Full wwPDB NMR Structure Validation Report (i)

Jun 3, 2023 – 08:19 PM EDT

PDB ID	:	2N3T
BMRB ID	:	25657
Title	:	Solution structure of the Rpn1 substrate receptor site toroid 1 (T1)
Authors	:	Chen, X.; Walters, K.J.
Deposited on	:	2015-06-10

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

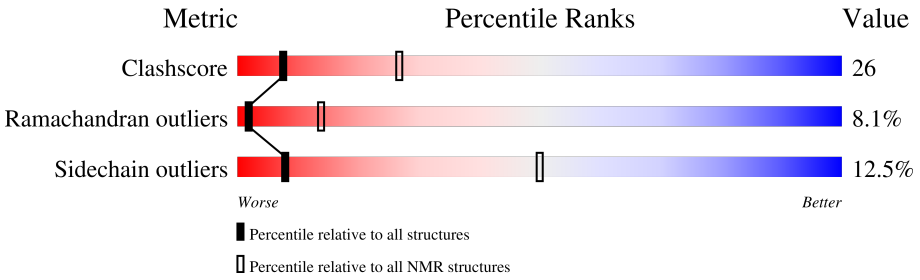
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

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

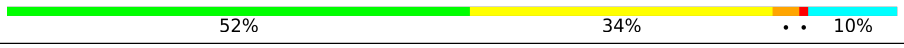
The overall completeness of chemical shifts assignment is 66%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	131	

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 3 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:490-A:607 (118)	1.45	3

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. No single-model clusters were found.

Cluster number	Models
1	1, 6, 7, 9, 10
2	2, 3, 4
3	5, 8

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1921 atoms, of which 967 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	1921	606	967	150	192	6	0

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 52% 34% • • 10%

D482 T483 K484 I485 S486 S487 A488 A489 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 D503 G507 L508 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 T560

D561 W562 V563 R564 Y574 M575 G576 Q577 G578 E592 H593 P594 M595 T596 S597 Y608 T609 G610 T611 G612

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: 26S proteasome regulatory subunit RPN1

Chain A: 50% 28% 10% • 10%

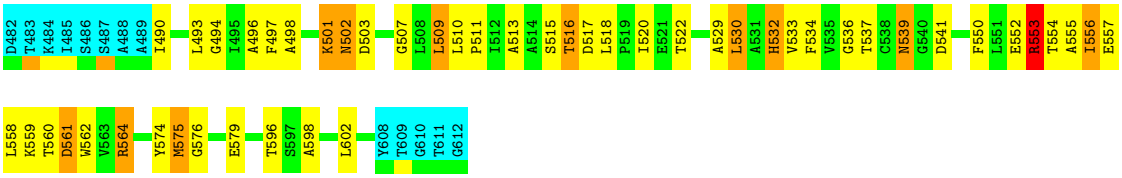
D482 T483 K484 I485 S486 S487 A488 A489 I490 L491 A496 F497 A498 G499 S500 K501 N502 D503 E504 G507 L508 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541 I542 T543 M547 F550 R553 T554 A555 I556 E557 L558 K559

T560 D561 W562 V563 R564 Y574 Q577 D582 E592 H593 P594 M595 T596 S597 L602 Y608 T609 G610 T611 G612

4.2.2 Score per residue for model 2

• Molecule 1: 26S proteasome regulatory subunit RPN1

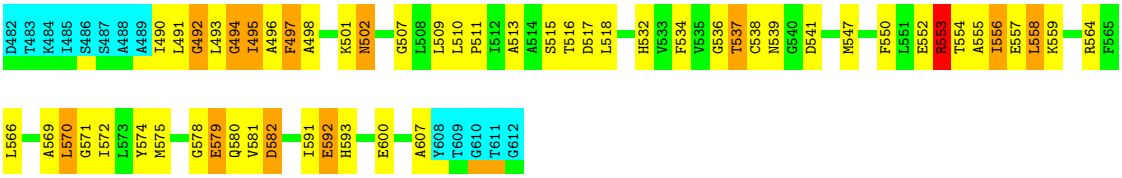
Chain A: 53% 28% 8% • 10%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: 26S proteasome regulatory subunit RPN1

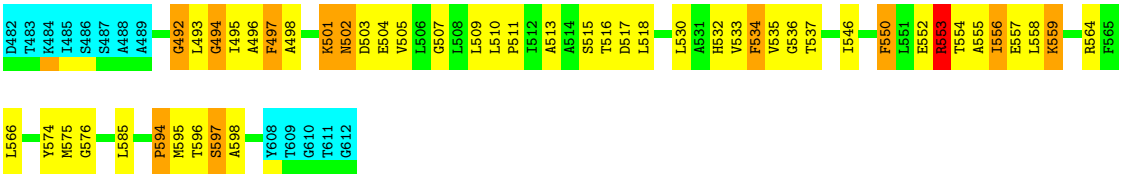
Chain A: 48% 32% 9% • 10%



4.2.4 Score per residue for model 4

- Molecule 1: 26S proteasome regulatory subunit RPN1

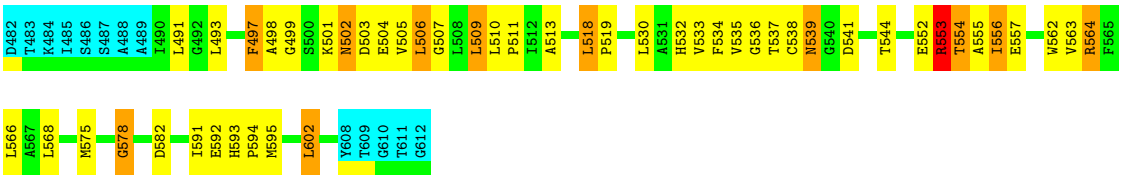
Chain A: 53% 28% 8% • 10%



4.2.5 Score per residue for model 5

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 53% 28% 8% • 10%



4.2.6 Score per residue for model 6

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 50% 32% 8% • 10%

D482 T483 K484 I485 S486 S487 A488 A489 I490 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 D503 E504 V505 L506 G507 L508 L509 L510 P511 I512 A513 A514 S515 L518 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541 T544 S545 I546 N549 R553 T554 A555 I556 E557

D561 W562 V563 I572 L573 Y574 M575 G576 Q577 L585 E586 I591 E592 H593 P594 A607 Y608 T609 G610 T611 G612

4.2.7 Score per residue for model 7

• Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 52% 30% 6% • 10%

D482 T483 K484 I485 S486 S487 A488 A489 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 D503 E504 V505 L506 L510 P511 A514 D517 L518 P519 I520 E521 T522 A523 A524 M525 L530 V533 F534 C538 N539 G540 D541 S545 I546 F550 L551 E552 R553 T554 A555

I556 E557 L558 K559 T560 D561 R564 G576 Q577 G578 E579 Q580 T596 S597 A598 I599 E600 A607 Y608 T609 G610 T611 G612

4.2.8 Score per residue for model 8

• Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 53% 29% 7% • 10%

D482 T483 K484 I485 S486 S487 A488 A489 I490 L491 G492 L493 A496 F497 A498 G499 S500 K501 N502 D503 E504 V505 L508 L509 L510 P511 L518 L530 A531 H532 V533 F534 V535 G536 T537 C538 N539 G540 D541 I546 M547 D548 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 W562

V563 R564 Y574 M575 G576 Q577 G578 D582 A590 I591 E592 H593 P594 M595 E600 Y608 T609 G610 T611 G612

4.2.9 Score per residue for model 9

• Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A: 60% 25% • • 10%

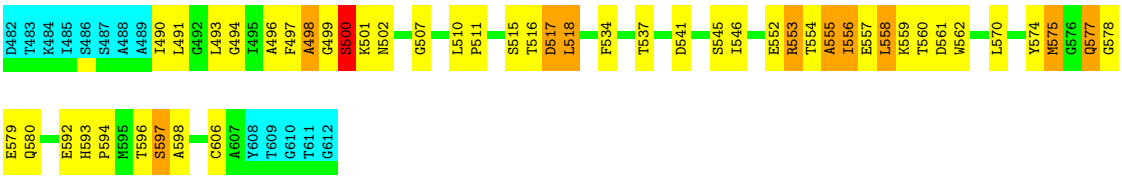
D482 T483 K484 I485 S486 S487 A488 A489 F497 A498 G499 S500 K501 N502 L509 L510 P511 T516 D517 L518 P519 I520 A524 L528 F534 V535 G536 T537 C538 S545 E552 R553 T554 A555 I556 E557 L558 K559 R564 I572 L573 Y574 M575 G576 E592 H593 P594 M595

E600 V601 L602 V603 G604 A607 Y608 T609 G610 T611 G612

4.2.10 Score per residue for model 10

- Molecule 1: 26S proteasome regulatory subunit RPN1

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 10 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
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1035
Number of shifts mapped to atoms	1035
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	66%

6 Model quality (i)

6.1 Standard geometry (i)

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

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

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.6±0.8
All	All	0	16

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	553	ARG	Sidechain	8
1	A	564	ARG	Sidechain	8

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	865	881	881	45±11
All	All	8650	8810	8810	450

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:497:PHE:CD1	1:A:498:ALA:N	0.71	2.58	2	1
1:A:494:GLY:O	1:A:497:PHE:CD1	0.71	2.44	3	1
1:A:494:GLY:C	1:A:497:PHE:CZ	0.69	2.66	3	1
1:A:494:GLY:O	1:A:497:PHE:CG	0.68	2.47	3	2
1:A:494:GLY:O	1:A:497:PHE:CE1	0.67	2.46	3	1
1:A:499:GLY:O	1:A:501:LYS:N	0.67	2.27	7	5
1:A:577:GLN:NE2	1:A:577:GLN:H	0.65	1.89	10	1
1:A:494:GLY:O	1:A:497:PHE:CD2	0.64	2.51	4	3
1:A:506:LEU:HD23	1:A:534:PHE:CE1	0.63	2.28	5	1
1:A:497:PHE:CZ	1:A:533:VAL:HG22	0.62	2.29	2	1
1:A:501:LYS:O	1:A:502:ASN:ND2	0.62	2.33	3	1
1:A:591:ILE:HD12	1:A:591:ILE:N	0.61	2.11	3	1
1:A:494:GLY:O	1:A:497:PHE:CZ	0.61	2.53	3	1
1:A:497:PHE:N	1:A:497:PHE:CD1	0.61	2.65	5	2
1:A:572:ILE:HD12	1:A:572:ILE:N	0.61	2.10	6	1
1:A:497:PHE:O	1:A:499:GLY:N	0.59	2.35	7	4
1:A:525:MET:SD	1:A:525:MET:N	0.59	2.76	7	1
1:A:494:GLY:O	1:A:496:ALA:N	0.59	2.36	4	2
1:A:494:GLY:HA2	1:A:497:PHE:CE2	0.59	2.32	3	1
1:A:494:GLY:O	1:A:497:PHE:CE2	0.58	2.57	3	3
1:A:508:LEU:HD12	1:A:508:LEU:N	0.58	2.14	8	1
1:A:497:PHE:CD1	1:A:505:VAL:HG21	0.57	2.33	8	1
1:A:554:THR:O	1:A:556:ILE:N	0.57	2.38	7	9
1:A:502:ASN:N	1:A:502:ASN:OD1	0.56	2.38	8	3
1:A:497:PHE:CE1	1:A:533:VAL:HG22	0.56	2.35	2	1
1:A:593:HIS:O	1:A:594:PRO:O	0.56	2.23	1	1
1:A:490:ILE:HD12	1:A:490:ILE:N	0.56	2.16	3	1
1:A:591:ILE:N	1:A:591:ILE:CD1	0.55	2.69	3	1
1:A:572:ILE:HG23	1:A:573:LEU:N	0.55	2.17	9	1
1:A:562:TRP:CD2	1:A:563:VAL:N	0.55	2.75	1	2
1:A:501:LYS:O	1:A:502:ASN:CB	0.55	2.55	3	3
1:A:493:LEU:O	1:A:497:PHE:CE1	0.55	2.60	8	2
1:A:498:ALA:C	1:A:500:SER:H	0.55	2.05	7	1
1:A:574:TYR:O	1:A:576:GLY:N	0.54	2.40	6	5
1:A:595:MET:SD	1:A:595:MET:N	0.54	2.80	8	1
1:A:579:GLU:H	1:A:579:GLU:CD	0.54	2.06	3	2
1:A:508:LEU:N	1:A:508:LEU:CD1	0.54	2.71	8	1
1:A:557:GLU:O	1:A:559:LYS:N	0.54	2.40	7	5
1:A:496:ALA:C	1:A:498:ALA:H	0.53	2.06	7	6
1:A:493:LEU:O	1:A:497:PHE:CD1	0.53	2.61	6	2
1:A:497:PHE:CD1	1:A:533:VAL:HG21	0.53	2.38	4	1
1:A:558:LEU:HD23	1:A:558:LEU:N	0.53	2.17	3	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:501:LYS:O	1:A:502:ASN:CG	0.53	2.47	4	2
1:A:516:THR:O	1:A:518:LEU:N	0.53	2.42	10	1
1:A:497:PHE:C	1:A:499:GLY:N	0.53	2.62	7	5
1:A:494:GLY:C	1:A:496:ALA:N	0.53	2.62	4	3
1:A:502:ASN:OD1	1:A:534:PHE:CZ	0.53	2.61	3	1
1:A:530:LEU:O	1:A:533:VAL:N	0.53	2.42	8	1
1:A:539:ASN:ND2	1:A:541:ASP:OD2	0.53	2.41	3	1
1:A:502:ASN:HD22	1:A:533:VAL:CG1	0.53	2.17	5	1
1:A:554:THR:C	1:A:556:ILE:N	0.52	2.62	7	10
1:A:498:ALA:O	1:A:500:SER:N	0.52	2.43	7	1
1:A:497:PHE:CD1	1:A:533:VAL:CG2	0.52	2.93	4	1
1:A:491:LEU:O	1:A:494:GLY:N	0.52	2.42	7	2
1:A:499:GLY:O	1:A:502:ASN:ND2	0.52	2.43	10	1
1:A:574:TYR:CD1	1:A:574:TYR:N	0.52	2.78	3	2
1:A:551:LEU:N	1:A:551:LEU:HD12	0.52	2.19	8	1
1:A:569:ALA:O	1:A:571:GLY:N	0.52	2.42	3	1
1:A:593:HIS:O	1:A:593:HIS:CG	0.52	2.62	5	2
1:A:497:PHE:C	1:A:499:GLY:H	0.52	2.08	8	3
1:A:499:GLY:C	1:A:501:LYS:N	0.51	2.62	7	5
1:A:507:GLY:O	1:A:511:PRO:CD	0.51	2.57	10	7
1:A:554:THR:C	1:A:556:ILE:H	0.51	2.08	5	7
1:A:593:HIS:ND1	1:A:597:SER:OG	0.51	2.43	10	1
1:A:557:GLU:C	1:A:559:LYS:H	0.51	2.09	1	6
1:A:502:ASN:O	1:A:504:GLU:N	0.51	2.43	1	2
1:A:550:PHE:O	1:A:553:ARG:NE	0.51	2.43	1	1
1:A:538:CYS:O	1:A:539:ASN:ND2	0.51	2.41	5	1
1:A:534:PHE:CD2	1:A:537:THR:OG1	0.51	2.64	2	2
1:A:498:ALA:C	1:A:500:SER:N	0.51	2.63	7	1
1:A:497:PHE:CG	1:A:498:ALA:N	0.51	2.78	2	1
1:A:520:ILE:O	1:A:524:ALA:N	0.51	2.44	9	1
1:A:501:LYS:O	1:A:502:ASN:OD1	0.51	2.29	4	1
1:A:520:ILE:HD11	1:A:556:ILE:CG2	0.51	2.35	2	1
1:A:537:THR:OG1	1:A:538:CYS:N	0.50	2.44	3	2
1:A:578:GLY:O	1:A:582:ASP:N	0.50	2.44	8	1
1:A:541:ASP:N	1:A:541:ASP:OD1	0.50	2.43	1	2
1:A:494:GLY:C	1:A:497:PHE:CE2	0.50	2.85	3	2
1:A:560:THR:O	1:A:561:ASP:CB	0.50	2.59	10	1
1:A:494:GLY:C	1:A:496:ALA:H	0.50	2.10	4	3
1:A:510:LEU:CB	1:A:511:PRO:CD	0.50	2.90	2	10
1:A:507:GLY:O	1:A:511:PRO:CG	0.50	2.60	3	5
1:A:515:SER:O	1:A:517:ASP:N	0.50	2.44	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:503:ASP:CG	1:A:504:GLU:N	0.50	2.66	5	1
1:A:510:LEU:O	1:A:514:ALA:N	0.50	2.43	7	1
1:A:494:GLY:CA	1:A:497:PHE:CE2	0.49	2.94	3	1
1:A:572:ILE:N	1:A:572:ILE:CD1	0.49	2.75	6	1
1:A:559:LYS:O	1:A:562:TRP:CD1	0.49	2.65	10	1
1:A:557:GLU:C	1:A:559:LYS:N	0.49	2.66	7	7
1:A:502:ASN:C	1:A:504:GLU:N	0.49	2.65	1	2
1:A:541:ASP:O	1:A:544:THR:N	0.49	2.44	6	1
1:A:492:GLY:O	1:A:494:GLY:N	0.49	2.46	3	2
1:A:569:ALA:C	1:A:571:GLY:N	0.49	2.66	3	1
1:A:558:LEU:N	1:A:558:LEU:CD2	0.49	2.75	3	3
1:A:502:ASN:OD1	1:A:502:ASN:C	0.49	2.51	3	2
1:A:571:GLY:O	1:A:575:MET:N	0.49	2.46	3	1
1:A:497:PHE:O	1:A:502:ASN:OD1	0.49	2.31	5	3
1:A:578:GLY:O	1:A:580:GLN:N	0.49	2.46	3	2
1:A:493:LEU:O	1:A:497:PHE:CD2	0.49	2.65	10	1
1:A:530:LEU:HD23	1:A:530:LEU:O	0.49	2.08	2	3
1:A:585:LEU:N	1:A:585:LEU:HD12	0.49	2.23	4	2
1:A:500:SER:HB2	1:A:533:VAL:HG11	0.49	1.83	1	1
1:A:515:SER:C	1:A:517:ASP:N	0.48	2.66	2	4
1:A:568:LEU:N	1:A:568:LEU:CD2	0.48	2.76	5	1
1:A:606:CYS:SG	1:A:606:CYS:O	0.48	2.71	10	1
1:A:579:GLU:O	1:A:582:ASP:OD2	0.48	2.31	3	1
1:A:552:GLU:O	1:A:553:ARG:C	0.48	2.51	5	5
1:A:592:GLU:O	1:A:593:HIS:ND1	0.48	2.45	3	1
1:A:534:PHE:C	1:A:536:GLY:N	0.48	2.67	2	8
1:A:594:PRO:C	1:A:596:THR:H	0.48	2.11	1	1
1:A:509:LEU:HD23	1:A:530:LEU:HD23	0.48	1.84	6	1
1:A:497:PHE:CD1	1:A:533:VAL:HG13	0.48	2.43	2	1
1:A:521:GLU:O	1:A:525:MET:SD	0.48	2.72	7	1
1:A:502:ASN:C	1:A:504:GLU:H	0.48	2.12	7	2
1:A:560:THR:OG1	1:A:561:ASP:N	0.48	2.46	10	1
1:A:561:ASP:OD1	1:A:562:TRP:N	0.48	2.47	2	1
1:A:496:ALA:C	1:A:498:ALA:N	0.48	2.67	1	6
1:A:496:ALA:O	1:A:498:ALA:N	0.48	2.47	6	4
1:A:550:PHE:CE1	1:A:566:LEU:HD21	0.48	2.44	3	1
1:A:492:GLY:C	1:A:494:GLY:N	0.47	2.66	3	2
1:A:555:ALA:C	1:A:557:GLU:H	0.47	2.12	8	5
1:A:575:MET:SD	1:A:575:MET:O	0.47	2.72	10	1
1:A:531:ALA:O	1:A:535:VAL:N	0.47	2.48	1	2
1:A:506:LEU:O	1:A:510:LEU:HD13	0.47	2.09	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:509:LEU:O	1:A:513:ALA:N	0.47	2.48	6	6
1:A:555:ALA:C	1:A:557:GLU:N	0.47	2.67	8	8
1:A:520:ILE:O	1:A:523:ALA:N	0.47	2.48	7	1
1:A:552:GLU:O	1:A:554:THR:N	0.47	2.47	8	1
1:A:509:LEU:CD2	1:A:530:LEU:HD23	0.47	2.40	6	1
1:A:520:ILE:HD12	1:A:556:ILE:CG2	0.47	2.39	9	1
1:A:595:MET:SD	1:A:595:MET:O	0.47	2.73	9	1
1:A:534:PHE:O	1:A:537:THR:O	0.47	2.33	3	8
1:A:504:GLU:N	1:A:504:GLU:CD	0.47	2.68	4	1
1:A:502:ASN:ND2	1:A:534:PHE:CD1	0.47	2.83	4	1
1:A:575:MET:SD	1:A:575:MET:C	0.47	2.93	10	1
1:A:503:ASP:OD1	1:A:504:GLU:N	0.47	2.47	5	1
1:A:568:LEU:N	1:A:568:LEU:HD22	0.47	2.25	5	1
1:A:594:PRO:C	1:A:596:THR:N	0.46	2.68	1	1
1:A:490:ILE:O	1:A:494:GLY:N	0.46	2.49	3	5
1:A:562:TRP:CE3	1:A:563:VAL:N	0.46	2.82	6	1
1:A:516:THR:C	1:A:518:LEU:N	0.46	2.67	10	1
1:A:578:GLY:C	1:A:580:GLN:N	0.46	2.68	3	3
1:A:577:GLN:H	1:A:577:GLN:CD	0.46	2.11	10	1
1:A:554:THR:HG22	1:A:555:ALA:N	0.46	2.25	3	1
1:A:581:VAL:CG1	1:A:582:ASP:N	0.46	2.78	3	1
1:A:538:CYS:O	1:A:539:ASN:OD1	0.46	2.34	8	1
1:A:499:GLY:C	1:A:501:LYS:H	0.46	2.14	7	5
1:A:579:GLU:OE1	1:A:579:GLU:N	0.46	2.49	3	1
1:A:532:HIS:ND1	1:A:532:HIS:O	0.46	2.49	6	1
1:A:595:MET:SD	1:A:595:MET:C	0.46	2.94	9	1
1:A:574:TYR:O	1:A:575:MET:C	0.46	2.54	2	1
1:A:532:HIS:O	1:A:535:VAL:HG12	0.46	2.11	4	1
1:A:502:ASN:ND2	1:A:534:PHE:CE1	0.45	2.83	4	1
1:A:503:ASP:O	1:A:506:LEU:CB	0.45	2.64	5	1
1:A:593:HIS:N	1:A:593:HIS:CD2	0.45	2.83	10	1
1:A:534:PHE:O	1:A:536:GLY:N	0.45	2.49	2	7
1:A:569:ALA:O	1:A:572:ILE:N	0.45	2.49	3	1
1:A:575:MET:C	1:A:575:MET:SD	0.45	2.94	5	1
1:A:555:ALA:O	1:A:557:GLU:N	0.45	2.49	8	3
1:A:602:LEU:C	1:A:602:LEU:HD23	0.45	2.32	1	1
1:A:596:THR:O	1:A:598:ALA:N	0.45	2.50	10	4
1:A:502:ASN:OD1	1:A:502:ASN:O	0.45	2.35	3	1
1:A:575:MET:O	1:A:575:MET:CG	0.45	2.64	3	1
1:A:586:GLU:OE2	1:A:586:GLU:O	0.45	2.35	6	1
1:A:572:ILE:CG2	1:A:573:LEU:N	0.45	2.80	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:552:GLU:O	1:A:553:ARG:O	0.45	2.35	2	3
1:A:556:ILE:O	1:A:556:ILE:HG23	0.45	2.12	3	1
1:A:500:SER:HB3	1:A:533:VAL:HG11	0.45	1.88	6	1
1:A:520:ILE:HD11	1:A:556:ILE:HG21	0.45	1.89	2	1
1:A:490:ILE:N	1:A:490:ILE:CD1	0.45	2.80	3	1
1:A:497:PHE:O	1:A:500:SER:OG	0.45	2.35	1	1
1:A:551:LEU:N	1:A:551:LEU:CD1	0.44	2.80	8	1
1:A:570:LEU:O	1:A:574:TYR:CE2	0.44	2.71	10	1
1:A:561:ASP:OD1	1:A:561:ASP:N	0.44	2.47	2	1
1:A:582:ASP:OD1	1:A:582:ASP:C	0.44	2.55	3	1
1:A:593:HIS:O	1:A:595:MET:N	0.44	2.50	9	1
1:A:506:LEU:HD13	1:A:506:LEU:O	0.44	2.13	5	1
1:A:491:LEU:HD12	1:A:491:LEU:N	0.44	2.28	8	1
1:A:550:PHE:CE2	1:A:566:LEU:HD21	0.44	2.48	4	1
1:A:497:PHE:C	1:A:497:PHE:CD1	0.44	2.87	7	1
1:A:493:LEU:O	1:A:496:ALA:HB3	0.44	2.13	8	1
1:A:592:GLU:H	1:A:592:GLU:CD	0.44	2.15	10	1
1:A:500:SER:OG	1:A:505:VAL:HG11	0.44	2.13	6	1
1:A:561:ASP:O	1:A:561:ASP:OD1	0.44	2.36	7	1
1:A:497:PHE:O	1:A:500:SER:N	0.44	2.50	10	1
1:A:596:THR:C	1:A:598:ALA:N	0.43	2.71	7	4
1:A:504:GLU:CD	1:A:504:GLU:H	0.43	2.16	4	1
1:A:518:LEU:CB	1:A:519:PRO:CD	0.43	2.96	5	1
1:A:595:MET:O	1:A:597:SER:N	0.43	2.51	1	2
1:A:503:ASP:N	1:A:503:ASP:OD1	0.43	2.51	6	2
1:A:539:ASN:ND2	1:A:541:ASP:CB	0.43	2.82	2	1
1:A:516:THR:O	1:A:517:ASP:OD1	0.43	2.37	9	1
1:A:594:PRO:O	1:A:596:THR:N	0.43	2.51	1	1
1:A:592:GLU:OE2	1:A:600:GLU:OE1	0.43	2.36	8	1
1:A:550:PHE:CE1	1:A:570:LEU:HD11	0.43	2.49	3	1
1:A:513:ALA:O	1:A:549:ASN:ND2	0.43	2.49	6	1
1:A:592:GLU:O	1:A:592:GLU:OE2	0.43	2.37	9	1
1:A:556:ILE:O	1:A:556:ILE:CG2	0.43	2.66	10	1
1:A:515:SER:C	1:A:517:ASP:H	0.43	2.17	3	3
1:A:590:ALA:HB3	1:A:591:ILE:HD12	0.43	1.91	8	1
1:A:581:VAL:HG13	1:A:582:ASP:N	0.43	2.29	3	1
1:A:506:LEU:HD13	1:A:534:PHE:CZ	0.43	2.49	6	1
1:A:514:ALA:O	1:A:549:ASN:OD1	0.43	2.37	6	1
1:A:490:ILE:O	1:A:494:GLY:CA	0.43	2.67	10	1
1:A:585:LEU:N	1:A:585:LEU:CD1	0.43	2.82	4	2
1:A:538:CYS:SG	1:A:539:ASN:N	0.43	2.92	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:539:ASN:OD1	1:A:540:GLY:N	0.42	2.52	1	1
1:A:600:GLU:O	1:A:600:GLU:OE2	0.42	2.37	3	1
1:A:532:HIS:O	1:A:535:VAL:CG1	0.42	2.67	5	1
1:A:600:GLU:O	1:A:604:GLY:N	0.42	2.52	9	1
1:A:563:VAL:HG13	1:A:564:ARG:N	0.42	2.29	1	2
1:A:501:LYS:C	1:A:502:ASN:OD1	0.42	2.58	2	1
1:A:534:PHE:C	1:A:536:GLY:H	0.42	2.18	2	4
1:A:541:ASP:O	1:A:544:THR:OG1	0.42	2.32	5	1
1:A:592:GLU:CD	1:A:592:GLU:N	0.42	2.72	10	1
1:A:500:SER:C	1:A:502:ASN:H	0.42	2.18	7	3
1:A:491:LEU:C	1:A:491:LEU:HD23	0.42	2.35	1	1
1:A:595:MET:C	1:A:597:SER:N	0.42	2.73	4	2
1:A:592:GLU:OE2	1:A:593:HIS:O	0.42	2.37	1	1
1:A:591:ILE:HG22	1:A:592:GLU:N	0.42	2.30	5	1
1:A:582:ASP:OD1	1:A:582:ASP:O	0.42	2.38	1	1
1:A:529:ALA:O	1:A:532:HIS:N	0.41	2.53	2	1
1:A:562:TRP:CD1	1:A:563:VAL:N	0.41	2.88	5	1
1:A:602:LEU:C	1:A:602:LEU:CD1	0.41	2.89	5	1
1:A:528:LEU:HD23	1:A:528:LEU:O	0.41	2.16	9	1
1:A:543:THR:O	1:A:547:MET:N	0.41	2.53	1	1
1:A:499:GLY:O	1:A:502:ASN:OD1	0.41	2.38	6	1
1:A:502:ASN:ND2	1:A:533:VAL:CG1	0.41	2.84	5	1
1:A:495:ILE:O	1:A:498:ALA:HB3	0.41	2.16	3	1
1:A:594:PRO:O	1:A:597:SER:CB	0.41	2.68	4	1
1:A:501:LYS:N	1:A:501:LYS:CD	0.41	2.84	7	1
1:A:531:ALA:O	1:A:533:VAL:N	0.40	2.54	1	1
1:A:539:ASN:OD1	1:A:541:ASP:HB2	0.40	2.15	6	1
1:A:578:GLY:O	1:A:582:ASP:OD2	0.40	2.39	5	1
1:A:539:ASN:OD1	1:A:541:ASP:N	0.40	2.55	7	1
1:A:491:LEU:N	1:A:491:LEU:CD1	0.40	2.85	8	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	118/131 (90%)	91±4 (77±4%)	18±4 (15±4%)	10±3 (8±3%)	2 14
All	All	1180/1310 (90%)	910 (77%)	175 (15%)	95 (8%)	2 14

All 35 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	553	ARG	10
1	A	555	ALA	7
1	A	500	SER	5
1	A	558	LEU	5
1	A	594	PRO	5
1	A	575	MET	5
1	A	517	ASP	4
1	A	607	ALA	4
1	A	498	ALA	4
1	A	497	PHE	3
1	A	561	ASP	3
1	A	516	THR	3
1	A	597	SER	3
1	A	576	GLY	3
1	A	503	ASP	2
1	A	515	SER	2
1	A	577	GLN	2
1	A	492	GLY	2
1	A	493	LEU	2
1	A	494	GLY	2
1	A	495	ILE	2
1	A	579	GLU	2
1	A	559	LYS	2
1	A	556	ILE	2
1	A	595	MET	1
1	A	596	THR	1
1	A	491	LEU	1
1	A	570	LEU	1
1	A	592	GLU	1
1	A	502	ASN	1
1	A	578	GLY	1
1	A	535	VAL	1
1	A	591	ILE	1
1	A	499	GLY	1
1	A	539	ASN	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	93/102 (91%)	81±3 (88±4%)	12±3 (12±4%)	8 50
All	All	930/1020 (91%)	814 (88%)	116 (12%)	8 50

All 44 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	518	LEU	10
1	A	556	ILE	10
1	A	497	PHE	7
1	A	530	LEU	6
1	A	501	LYS	6
1	A	502	ASN	5
1	A	546	ILE	5
1	A	550	PHE	4
1	A	558	LEU	4
1	A	509	LEU	4
1	A	541	ASP	3
1	A	562	TRP	3
1	A	532	HIS	3
1	A	602	LEU	3
1	A	503	ASP	3
1	A	557	GLU	3
1	A	545	SER	3
1	A	577	GLN	2
1	A	593	HIS	2
1	A	539	ASN	2
1	A	505	VAL	2
1	A	534	PHE	2
1	A	595	MET	2
1	A	500	SER	2
1	A	542	ILE	1
1	A	493	LEU	1
1	A	516	THR	1
1	A	522	THR	1
1	A	560	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	564	ARG	1
1	A	537	THR	1
1	A	547	MET	1
1	A	582	ASP	1
1	A	491	LEU	1
1	A	506	LEU	1
1	A	554	THR	1
1	A	566	LEU	1
1	A	544	THR	1
1	A	533	VAL	1
1	A	600	GLU	1
1	A	548	ASP	1
1	A	549	ASN	1
1	A	517	ASP	1
1	A	575	MET	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 66% for the well-defined parts and 62% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1035
Number of shifts mapped to atoms	1035
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

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	573	LEU	HD11	0.970	0.000	.

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	96	-0.46 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	92	0.23 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	63	0.80 ± 0.53	None needed (imprecise)

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 66%, i.e. 1004 atoms were assigned a chemical shift out of a possible 1532. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	318/594 (54%)	162/243 (67%)	93/236 (39%)	63/115 (55%)
Sidechain	666/863 (77%)	464/577 (80%)	202/273 (74%)	0/13 (0%)
Aromatic	20/75 (27%)	20/38 (53%)	0/34 (0%)	0/3 (0%)
Overall	1004/1532 (66%)	646/858 (75%)	295/543 (54%)	63/131 (48%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 1034 atoms were assigned a chemical shift out of a possible 1673. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	324/661 (49%)	165/271 (61%)	96/262 (37%)	63/128 (49%)
Sidechain	686/928 (74%)	478/620 (77%)	208/294 (71%)	0/14 (0%)
Aromatic	24/84 (29%)	24/42 (57%)	0/39 (0%)	0/3 (0%)
Overall	1034/1673 (62%)	667/933 (71%)	304/595 (51%)	63/145 (43%)

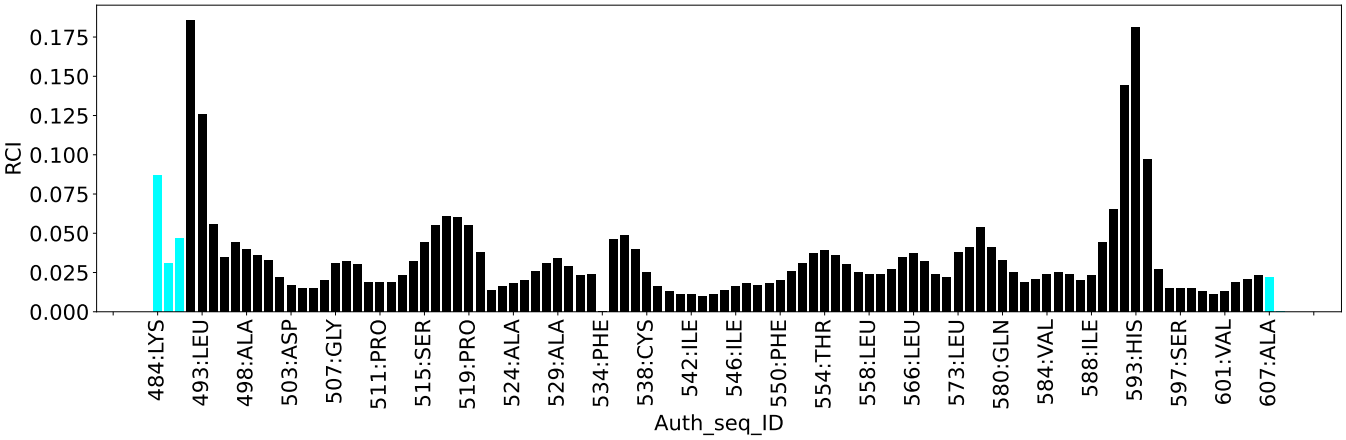
7.1.4 Statistically unusual chemical shifts (i)

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:


RCI
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
484:LYS
493:LEU
498:ALA
503:ASP
507:GLY
511:PRO
515:SER
519:PRO
524:ALA
529:ALA
534:PHE
538:CYS
542:ILE
546:ILE
550:PHE
554:THR
558:LEU
566:LEU
573:LEU
580:GLN
584:VAL
588:ILE
593:HIS
597:SER
601:VAL
607:ALA
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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

Description	Value
Total distance restraints	1360
Intra-residue (|i-j|=0)	576
Sequential (|i-j|=1)	178
Medium range (|i-j|>1 and |i-j|<5)	241
Long range (|i-j|≥5)	247
Inter-chain	0
Hydrogen bond restraints	118
Disulfide bond restraints	0
Total dihedral-angle restraints	182
Number of unmapped restraints	0
Number of restraints per residue	11.8
Number of long range restraints per residue[1]	1.9

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

8.2 Residual restraint violations (i)

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

8.2.1 Average number of distance violations per model (i)

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

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	0.2	0.18
0.2-0.5 (Medium)	0.1	0.44
>0.5 (Large)	1.6	1.7

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)	3.6	5.0
10.0-20.0 (Medium)	None	None
>20.0 (Large)	1.0	126.7

9 Distance violation analysis (i)

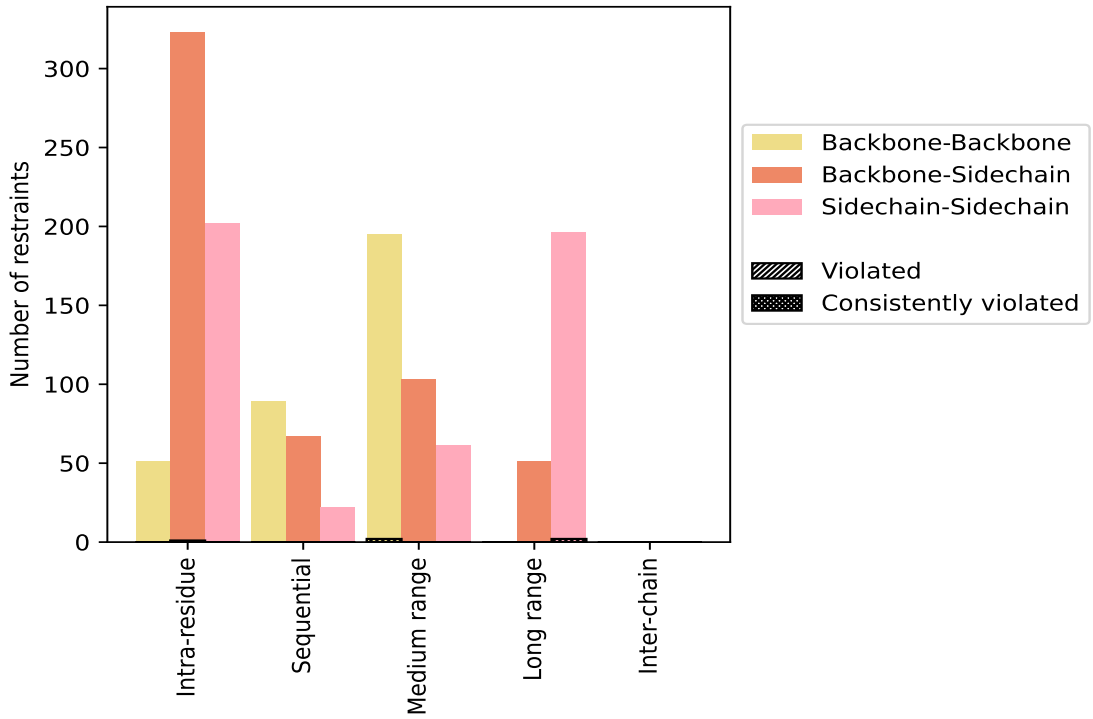
9.1 Summary of distance violations (i)

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

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	576	42.4	1	0.2	0.1	0	0.0	0.0
Backbone-Backbone	51	3.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	323	23.8	1	0.3	0.1	0	0.0	0.0
Sidechain-Sidechain	202	14.9	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	178	13.1	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	89	6.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	67	4.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	22	1.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	241	17.7	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	77	5.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	103	7.6	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	61	4.5	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	247	18.2	2	0.8	0.1	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	51	3.8	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	196	14.4	2	1.0	0.1	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	118	8.7	2	1.7	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1360	100.0	5	0.4	0.4	0	0.0	0.0
Backbone-Backbone	335	24.6	2	0.6	0.1	0	0.0	0.0
Backbone-Sidechain	544	40.0	1	0.2	0.1	0	0.0	0.0
Sidechain-Sidechain	481	35.4	2	0.4	0.1	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)

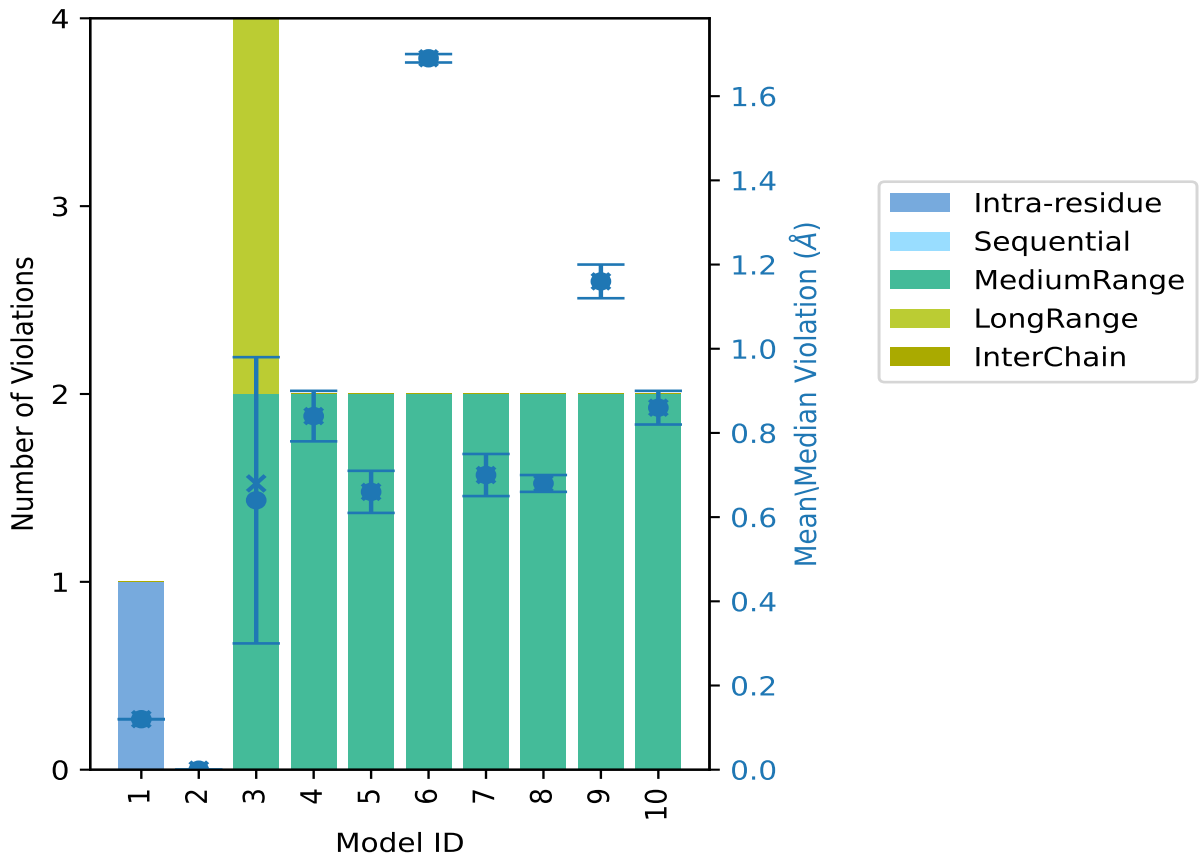
The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

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	1	0	0	0	0	1	0.12	0.12	0.0	0.12
2	0	0	0	0	0	0	0.0	0.0	0.0	0.0
3	0	0	2	2	0	4	0.64	1.01	0.34	0.68
4	0	0	2	0	0	2	0.84	0.9	0.06	0.84
5	0	0	2	0	0	2	0.66	0.71	0.05	0.66
6	0	0	2	0	0	2	1.69	1.7	0.01	1.69
7	0	0	2	0	0	2	0.7	0.75	0.05	0.7
8	0	0	2	0	0	2	0.68	0.71	0.02	0.68
9	0	0	2	0	0	2	1.16	1.21	0.04	1.16
10	0	0	2	0	0	2	0.86	0.9	0.04	0.86

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

[5]Inter-chain restraints, [6]Standard deviation

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



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

9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1239(IR:575, SQ:178, MR:241, LR:245, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
1	0	0	2	0	3	1	10.0
0	0	0	0	0	0	2	20.0
0	0	0	0	0	0	3	30.0
0	0	0	0	0	0	4	40.0

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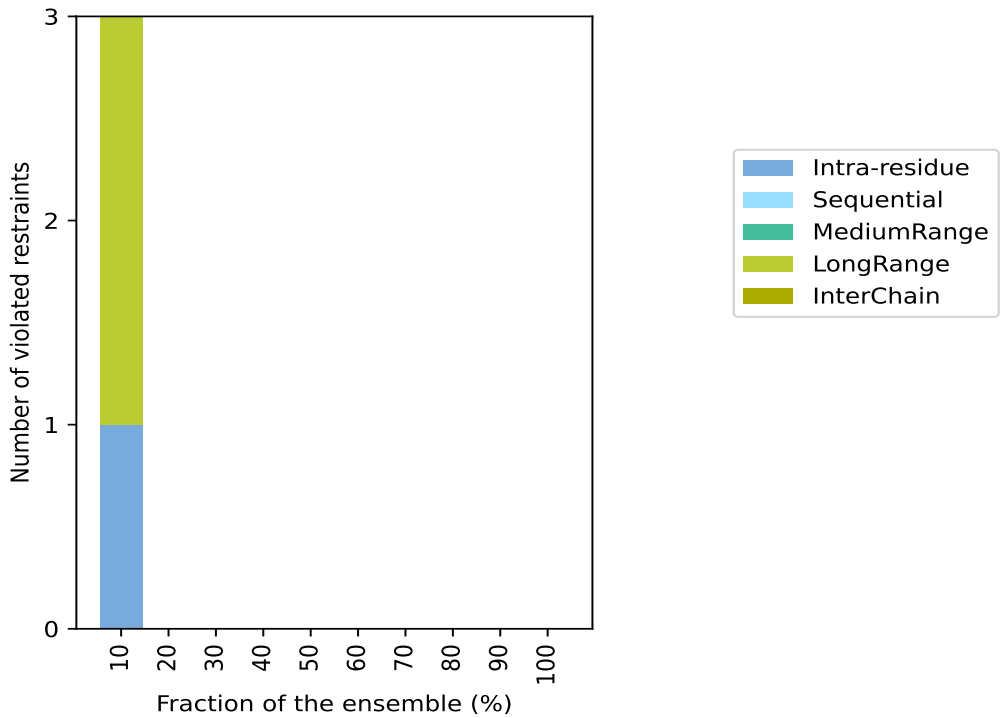
Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
0	0	0	0	0	0	5	50.0
0	0	0	0	0	0	6	60.0
0	0	0	0	0	0	7	70.0
0	0	0	0	0	0	8	80.0
0	0	0	0	0	0	9	90.0
0	0	0	0	0	0	10	100.0

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

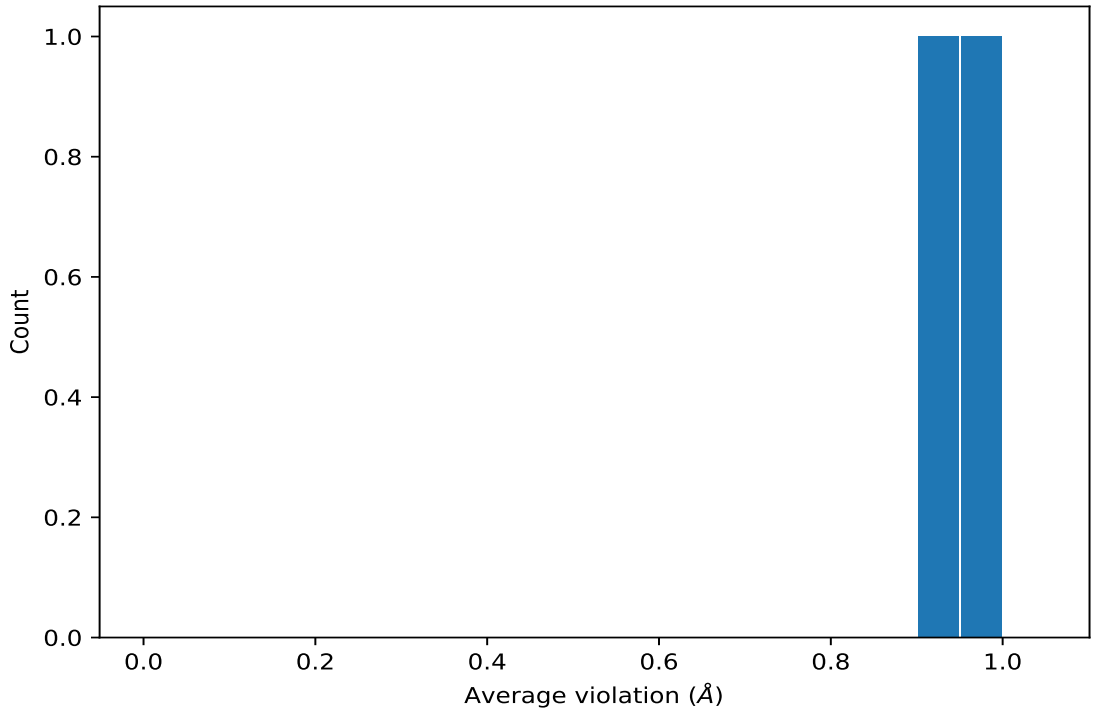
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

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

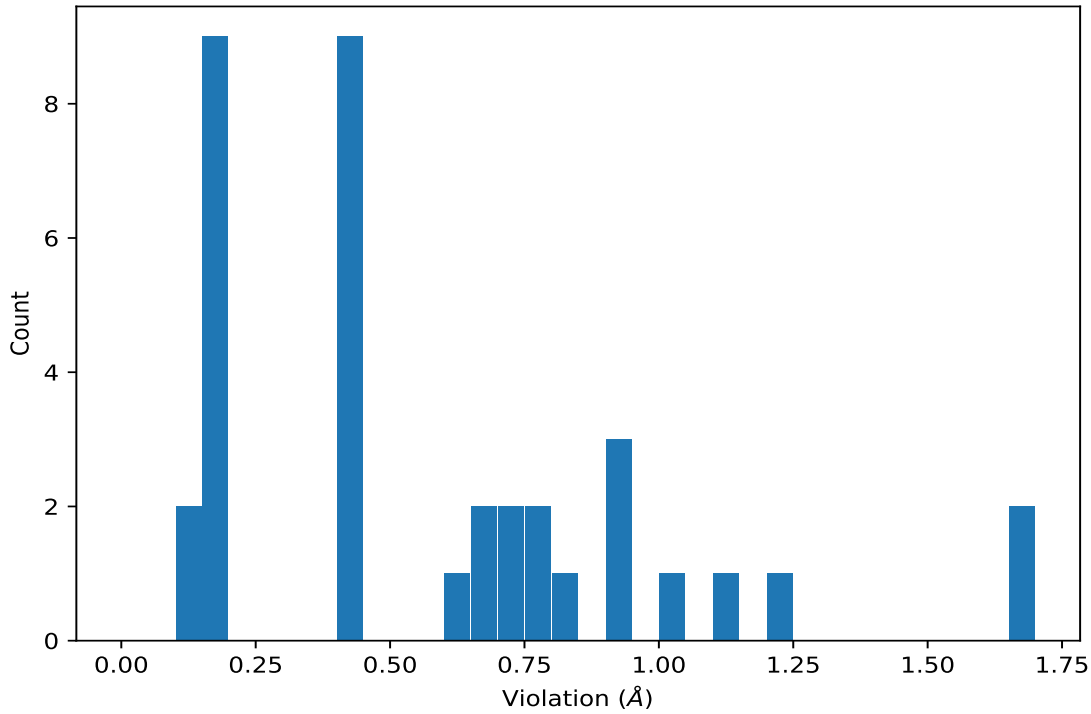
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	8	0.98	0.31	0.9
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	8	0.9	0.34	0.79

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	6	1.7
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	6	1.68
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	9	1.21
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	9	1.12
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	3	1.01
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	3	0.91
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	4	0.9
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	10	0.9
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	10	0.81
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	4	0.77
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	7	0.75
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	5	0.71
(2,2)	1:A:484:LYS:O	1:A:488:ALA:N	8	0.71
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	8	0.66
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	7	0.65
(2,1)	1:A:484:LYS:O	1:A:488:ALA:H	5	0.61

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,453)	1:A:490:ILE:HG21	1:A:526:ALA:HB1	3	0.44
(1,453)	1:A:490:ILE:HG21	1:A:526:ALA:HB2	3	0.44
(1,453)	1:A:490:ILE:HG21	1:A:526:ALA:HB3	3	0.44
(1,453)	1:A:490:ILE:HG22	1:A:526:ALA:HB1	3	0.44
(1,453)	1:A:490:ILE:HG22	1:A:526:ALA:HB2	3	0.44
(1,453)	1:A:490:ILE:HG22	1:A:526:ALA:HB3	3	0.44
(1,453)	1:A:490:ILE:HG23	1:A:526:ALA:HB1	3	0.44
(1,453)	1:A:490:ILE:HG23	1:A:526:ALA:HB2	3	0.44
(1,453)	1:A:490:ILE:HG23	1:A:526:ALA:HB3	3	0.44
(1,449)	1:A:490:ILE:HD11	1:A:509:LEU:HD11	3	0.18
(1,449)	1:A:490:ILE:HD11	1:A:509:LEU:HD12	3	0.18
(1,449)	1:A:490:ILE:HD11	1:A:509:LEU:HD13	3	0.18
(1,449)	1:A:490:ILE:HD12	1:A:509:LEU:HD11	3	0.18
(1,449)	1:A:490:ILE:HD12	1:A:509:LEU:HD12	3	0.18
(1,449)	1:A:490:ILE:HD12	1:A:509:LEU:HD13	3	0.18
(1,449)	1:A:490:ILE:HD13	1:A:509:LEU:HD11	3	0.18
(1,449)	1:A:490:ILE:HD13	1:A:509:LEU:HD12	3	0.18
(1,449)	1:A:490:ILE:HD13	1:A:509:LEU:HD13	3	0.18
(1,216)	1:A:542:ILE:HG12	1:A:542:ILE:H	1	0.12
(1,216)	1:A:542:ILE:HG13	1:A:542:ILE:H	1	0.12

10 Dihedral-angle violation analysis (i)

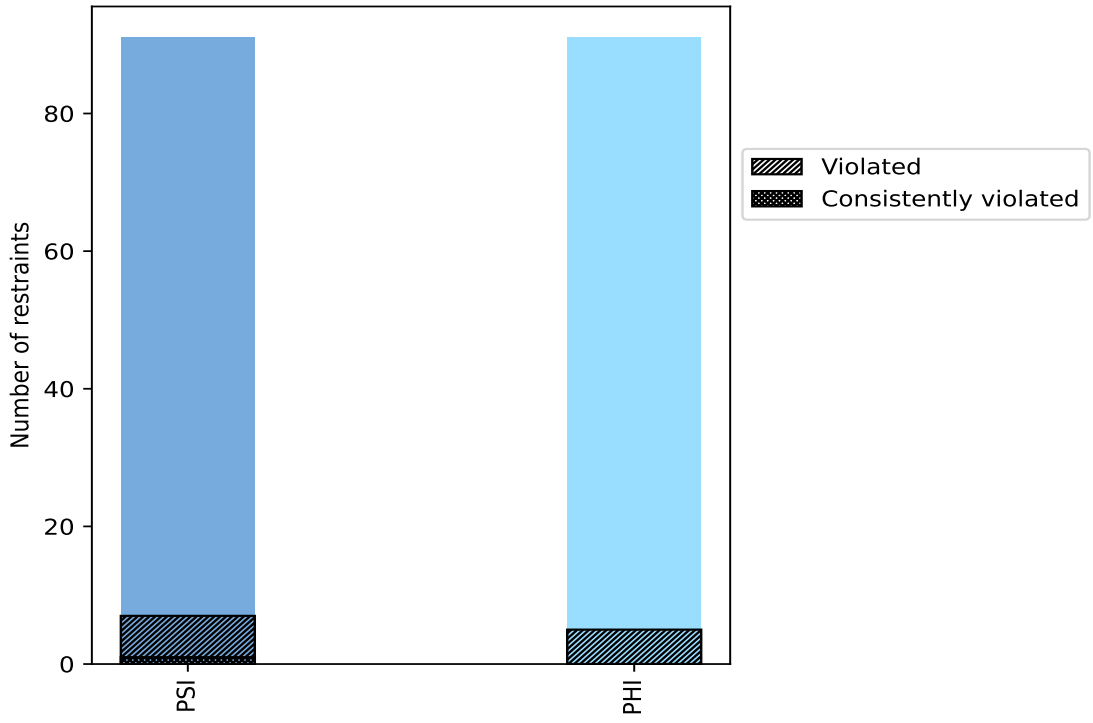
10.1 Summary of dihedral-angle violations (i)

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

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PSI	91	50.0	7	7.7	3.8	1	1.1	0.5
PHI	91	50.0	5	5.5	2.7	0	0.0	0.0
Total	182	100.0	12	6.6	6.6	1	0.5	0.5

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

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



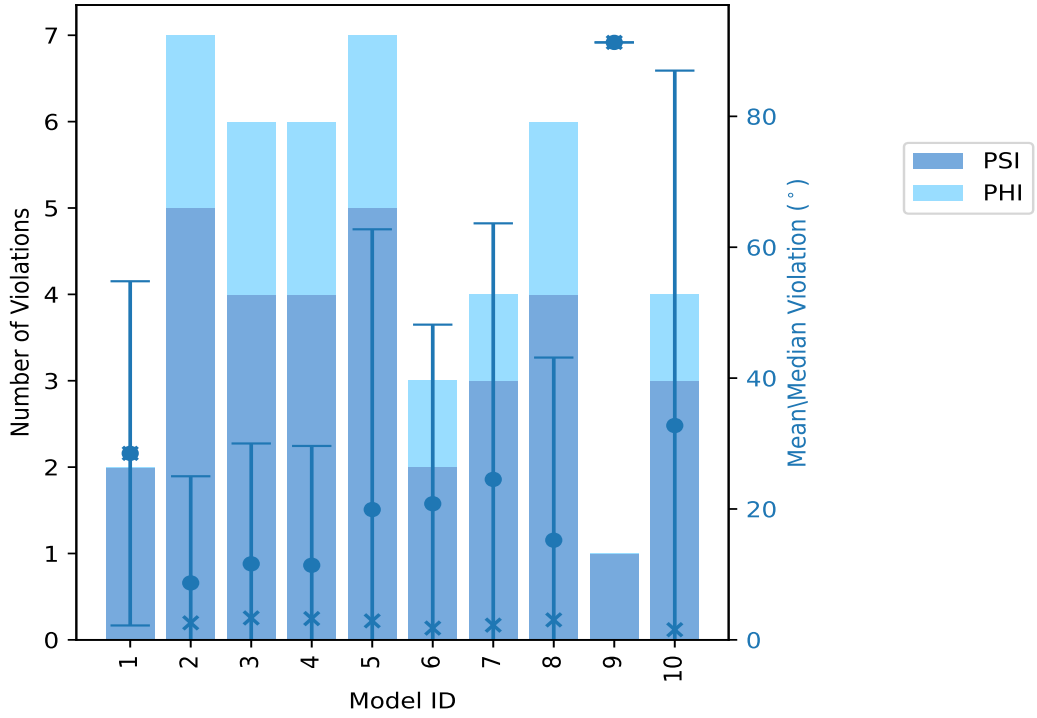
Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

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

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

Model ID	Number of violations			Mean (°)	Max (°)	SD (°)	Median (°)
	PSI	PHI	Total				
1	2	0	2	28.5	54.8	26.3	28.5
2	5	2	7	8.7	48.6	16.3	2.6
3	4	2	6	11.62	52.7	18.39	3.35
4	4	2	6	11.4	52.1	18.23	3.25
5	5	2	7	19.91	124.8	42.83	2.9
6	2	1	3	20.8	59.5	27.37	1.8
7	3	1	4	24.52	92.3	39.13	2.25
8	4	2	6	15.23	77.6	27.91	3.05
9	1	0	1	91.3	91.3	0.0	91.3
10	3	1	4	32.75	126.7	54.24	1.55

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

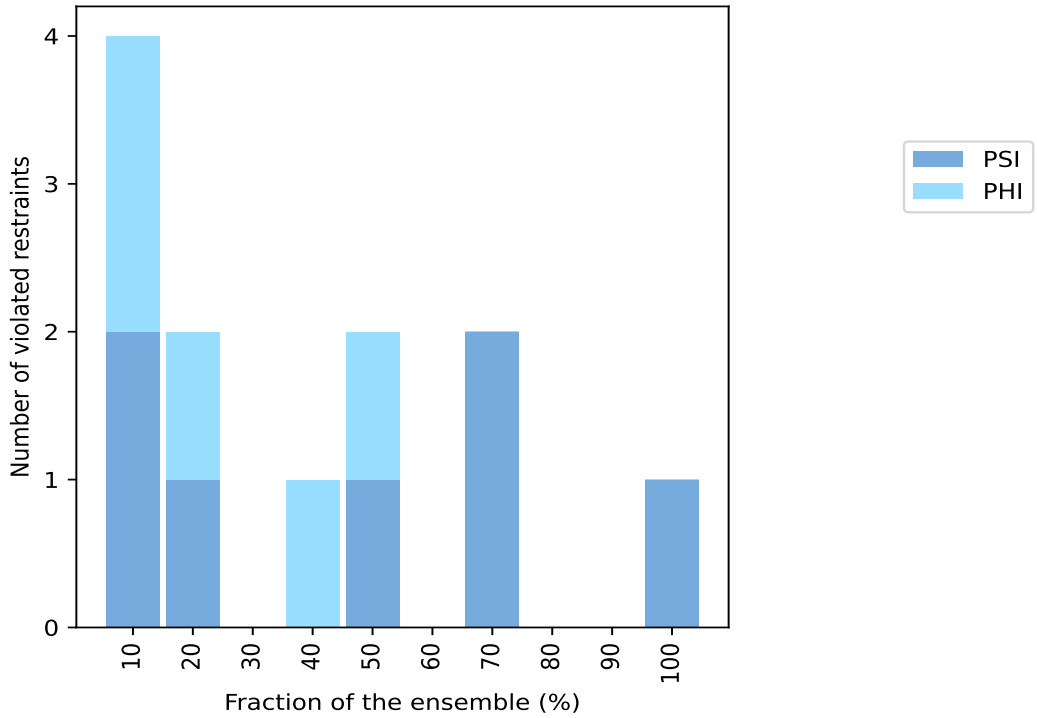
10.3 Dihedral-angle violation statistics for the ensemble (i)

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	
PSI	PHI	Total	Count[1]	%
2	2	4	1	10.0
1	1	2	2	20.0
0	0	0	3	30.0
0	1	1	4	40.0
1	1	2	5	50.0
0	0	0	6	60.0
2	0	2	7	70.0
0	0	0	8	80.0
0	0	0	9	90.0
1	0	1	10	100.0

[1] Number of models with violations

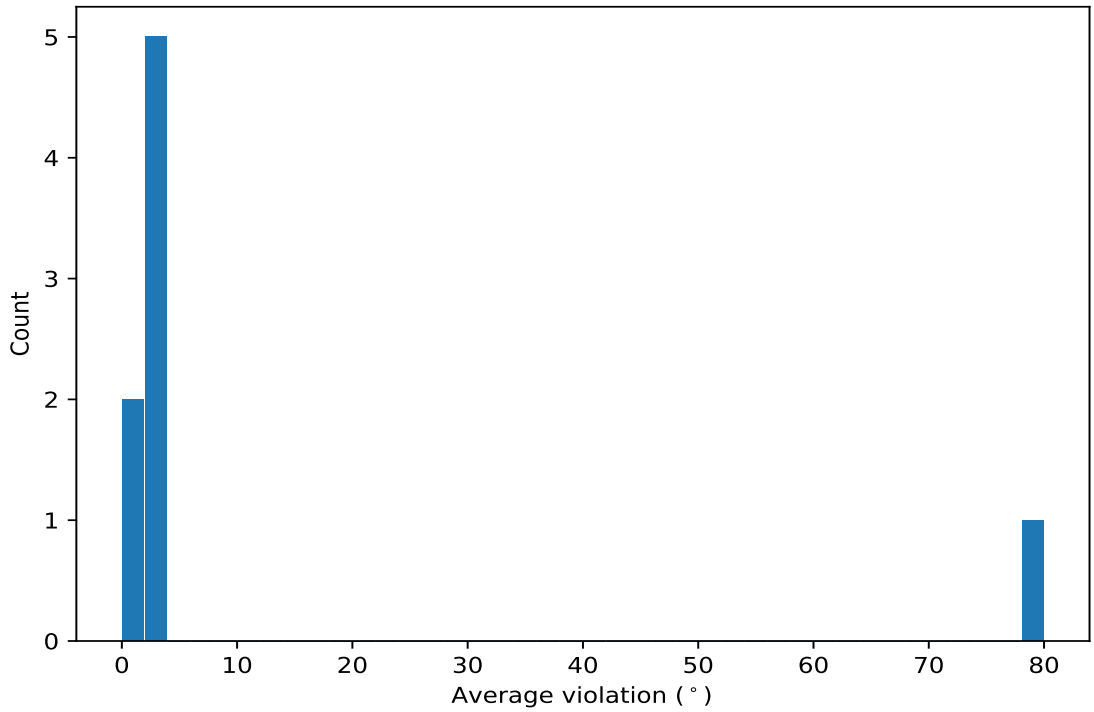
10.3.1 Bar graph : Dihedral-angle Violation statistics for the ensemble (i)



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

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

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



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

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

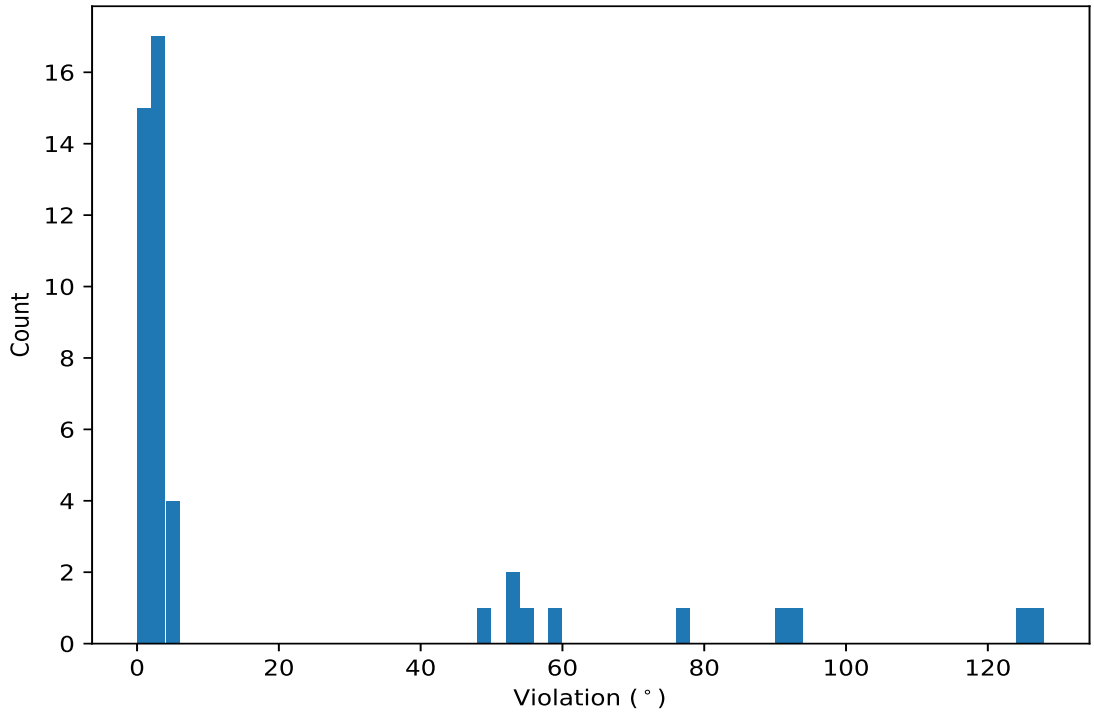
Key	Atom-1	Atom-2	Atom-3	Atom-4	Models[1]	Mean	SD[2]	Median
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	10	78.04	28.28	68.55
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	7	3.63	1.25	4.4
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	7	2.0	0.61	1.7
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	5	3.16	0.73	3.3
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	5	2.26	0.44	2.4
(1,13)	1:A:498:ALA:C	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	4	2.72	0.13	2.7
(1,27)	1:A:507:GLY:C	1:A:508:LEU:N	1:A:508:LEU:CA	1:A:508:LEU:C	2	1.4	0.3	1.4
(1,74)	1:A:534:PHE:N	1:A:534:PHE:CA	1:A:534:PHE:C	1:A:535:VAL:N	2	1.15	0.05	1.15

[1] Number of violated models, [2]Standard deviation, All angle values are in degree (°)

10.5 All violated dihedral-angle restraints (i)

10.5.1 Histogram : Distribution of violations (i)

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



10.5.2 Table: All violated dihedral-angle restraints (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint.

Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	10	126.7
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	5	124.8
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	7	92.3
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	9	91.3
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	8	77.6
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	6	59.5
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	1	54.8
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	3	52.7
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	4	52.1
(1,182)	1:A:606:CYS:N	1:A:606:CYS:CA	1:A:606:CYS:C	1:A:607:ALA:N	2	48.6
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	4	5.0
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	3	4.9
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	5	4.4
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	8	4.4

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Key	Atom-1	Atom-2	Atom-3	Atom-4	Model ID	Violation (°)
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	4	3.9
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	3	3.8
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	8	3.3
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	3	2.9
(1,13)	1:A:498:ALA:C	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	5	2.9
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	5	2.9
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	3	2.8
(1,13)	1:A:498:ALA:C	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	8	2.8
(1,10)	1:A:497:PHE:N	1:A:497:PHE:CA	1:A:497:PHE:C	1:A:498:ALA:N	7	2.8
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	2	2.7
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	2	2.7
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	2	2.6
(1,13)	1:A:498:ALA:C	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	3	2.6
(1,13)	1:A:498:ALA:C	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	4	2.6
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	4	2.4
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	4	2.4
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	1	2.2
(1,12)	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	1:A:499:GLY:N	2	1.9
(1,16)	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	1:A:501:LYS:N	6	1.8
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	5	1.8
(1,27)	1:A:507:GLY:C	1:A:508:LEU:N	1:A:508:LEU:CA	1:A:508:LEU:C	10	1.7
(1,15)	1:A:499:GLY:C	1:A:500:SER:N	1:A:500:SER:CA	1:A:500:SER:C	8	1.7
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	7	1.7
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	8	1.6
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	5	1.5
(1,18)	1:A:503:ASP:N	1:A:503:ASP:CA	1:A:503:ASP:C	1:A:504:GLU:N	10	1.4
(1,11)	1:A:497:PHE:C	1:A:498:ALA:N	1:A:498:ALA:CA	1:A:498:ALA:C	7	1.3
(1,75)	1:A:534:PHE:C	1:A:535:VAL:N	1:A:535:VAL:CA	1:A:535:VAL:C	2	1.2
(1,74)	1:A:534:PHE:N	1:A:534:PHE:CA	1:A:534:PHE:C	1:A:535:VAL:N	2	1.2
(1,14)	1:A:499:GLY:N	1:A:499:GLY:CA	1:A:499:GLY:C	1:A:500:SER:N	10	1.2
(1,74)	1:A:534:PHE:N	1:A:534:PHE:CA	1:A:534:PHE:C	1:A:535:VAL:N	5	1.1
(1,27)	1:A:507:GLY:C	1:A:508:LEU:N	1:A:508:LEU:CA	1:A:508:LEU:C	6	1.1