



Full wwPDB NMR Structure Validation Report ⓘ

Mar 8, 2026 – 02:06 AM UTC

PDB ID : 5W4S / pdb_00005w4s
BMRB ID : 30305
Title : Solution structure of C2 domain from protein kinase C alpha in ternary complex with calcium and V5-pHM peptide
Authors : Yang, Y.; Igumenova, T.I.
Deposited on : 2017-06-12

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

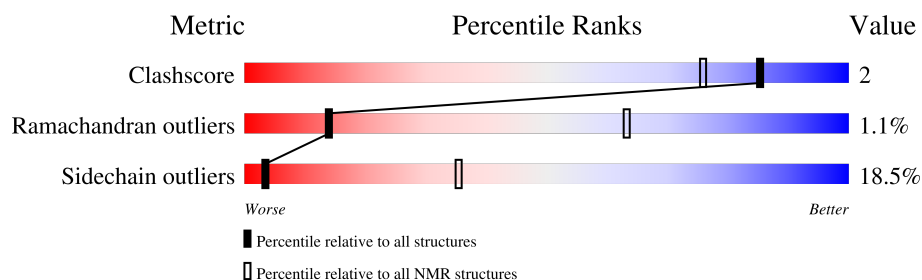
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 1%.

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	139	
2	B	12	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:156-A:293, B:653-B:656 (142)	0.43	2

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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2446 atoms, of which 1209 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein kinase C alpha type.

Mol	Chain	Residues	Atoms						Trace
1	A	139	Total	C	H	N	O	S	0
			2286	725	1143	197	217	4	

- Molecule 2 is a protein called V5-pHM peptide.

Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	1
			158	55	66	12	24	1	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

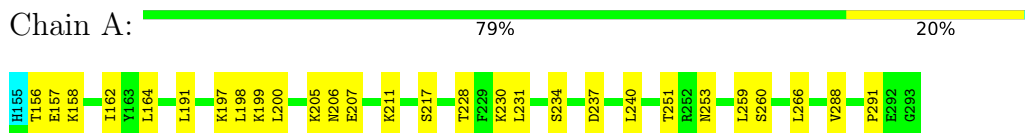
Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

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: Protein kinase C alpha type



- Molecule 2: V5-pHM peptide

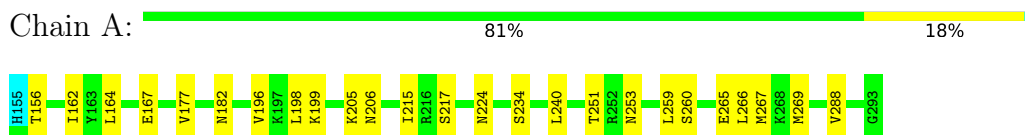


4.2 Scores per residue for each member of the ensemble

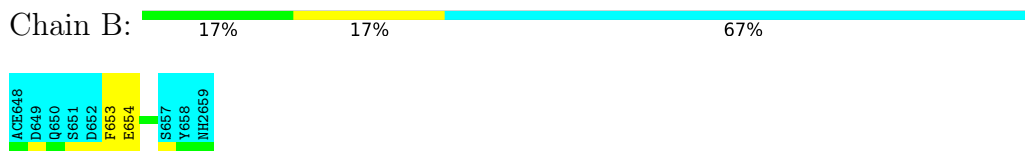
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein kinase C alpha type



- Molecule 2: V5-pHM peptide



4.2.2 Score per residue for model 2 (medoid)

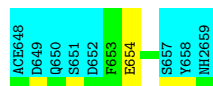
- Molecule 1: Protein kinase C alpha type

Chain A:  80% 18% ..



- Molecule 2: V5-pHM peptide

Chain B:  25% 8% 67%



4.2.3 Score per residue for model 3

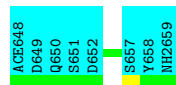
- Molecule 1: Protein kinase C alpha type

Chain A:  77% 22% ..



- Molecule 2: V5-pHM peptide

Chain B:  33% 67%



4.2.4 Score per residue for model 4

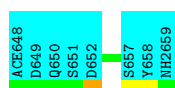
- Molecule 1: Protein kinase C alpha type

Chain A:  79% 19% ..



- Molecule 2: V5-pHM peptide

Chain B:  33% 67%



4.2.5 Score per residue for model 5

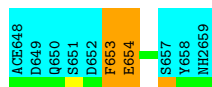
- Molecule 1: Protein kinase C alpha type

Chain A: 75% 24% ..



- Molecule 2: V5-pHM peptide

Chain B: 17% 17% 67%



4.2.6 Score per residue for model 6

- Molecule 1: Protein kinase C alpha type

Chain A: 74% 22% ..



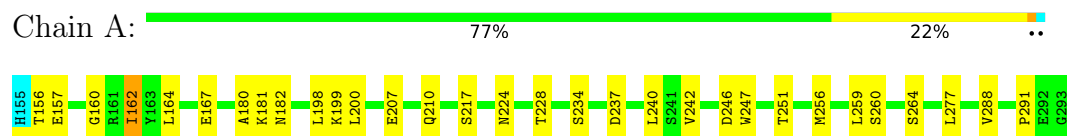
- Molecule 2: V5-pHM peptide

Chain B: 25% 8% 67%

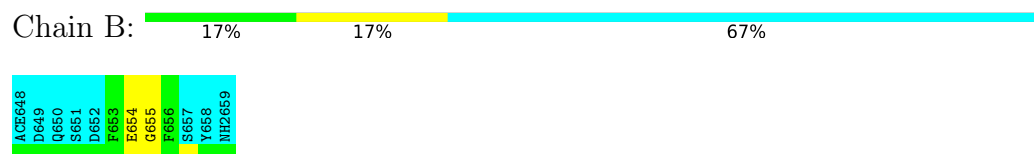


4.2.7 Score per residue for model 7

- Molecule 1: Protein kinase C alpha type

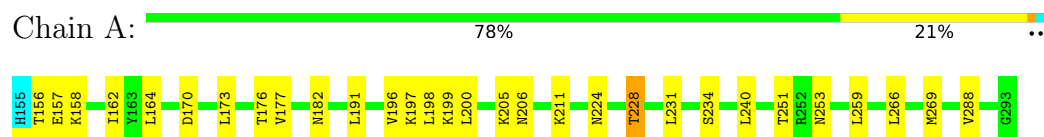


- Molecule 2: V5-pHM peptide



4.2.8 Score per residue for model 8

- Molecule 1: Protein kinase C alpha type

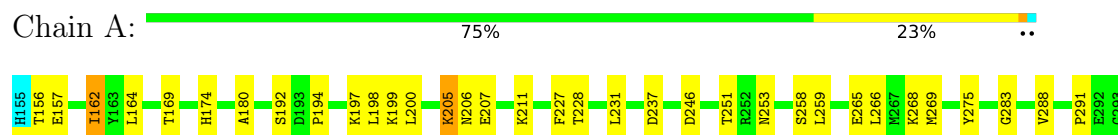


- Molecule 2: V5-pHM peptide

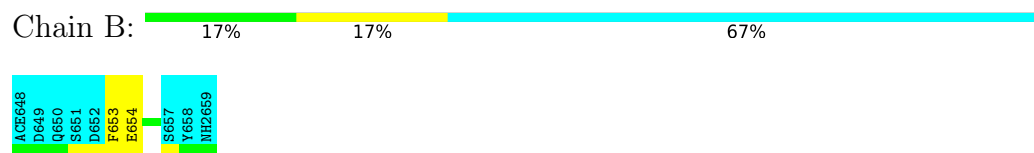


4.2.9 Score per residue for model 9

- Molecule 1: Protein kinase C alpha type

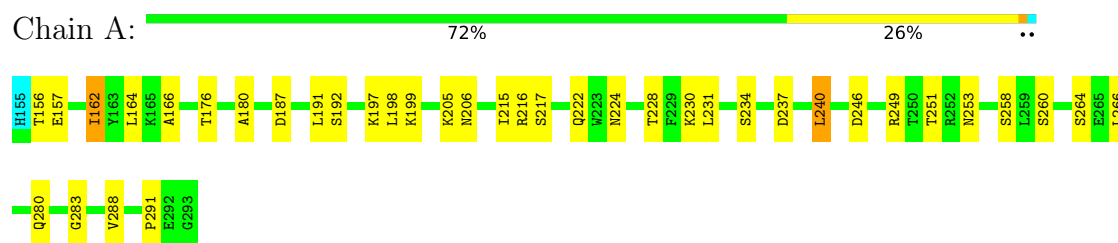


- Molecule 2: V5-pHM peptide

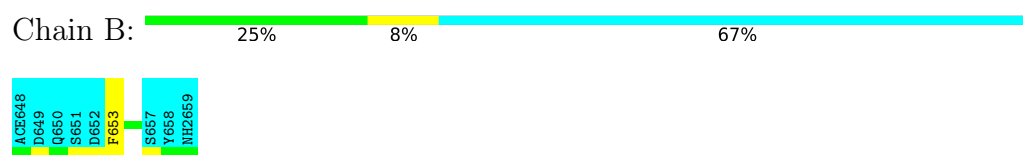


4.2.10 Score per residue for model 10

- Molecule 1: Protein kinase C alpha type

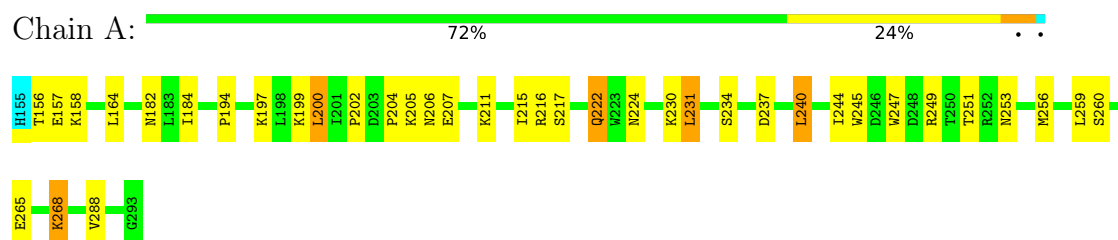


- Molecule 2: V5-pHM peptide

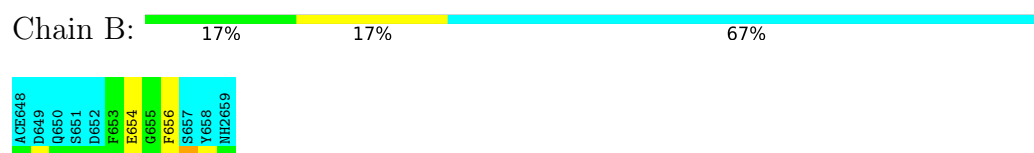


4.2.11 Score per residue for model 11

- Molecule 1: Protein kinase C alpha type



- Molecule 2: V5-pHM peptide



4.2.12 Score per residue for model 12

- Molecule 1: Protein kinase C alpha type



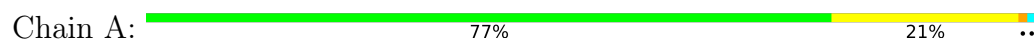


- Molecule 2: V5-pHM peptide

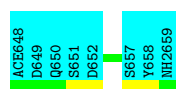


4.2.13 Score per residue for model 13

- Molecule 1: Protein kinase C alpha type

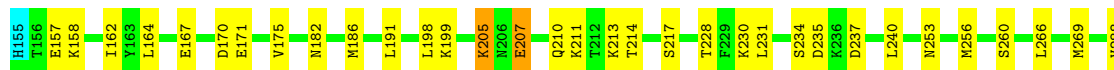
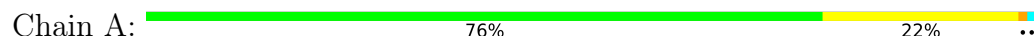


- Molecule 2: V5-pHM peptide

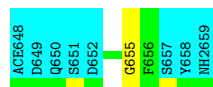


4.2.14 Score per residue for model 14

- Molecule 1: Protein kinase C alpha type

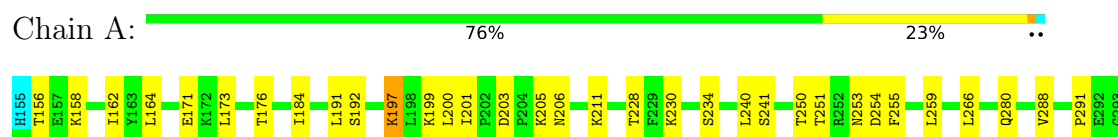


- Molecule 2: V5-pHM peptide



4.2.15 Score per residue for model 15

- Molecule 1: Protein kinase C alpha type

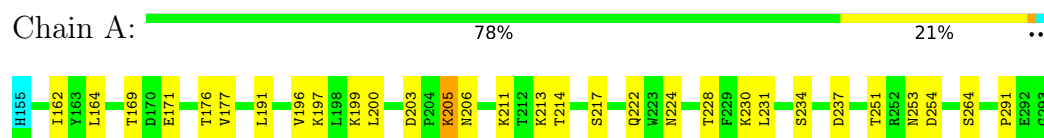


- Molecule 2: V5-pHM peptide

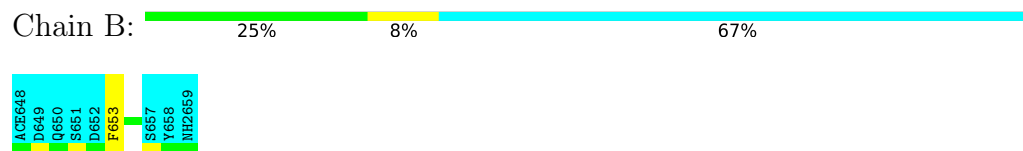


4.2.16 Score per residue for model 16

- Molecule 1: Protein kinase C alpha type

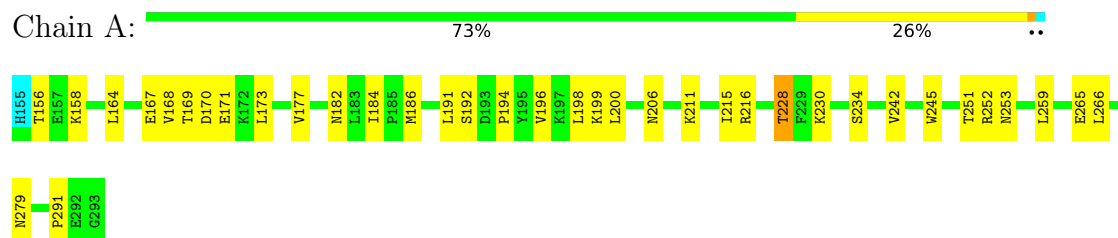


- Molecule 2: V5-pHM peptide



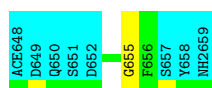
4.2.17 Score per residue for model 17

- Molecule 1: Protein kinase C alpha type



- Molecule 2: V5-pHM peptide





4.2.18 Score per residue for model 18

- Molecule 1: Protein kinase C alpha type

Chain A: 81% 17% ..



- Molecule 2: V5-pHM peptide

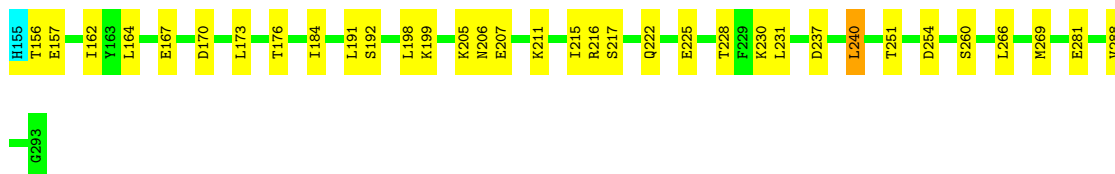
Chain B: 17% 17% 67%



4.2.19 Score per residue for model 19

- Molecule 1: Protein kinase C alpha type

Chain A: 75% 24% ..



- Molecule 2: V5-pHM peptide

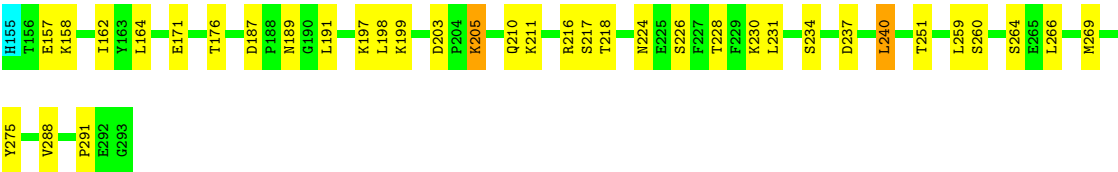
Chain B: 25% 8% 67%



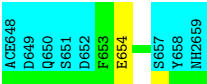
4.2.20 Score per residue for model 20

- Molecule 1: Protein kinase C alpha type

Chain A: 73% 24% ..



• Molecule 2: V5-pHM peptide



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure calculation	
CNS	refinement	
HADDOCK	structure calculation	

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	59
Number of shifts mapped to atoms	59
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

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: ACE, NH2, CA, SEP

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	1133	1133	1132	5±2
2	B	35	27	27	0±0
All	All	23400	23200	23180	103

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:VAL:HG21	1:A:196:VAL:HG21	0.65	1.67	17	7
1:A:258:SER:O	1:A:283:GLY:HA3	0.57	2.00	10	2
1:A:266:LEU:HA	1:A:269:MET:O	0.56	1.99	20	8
1:A:191:LEU:HD21	1:A:217:SER:HA	0.53	1.79	12	5
1:A:215:ILE:HG22	1:A:216:ARG:H	0.53	1.62	11	4
1:A:222:GLN:HG2	1:A:224:ASN:OD1	0.53	2.04	13	5
1:A:203:ASP:OD2	1:A:205:LYS:HD2	0.51	2.04	6	2
1:A:240:LEU:O	1:A:260:SER:HA	0.51	2.04	10	13
1:A:166:ALA:HB1	1:A:266:LEU:HD21	0.50	1.83	12	2
1:A:162:ILE:HG12	1:A:180:ALA:HB2	0.50	1.84	7	5
1:A:187:ASP:HB2	1:A:191:LEU:O	0.49	2.08	20	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:LEU:HG	1:A:192:SER:N	0.49	2.21	10	1
1:A:160:GLY:O	1:A:277:LEU:HG	0.49	2.07	7	2
1:A:275:TYR:OH	1:A:287:ASN:HA	0.48	2.09	3	1
1:A:203:ASP:OD2	1:A:205:LYS:HG3	0.47	2.08	15	2
1:A:192:SER:O	1:A:194:PRO:HD3	0.46	2.11	6	2
1:A:173:LEU:O	1:A:228:THR:HA	0.46	2.11	6	3
1:A:173:LEU:HD11	1:A:266:LEU:HD23	0.45	1.87	19	1
1:A:191:LEU:HG	1:A:192:SER:H	0.45	1.72	10	2
1:A:238:ARG:HA	1:A:238:ARG:NE	0.44	2.28	3	1
1:A:215:ILE:HG22	1:A:216:ARG:N	0.44	2.27	19	2
1:A:269:MET:O	1:A:269:MET:HG3	0.44	2.13	9	1
1:A:181:LYS:HE2	1:A:274:TRP:CH2	0.43	2.48	4	1
1:A:244:ILE:O	1:A:256:MET:HB2	0.43	2.14	11	2
1:A:246:ASP:HB3	1:A:254:ASP:HB2	0.43	1.89	2	1
1:A:194:PRO:HA	1:A:245:TRP:O	0.43	2.14	17	3
1:A:200:LEU:HB3	1:A:231:LEU:HD23	0.43	1.90	11	1
1:A:255:PHE:CZ	1:A:280:GLN:HG3	0.43	2.49	15	1
1:A:252:ARG:HD2	1:A:252:ARG:O	0.43	2.14	17	1
1:A:287:ASN:O	1:A:289:PRO:HD3	0.42	2.13	5	1
1:A:165:LYS:HG3	1:A:272:SER:OG	0.42	2.14	6	1
1:A:202:PRO:C	1:A:204:PRO:HD3	0.42	2.40	11	1
1:A:176:THR:HA	1:A:225:GLU:O	0.42	2.15	19	1
1:A:205:LYS:HD3	1:A:207:GLU:CG	0.42	2.45	14	3
1:A:174:HIS:HA	1:A:227:PHE:O	0.42	2.15	9	1
1:A:260:SER:OG	1:A:284:GLU:HA	0.42	2.15	5	1
1:A:265:GLU:O	1:A:268:LYS:HG3	0.41	2.15	11	1
1:A:216:ARG:O	1:A:218:THR:HG22	0.41	2.15	20	1
1:A:247:TRP:CE2	2:B:656:PHE:HB2	0.41	2.50	11	1
1:A:247:TRP:CH2	2:B:654:GLU:HA	0.41	2.51	7	1
1:A:265:GLU:OE1	1:A:268:LYS:HE2	0.40	2.16	9	1
2:B:653:PHE:HB3	2:B:654:GLU:OE1	0.40	2.16	5	1
1:A:213:LYS:HG3	1:A:214:THR:N	0.40	2.32	16	1
1:A:280:GLN:O	1:A:284:GLU:HG2	0.40	2.16	5	1
1:A:181:LYS:O	1:A:182:ASN:HB2	0.40	2.16	7	1
1:A:197:LYS:HE3	2:B:653:PHE:CE1	0.40	2.51	15	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	137/139 (99%)	123±2 (90±1%)	12±2 (9±1%)	1±1 (1±1%)	15	65
2	B	4/12 (33%)	2±1 (45±22%)	2±1 (50±25%)	0±0 (5±10%)	3	24
All	All	2820/3020 (93%)	2505 (89%)	283 (10%)	32 (1%)	14	63

All 5 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	253	ASN	14
1	A	291	PRO	11
2	B	655	GLY	4
1	A	249	ARG	2
1	A	215	ILE	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	128/129 (99%)	105±3 (82±3%)	23±3 (18±3%)	3	36
2	B	3/8 (38%)	2±1 (72±24%)	1±1 (28±24%)	1	19
All	All	2620/2740 (96%)	2136 (82%)	484 (18%)	3	35

All 67 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	164	LEU	20
1	A	199	LYS	19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	251	THR	17
1	A	288	VAL	17
1	A	228	THR	17
1	A	205	LYS	16
1	A	206	ASN	16
1	A	237	ASP	16
1	A	156	THR	15
1	A	162	ILE	15
1	A	198	LEU	15
1	A	234	SER	14
1	A	259	LEU	14
1	A	231	LEU	14
1	A	157	GLU	13
1	A	211	LYS	13
1	A	240	LEU	12
1	A	230	LYS	12
1	A	197	LYS	12
1	A	158	LYS	11
1	A	200	LEU	11
1	A	217	SER	10
1	A	207	GLU	10
2	B	653	PHE	9
1	A	167	GLU	8
1	A	182	ASN	8
2	B	654	GLU	8
1	A	176	THR	8
1	A	171	GLU	8
1	A	191	LEU	6
1	A	254	ASP	6
1	A	264	SER	6
1	A	256	MET	5
1	A	246	ASP	5
1	A	169	THR	5
1	A	266	LEU	5
1	A	170	ASP	5
1	A	224	ASN	4
1	A	265	GLU	4
1	A	226	SER	4
1	A	210	GLN	4
1	A	222	GLN	4
1	A	184	ILE	4
1	A	192	SER	3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	281	GLU	3
1	A	242	VAL	3
1	A	275	TYR	3
1	A	250	THR	3
1	A	175	VAL	2
1	A	173	LEU	2
1	A	279	ASN	2
1	A	241	SER	2
1	A	186	MET	2
1	A	267	MET	1
1	A	287	ASN	1
1	A	244	ILE	1
1	A	252	ARG	1
1	A	215	ILE	1
1	A	280	GLN	1
1	A	268	LYS	1
1	A	213	LYS	1
1	A	214	THR	1
1	A	235	ASP	1
1	A	201	ILE	1
1	A	168	VAL	1
1	A	269	MET	1
1	A	189	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	Counts	Bond lengths	
						RMSZ	#Z>2
2	SEP	B	657	2	8,9,10	1.55±0.01	1±0 (13±3%)

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	Counts	Bond angles	
						RMSZ	#Z>2
2	SEP	B	657	2	7,12,14	2.19±0.09	3±0 (42±0%)

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	SEP	B	657	2	-	0±0,6,8,10	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	657	SEP	P-O1P	3.22	1.60	1.50	20	20
2	B	657	SEP	P-O3P	2.02	1.47	1.54	10	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	657	SEP	OG-CB-CA	3.61	111.66	108.14	19	20
2	B	657	SEP	O3P-P-OG	3.11	114.77	106.67	17	20
2	B	657	SEP	O2P-P-OG	2.98	114.43	106.67	19	20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 1% for the well-defined parts and 3% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *pSer10_deposit_star3_v2.txt*

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	59
Number of shifts mapped to atoms	59
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 1%, i.e. 25 atoms were assigned a chemical shift out of a possible 1999. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	9/698 (1%)	9/282 (3%)	0/284 (0%)	0/132 (0%)
Sidechain	8/1140 (1%)	8/731 (1%)	0/359 (0%)	0/50 (0%)
Aromatic	8/161 (5%)	8/78 (10%)	0/77 (0%)	0/6 (0%)
Overall	25/1999 (1%)	25/1091 (2%)	0/720 (0%)	0/188 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 53 atoms were assigned a chemical shift out of a possible 2073. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	19/728 (3%)	19/294 (6%)	0/296 (0%)	0/138 (0%)
Sidechain	22/1167 (2%)	22/747 (3%)	0/369 (0%)	0/51 (0%)
Aromatic	12/178 (7%)	12/86 (14%)	0/84 (0%)	0/8 (0%)
Overall	53/2073 (3%)	53/1127 (5%)	0/749 (0%)	0/197 (0%)

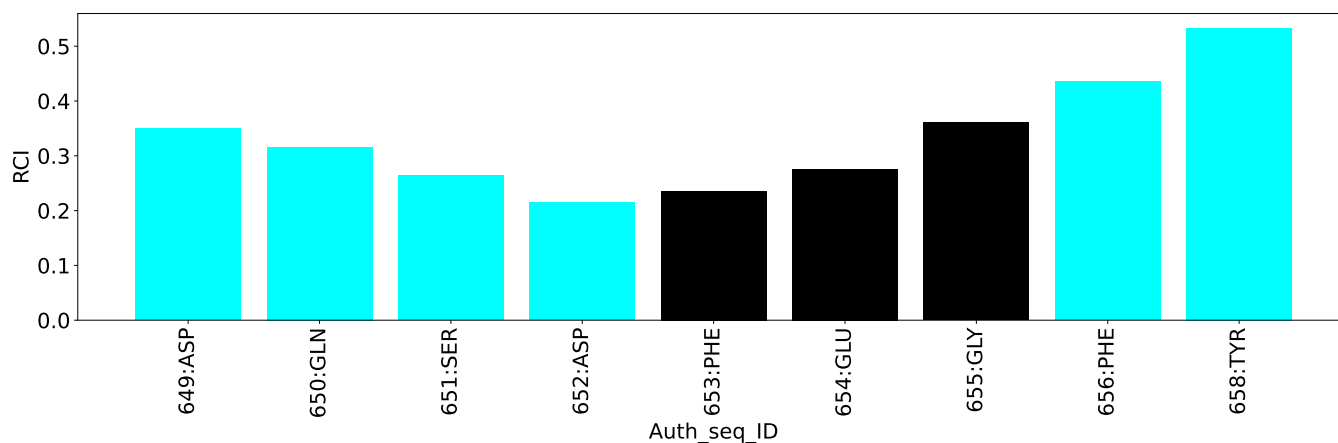
7.1.4 Statistically unusual chemical shifts [i](#)

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 B:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

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

Description	Value
Total distance restraints	49
Intra-residue ($ i-j =0$)	0
Sequential ($ i-j =1$)	0
Medium range ($ i-j >1$ and $ i-j <5$)	0
Long range ($ i-j \geq 5$)	2
Inter-chain	35
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	0.3
Number of long range restraints per residue ¹	0.0

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

8.2 Residual restraint violations

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

8.2.1 Average number of distance violations per model

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.3	0.2
0.2-0.5 (Medium)	0.3	0.43
>0.5 (Large)	2.0	4.5

8.2.2 Average number of dihedral-angle violations per model [i](#)

Dihedral-angle violations less than 1° are not included in the calculation. There are no dihedral-angle violations

9 Distance violation analysis

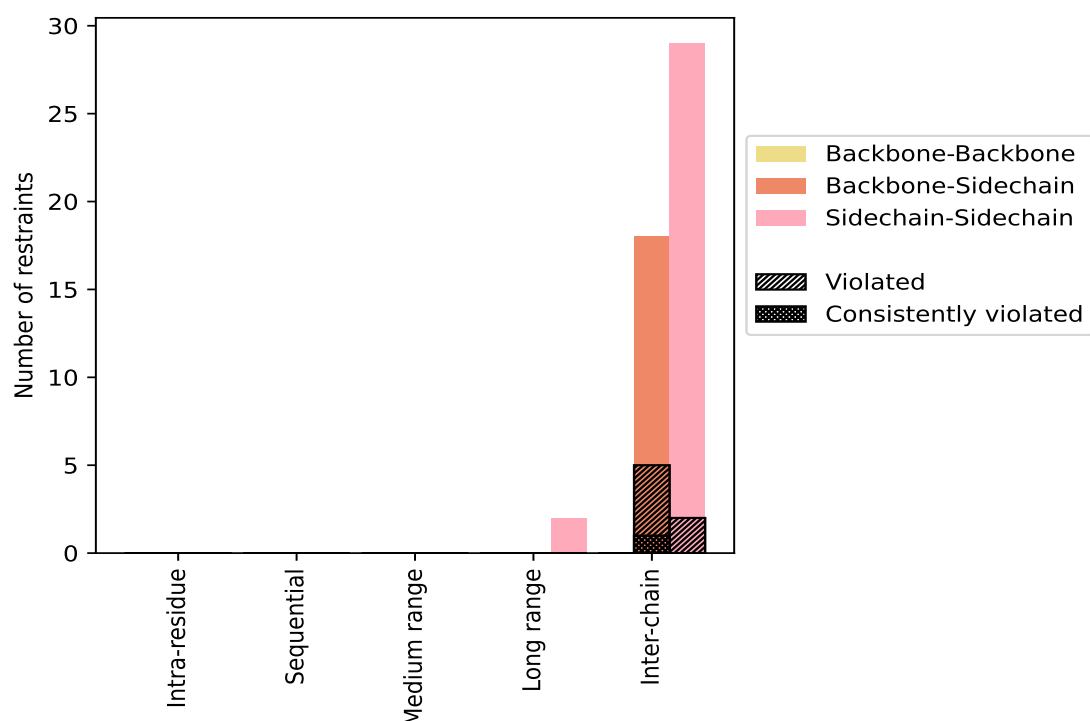
9.1 Summary of distance violations

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$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential ($ i-j =1$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Medium range ($ i-j >1$ & $ i-j <5$)	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Long range ($ i-j \geq 5$)	2	4.1	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	2	4.1	0	0.0	0.0	0	0.0	0.0
Inter-chain	35	71.4	6	17.1	12.2	1	2.9	2.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	36.7	5	27.8	10.2	1	5.6	2.0
Sidechain-Sidechain	17	34.7	1	5.9	2.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	49	100.0	7	14.3	14.3	1	2.0	2.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	18	36.7	5	27.8	10.2	1	5.6	2.0
Sidechain-Sidechain	31	63.3	2	6.5	4.1	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	0	0	0	2	2	2.62	4.43	1.8	2.62
2	0	0	0	0	2	2	2.37	4.37	2.0	2.37
3	0	0	0	0	3	3	1.75	4.35	1.86	0.78
4	0	0	0	0	3	3	1.61	3.71	1.5	0.87
5	0	0	0	0	2	2	2.24	4.22	1.98	2.24
6	0	0	0	0	3	3	1.52	4.08	1.81	0.34
7	0	0	0	0	3	3	1.92	4.42	1.77	0.76
8	0	0	0	0	3	3	1.95	4.22	1.69	1.48
9	0	0	0	0	2	2	2.7	4.32	1.63	2.7
10	0	0	0	0	4	4	1.72	4.04	1.42	1.3

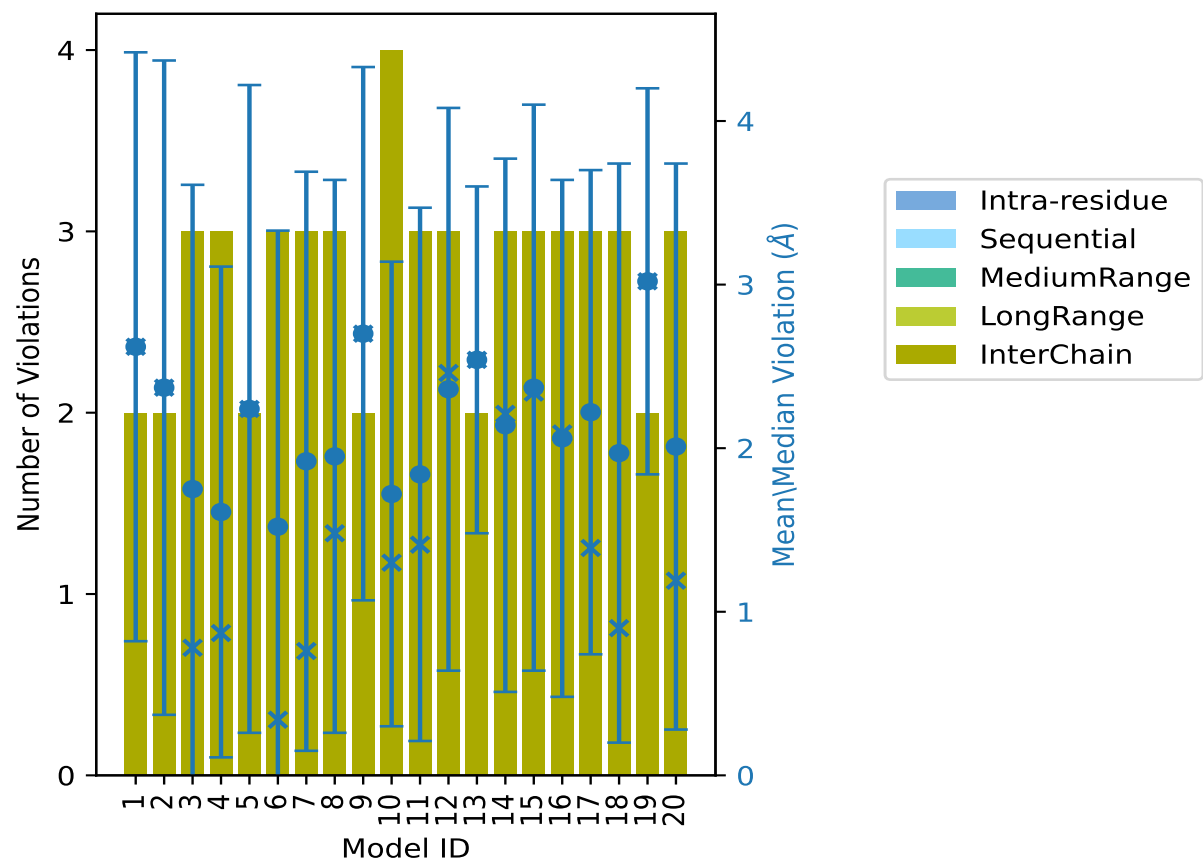
Continued on next page...

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	0	0	0	0	3	3	1.84	4.02	1.63	1.41
12	0	0	0	0	3	3	2.36	4.41	1.72	2.46
13	0	0	0	0	2	2	2.54	3.6	1.06	2.54
14	0	0	0	0	3	3	2.14	4.1	1.63	2.21
15	0	0	0	0	3	3	2.37	4.5	1.73	2.34
16	0	0	0	0	3	3	2.06	3.99	1.58	2.09
17	0	0	0	0	3	3	2.22	4.29	1.48	1.39
18	0	0	0	0	3	3	1.97	4.47	1.77	0.9
19	0	0	0	0	2	2	3.02	4.21	1.18	3.02
20	0	0	0	0	3	3	2.01	4.42	1.73	1.19

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

9.2.1 Bar graph : Distance Violation statistics for each model ⓘ



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

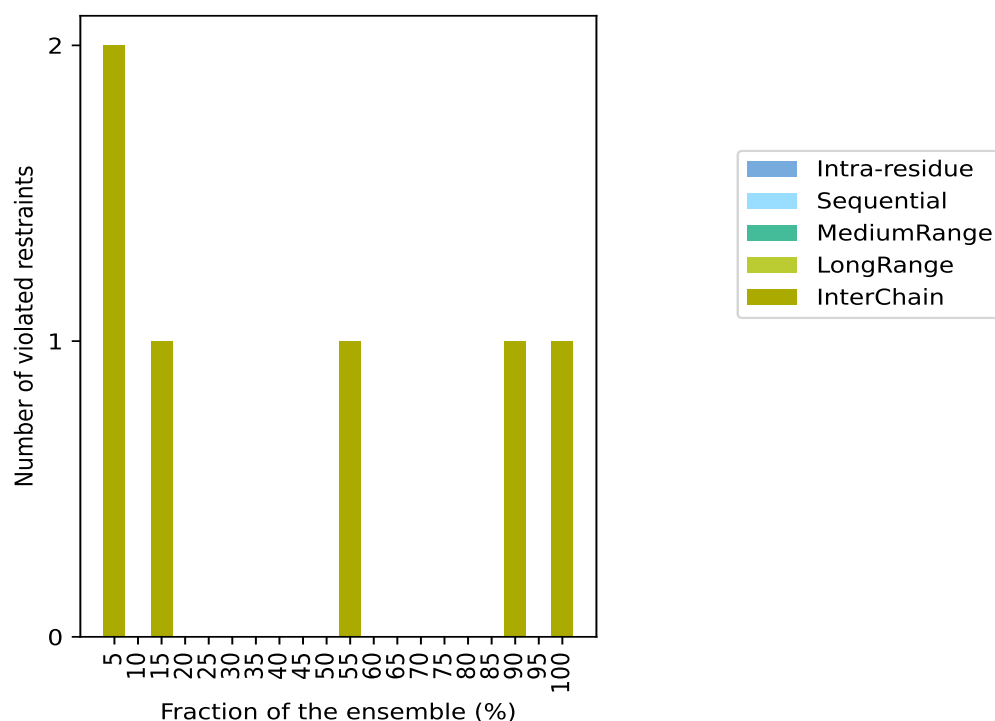
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 31(IR:0, SQ:0, MR:0, LR:2, IC:29) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵	Total	Count ⁶	%
0	0	0	0	2	2	1	5.0
0	0	0	0	0	0	2	10.0
0	0	0	0	1	1	3	15.0
0	0	0	0	0	0	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	1	1	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	1	1	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	1	1	20	100.0

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

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

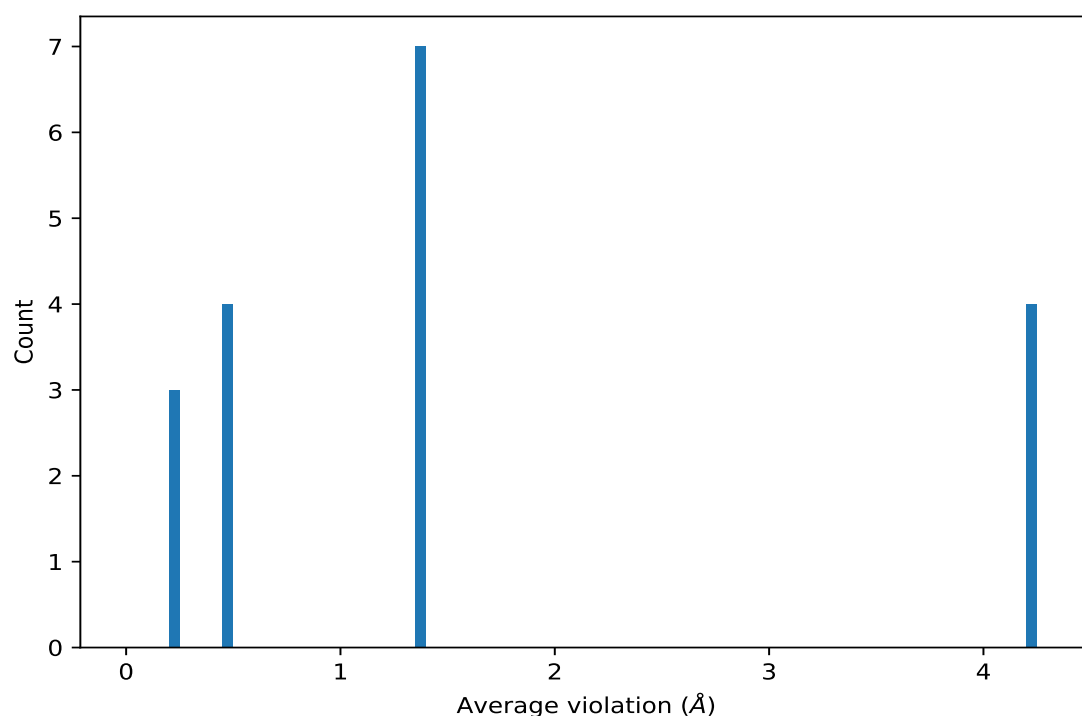
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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

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

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



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

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

Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	20	4.21	0.24	4.26
(1,34)	1:253:A:ASN:N	2:654:B:GLU:OE1	20	4.21	0.24	4.26
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	20	4.21	0.24	4.26
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	20	4.21	0.24	4.26
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:HA	2:658:B:TYR:O	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:HB	2:659:B:NH2:HN2	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:HA	2:659:B:NH2:N	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:O	2:654:B:GLU:HB3	18	1.36	0.62	1.4
(1,37)	1:250:A:THR:O	2:654:B:GLU:HG2	18	1.36	0.62	1.4
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	11	0.45	0.36	0.26
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HB3	11	0.45	0.36	0.26
(1,33)	1:251:A:THR:HG22	2:654:B:GLU:HG2	11	0.45	0.36	0.26
(1,33)	1:251:A:THR:HA	2:654:B:GLU:HG2	11	0.45	0.36	0.26
(1,35)	1:247:A:TRP:HZ3	2:654:B:GLU:HA	3	0.22	0.03	0.21

Continued on next page...

Continued from previous page...

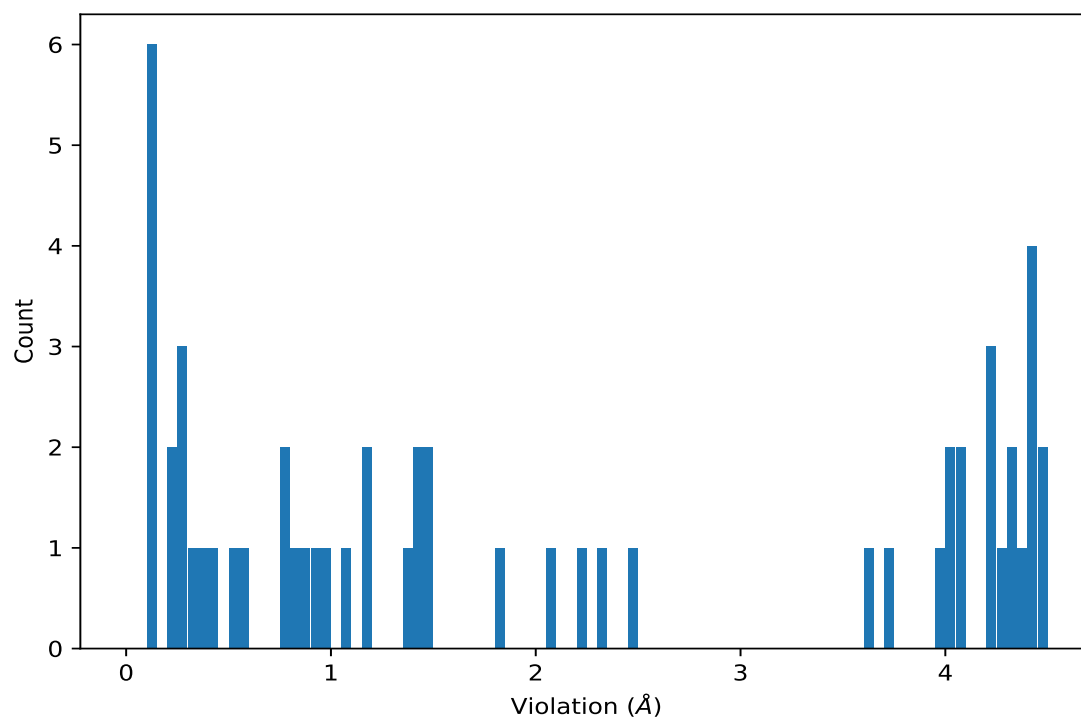
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,35)	1:247:A:TRP:HH2	2:654:B:GLU:HA	3	0.22	0.03	0.21
(1,35)	1:247:A:TRP:HZ2	2:657:B:SEP:H	3	0.22	0.03	0.21

¹Number of violated models, ²Standard deviation

9.5 All violated distance restraints [i](#)

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

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



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

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	15	4.5
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	18	4.47

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	1	4.43
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	7	4.42
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	20	4.42
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	12	4.41
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	2	4.37
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	3	4.35
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	9	4.32
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	17	4.29
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	5	4.22
(1,34)	1:253:A:ASN:N	2:653:B:PHE:HD2	8	4.22
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	19	4.21
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	14	4.1
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	6	4.08
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	10	4.04
(1,34)	1:253:A:ASN:N	2:654:B:GLU:HG3	11	4.02
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	16	3.99
(1,34)	1:253:A:ASN:N	2:654:B:GLU:OE1	4	3.71
(1,34)	1:253:A:ASN:H	2:653:B:PHE:HE2	13	3.6
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	12	2.46
(1,37)	1:250:A:THR:O	2:654:B:GLU:HB3	15	2.34
(1,37)	1:250:A:THR:O	2:654:B:GLU:HB3	14	2.21
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	16	2.09
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	19	1.84
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	8	1.48
(1,37)	1:250:A:THR:HA	2:659:B:NH2:N	13	1.48
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	10	1.43
(1,37)	1:250:A:THR:HA	2:658:B:TYR:O	11	1.41
(1,37)	1:250:A:THR:O	2:654:B:GLU:HG2	17	1.39
(1,37)	1:250:A:THR:O	2:654:B:GLU:HG2	20	1.19
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	10	1.18
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	9	1.07
(1,33)	1:251:A:THR:HA	2:654:B:GLU:HG2	17	0.97
(1,37)	1:250:A:THR:HA	2:657:B:SEP:O	18	0.9
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	4	0.87
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	1	0.82
(1,37)	1:250:A:THR:HA	2:658:B:TYR:O	3	0.78
(1,33)	1:251:A:THR:HA	2:654:B:GLU:HG2	7	0.76
(1,36)	1:209:A:LYS:HE3	2:652:B:ASP:OD2	7	0.58
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	18	0.54
(1,33)	1:251:A:THR:HA	2:654:B:GLU:HG2	20	0.43
(1,37)	1:250:A:THR:HA	2:659:B:NH2:HN1	2	0.37
(1,37)	1:250:A:THR:HB	2:659:B:NH2:HN2	6	0.34

Continued on next page...

Continued from previous page...

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,35)	1:247:A:TRP:HZ2	2:657:B:SEP:H	15	0.26
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HB3	4	0.26
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	5	0.26
(1,35)	1:247:A:TRP:HZ3	2:654:B:GLU:HA	10	0.21
(1,35)	1:247:A:TRP:HH2	2:654:B:GLU:HA	12	0.2
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	8	0.15
(1,33)	1:251:A:THR:HG22	2:654:B:GLU:HG2	6	0.13
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	3	0.12
(2,1)	3:301:A:CA:CA	1:187:A:ASP:OD1	16	0.11
(1,33)	1:251:A:THR:HG23	2:654:B:GLU:HG2	14	0.11
(1,3)	1:247:A:TRP:HE1	2:656:B:PHE:HE1	11	0.1

10 Dihedral-angle violation analysis ⓘ

No dihedral-angle restraints found