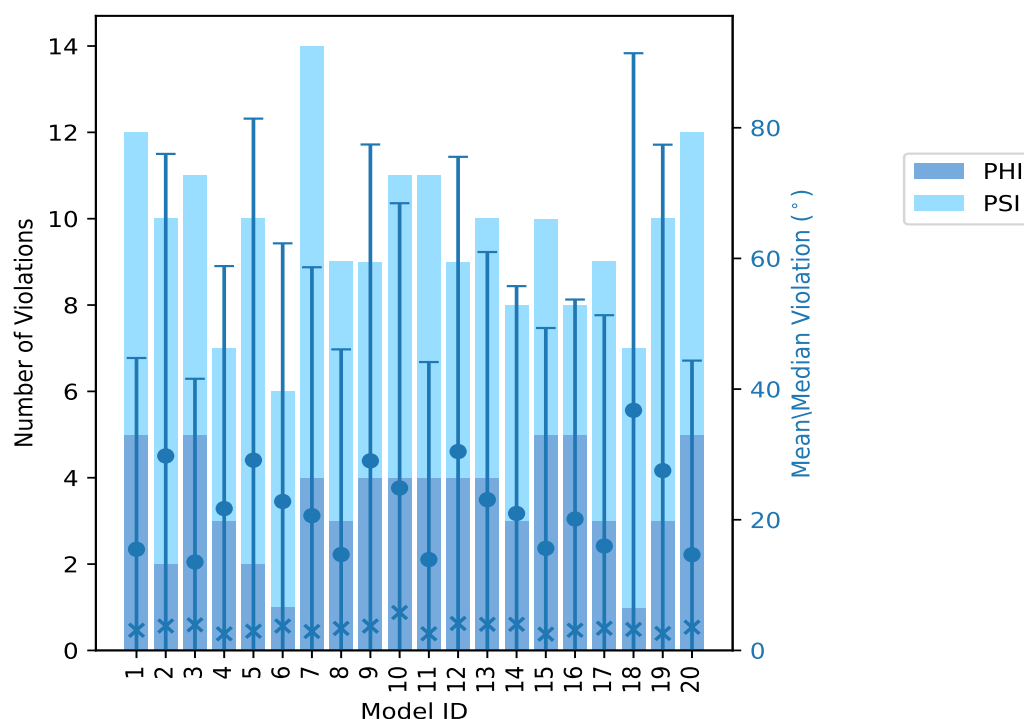
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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	5	7	12	15.48	108.12	29.28	3.09
2	2	8	10	29.77	127.21	46.23	3.74
3	5	6	11	13.53	101.46	28.05	3.92
4	3	4	7	21.71	109.27	37.12	2.54
5	2	8	10	29.12	150.82	52.28	2.94
6	1	5	6	22.8	110.45	39.51	3.74
7	4	10	14	20.63	117.53	38.02	2.9
8	3	6	9	14.68	103.3	31.4	3.37
9	4	5	9	29.02	131.14	48.42	3.73
10	4	7	11	24.86	124.59	43.59	5.81
11	4	7	11	13.91	108.58	30.23	2.55
12	4	5	9	30.44	114.54	45.11	4.13
13	4	6	10	23.07	109.22	37.91	4.0
14	3	5	8	20.96	109.86	34.8	4.0
15	5	5	10	15.63	115.97	33.72	2.49
16	5	3	8	20.11	105.07	33.6	3.09
17	3	6	9	15.98	115.62	35.33	3.39
18	1	6	7	36.75	134.86	54.66	3.21
19	3	7	10	27.52	144.96	49.89	2.6
20	5	7	12	14.65	110.3	29.71	3.55

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



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

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

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

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

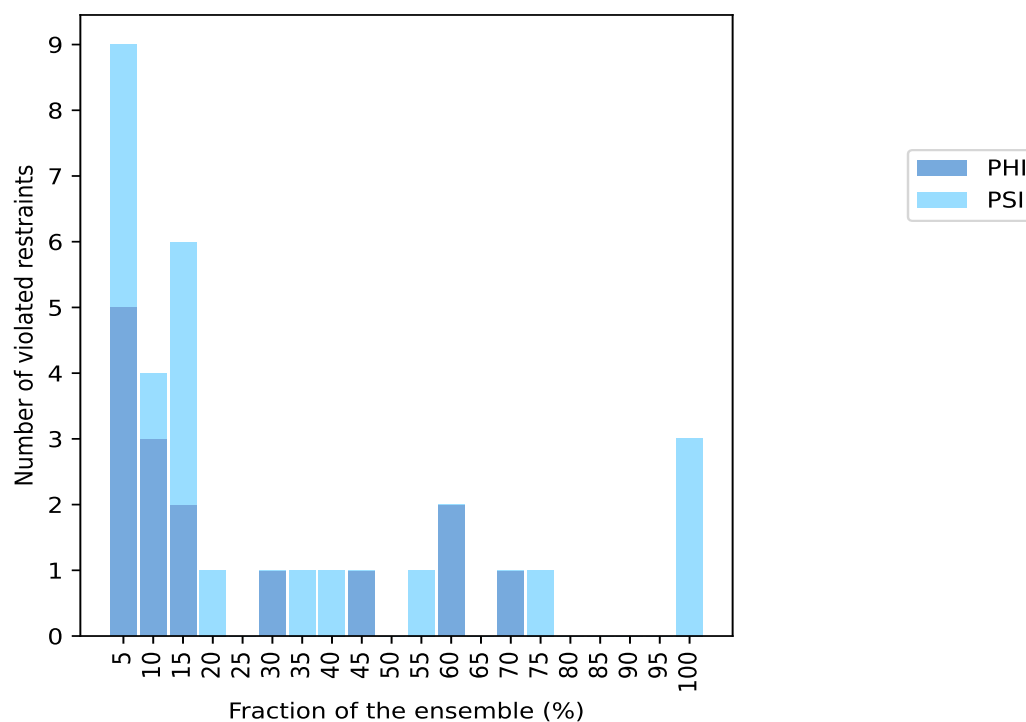
Continued on next page...

Continued from previous page...

Number of violated restraints			Fraction of the ensemble	
PHI	PSI	Total	Count ¹	%
2	0	2	12	60.0
0	0	0	13	65.0
1	0	1	14	70.0
0	1	1	15	75.0
0	0	0	16	80.0
0	0	0	17	85.0
0	0	0	18	90.0
0	0	0	19	95.0
0	3	3	20	100.0

¹ Number of models with violations

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

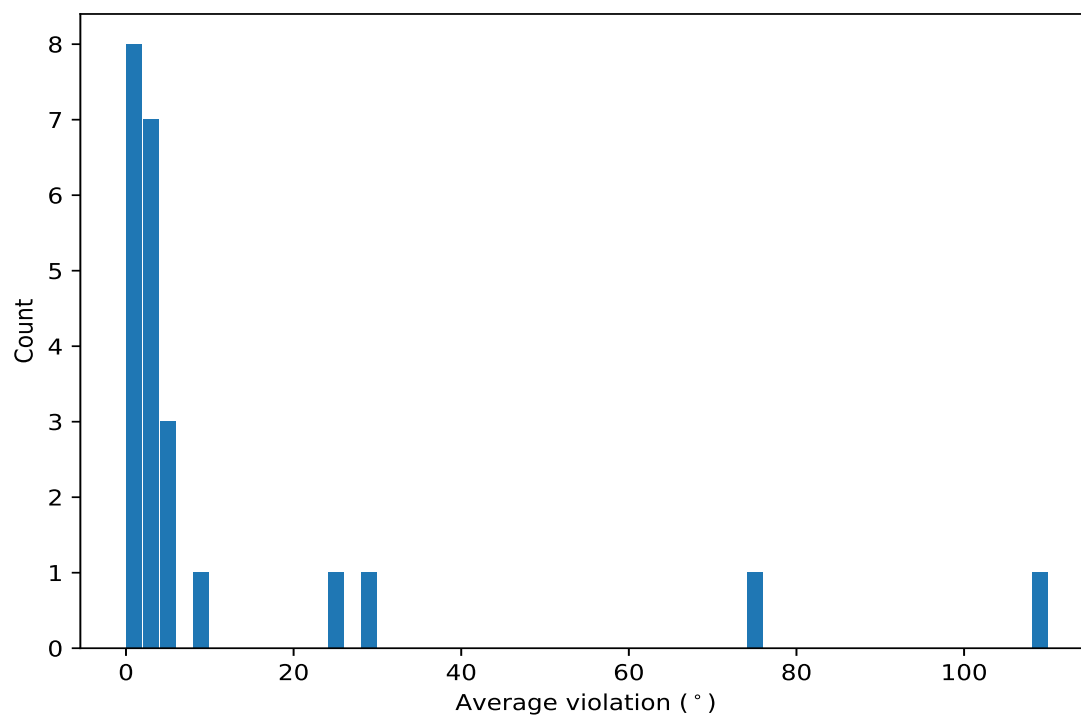


10.4 Most violated dihedral-angle restraints in the ensemble ⓘ

10.4.1 Histogram : Distribution of mean dihedral-angle violations ⓘ

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 violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

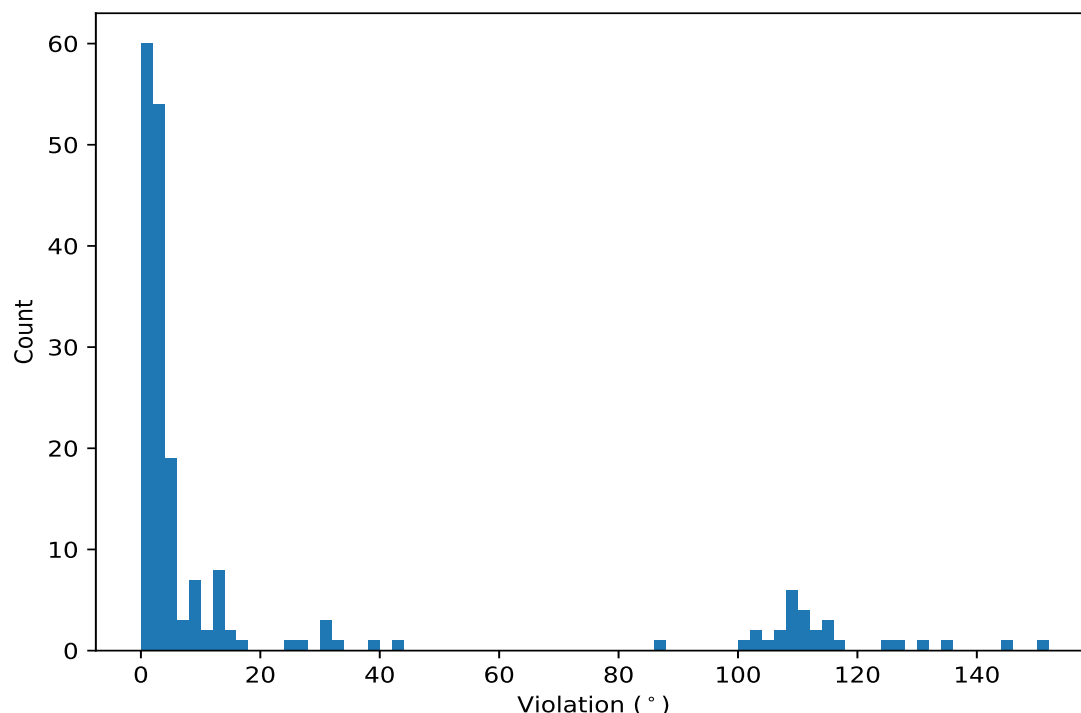
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models ¹	Mean	SD ²	Median
(1,50)	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	1:39:A:SER:N	20	109.03	3.79	109.3
(1,114)	1:75:A:GLY:N	1:75:A:GLY:CA	1:75:A:GLY:C	1:76:A:GLU:N	20	3.25	0.25	3.24
(1,112)	1:74:A:THR:N	1:74:A:THR:CA	1:74:A:THR:C	1:75:A:GLY:N	20	1.45	0.17	1.42
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	15	74.55	61.0	114.54
(1,43)	1:27:A:HIS:C	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	14	9.49	3.6	9.46
(1,89)	1:58:A:THR:C	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	12	28.27	19.91	26.08
(1,21)	1:15:A:GLY:C	1:16:A:LYS:N	1:16:A:LYS:CA	1:16:A:LYS:C	12	2.02	0.47	2.16
(1,92)	1:60:A:GLY:N	1:60:A:GLY:CA	1:60:A:GLY:C	1:61:A:GLN:N	11	4.45	0.75	4.1
(1,3)	1:2:A:THR:C	1:3:A:GLU:N	1:3:A:GLU:CA	1:3:A:GLU:C	9	2.6	0.83	2.35
(1,44)	1:28:A:PHE:N	1:28:A:PHE:CA	1:28:A:PHE:C	1:29:A:VAL:N	8	5.38	2.96	4.16

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 provides the list of violations for the 10 worst performing restraints, sorted by the violation 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 (°)
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	5	150.82
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	19	144.96
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	18	134.86
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	9	131.14
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	2	127.21
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	10	124.59
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	7	117.53
(1,50)	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	1:39:A:SER:N	15	115.97
(1,50)	1:38:A:ASP:N	1:38:A:ASP:CA	1:38:A:ASP:C	1:39:A:SER:N	17	115.62
(1,90)	1:59:A:ALA:N	1:59:A:ALA:CA	1:59:A:ALA:C	1:60:A:GLY:N	12	114.54