Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 10:25 PM EST

PDB ID	:	2JQE
BMRB ID	:	15275
Title	:	Soution Structure of Af54 M-domain
Authors	:	Ilangovan, U.; Hinck, A.P.; Zwieb, C.
Deposited on	:	2007-05-31

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

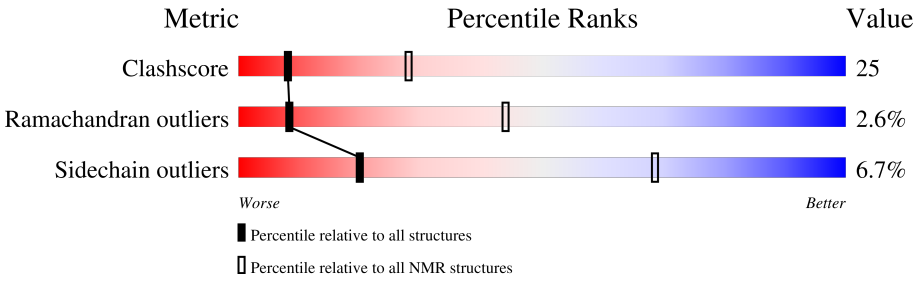
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 82%.

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	119	24% 24% · 45% ·

2 Ensemble composition and analysis

This entry contains 10 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:316-A:327, A:360-A:378, A:384-A:413 (61)	0.95	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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1033 atoms, of which 98 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Signal recognition 54 kDa protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	115	1033	597	98	157	169	12	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	GLY	-	expression tag	UNP O29633
A	308	SER	-	expression tag	UNP O29633
A	309	GLY	-	expression tag	UNP O29633
A	310	THR	-	expression tag	UNP O29633
A	311	MET	-	expression tag	UNP O29633
A	312	GLU	-	expression tag	UNP O29633

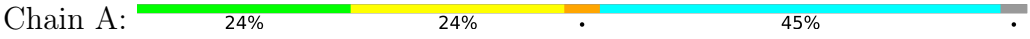
4 Residue-property plots

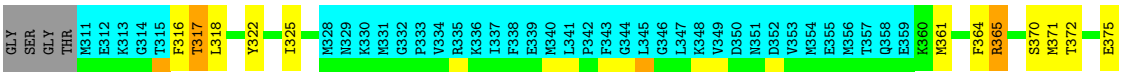
4.1 Average score per residue in the NMR ensemble

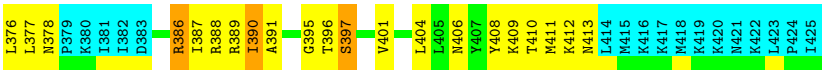
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for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

• Molecule 1: Signal recognition 54 kDa protein

Chain A:







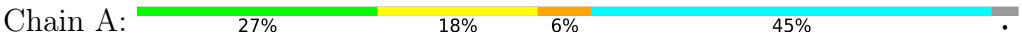
4.2 Scores per residue for each member of the ensemble

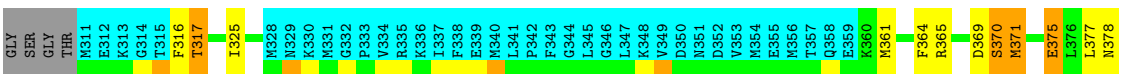
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Signal recognition 54 kDa protein

Chain A:

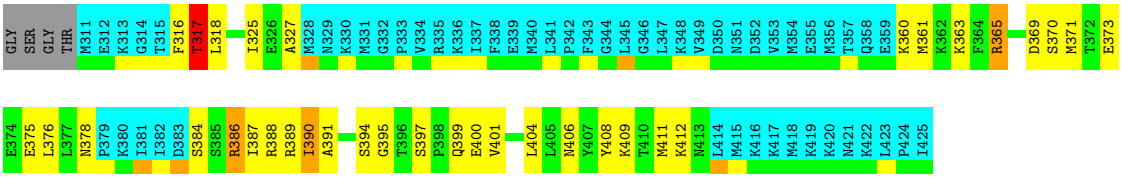




4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Signal recognition 54 kDa protein

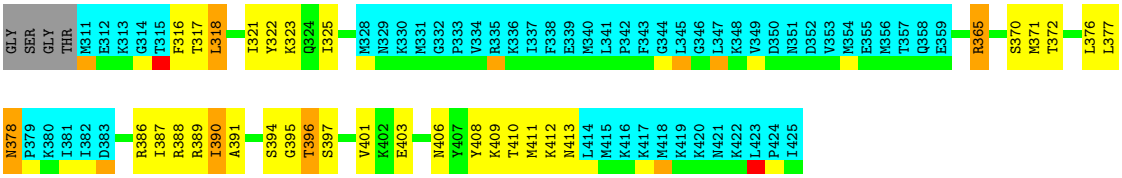
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Signal recognition 54 kDa protein

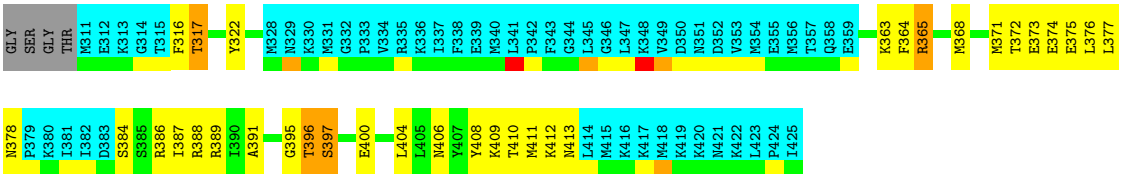
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Signal recognition 54 kDa protein

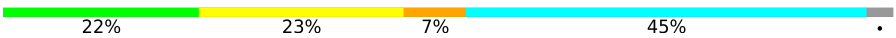
Chain A:

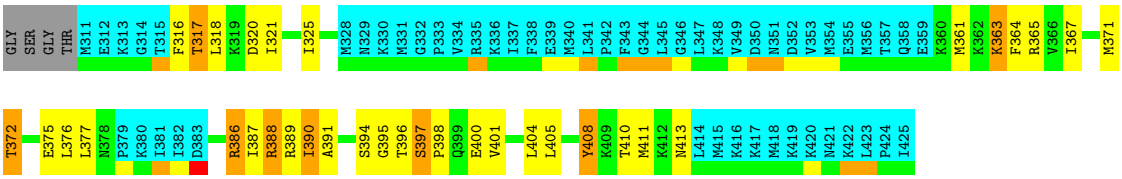


4.2.5 Score per residue for model 5

• Molecule 1: Signal recognition 54 kDa protein

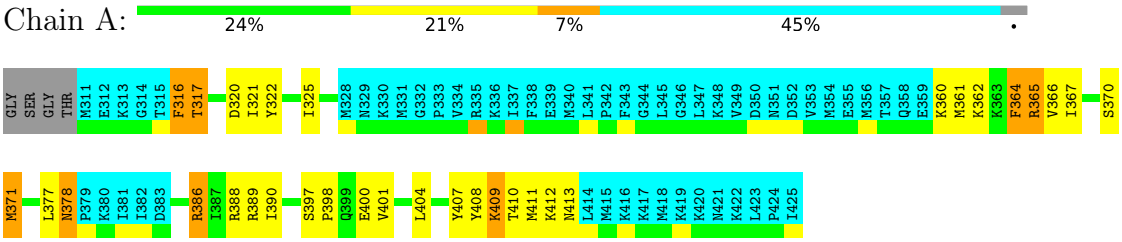
Chain A:





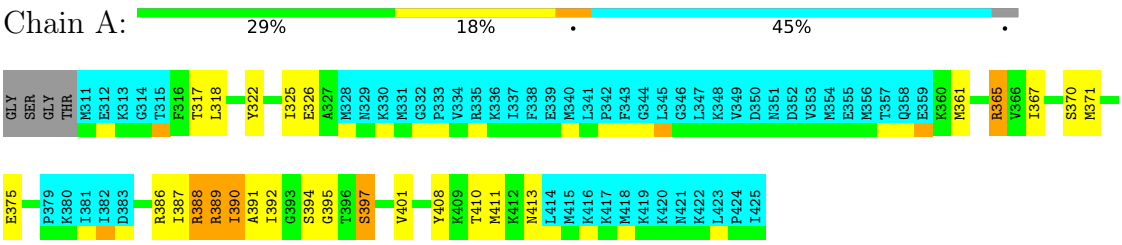
4.2.6 Score per residue for model 6

• Molecule 1: Signal recognition 54 kDa protein



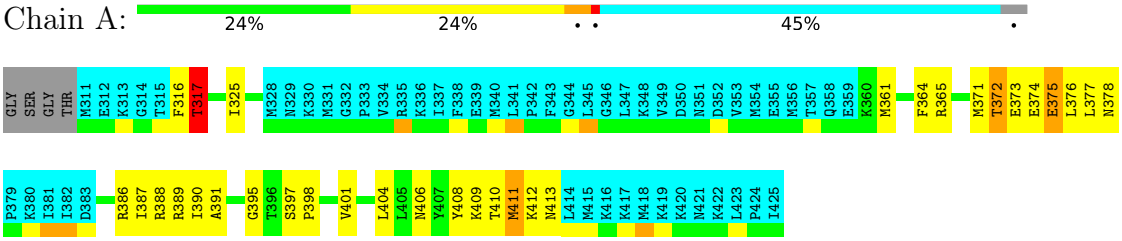
4.2.7 Score per residue for model 7

• Molecule 1: Signal recognition 54 kDa protein



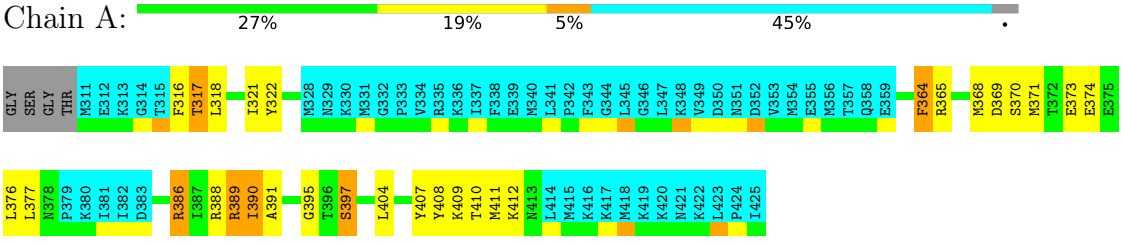
4.2.8 Score per residue for model 8

• Molecule 1: Signal recognition 54 kDa protein



4.2.9 Score per residue for model 9

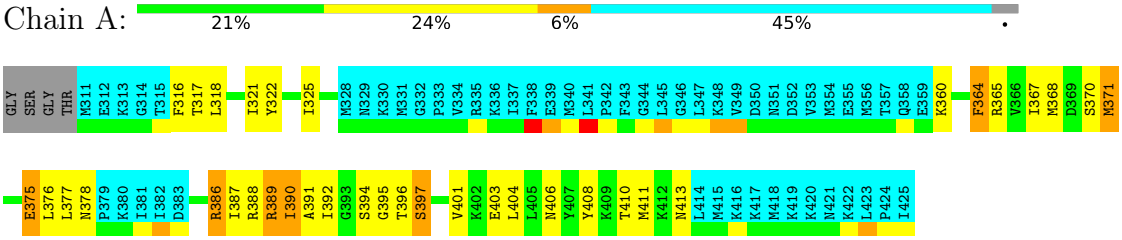
• Molecule 1: Signal recognition 54 kDa protein



4.2.10 Score per residue for model 10

• Molecule 1: Signal recognition 54 kDa protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 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	2.9.6
X-PLOR NIH	refinement	2.9.6

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	1084
Number of shifts mapped to atoms	562
Number of unparsed shifts	0
Number of shifts with mapping errors	522
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

6 Model quality

6.1 Standard geometry

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	3.9±0.3
All	All	0	39

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	365	ARG	Sidechain	10
1	A	388	ARG	Sidechain	10
1	A	389	ARG	Sidechain	10
1	A	386	ARG	Sidechain	9

6.2 Too-close contacts

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	503	54	530	26±3
All	All	5030	540	5300	255

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:321:ILE:HD13	1:A:408:TYR:CE1	0.92	2.00	10	2
1:A:387:ILE:HG23	1:A:401:VAL:CG1	0.85	2.01	10	1
1:A:318:LEU:O	1:A:321:ILE:HG22	0.83	1.72	5	1
1:A:317:THR:HG21	1:A:377:LEU:HD13	0.83	1.51	1	2
1:A:387:ILE:HG23	1:A:401:VAL:HG11	0.82	1.47	10	1
1:A:386:ARG:O	1:A:390:ILE:HD12	0.81	1.75	9	5
1:A:397:SER:O	1:A:401:VAL:HG23	0.81	1.75	10	1
1:A:364:PHE:CE2	1:A:404:LEU:HD11	0.79	2.12	5	2
1:A:372:THR:HG22	1:A:375:GLU:OE1	0.76	1.80	4	1
1:A:317:THR:C	1:A:318:LEU:HD12	0.69	2.08	2	2
1:A:367:ILE:HG21	1:A:401:VAL:HG12	0.69	1.64	6	1
1:A:325:ILE:HG23	1:A:361:MET:HG3	0.69	1.64	7	4
1:A:318:LEU:HD12	1:A:376:LEU:O	0.68	1.88	5	1
1:A:386:ARG:O	1:A:390:ILE:HD13	0.68	1.89	10	2
1:A:367:ILE:HD11	1:A:396:THR:HG21	0.68	1.63	10	1
1:A:372:THR:CG2	1:A:390:ILE:HD11	0.64	2.22	8	1
1:A:318:LEU:HD12	1:A:318:LEU:N	0.62	2.09	9	1
1:A:372:THR:HG22	1:A:390:ILE:HD11	0.61	1.71	8	1
1:A:364:PHE:CE1	1:A:404:LEU:HD22	0.61	2.31	4	1
1:A:364:PHE:CE1	1:A:404:LEU:HD11	0.60	2.31	6	1
1:A:387:ILE:HG13	1:A:401:VAL:HG11	0.59	1.74	7	1
1:A:373:GLU:HA	1:A:376:LEU:HD12	0.59	1.73	2	1
1:A:317:THR:HG21	1:A:377:LEU:CD1	0.58	2.26	1	1
1:A:389:ARG:HA	1:A:392:ILE:HD12	0.58	1.74	7	2
1:A:317:THR:CG2	1:A:377:LEU:HD13	0.57	2.27	1	1
1:A:374:GLU:HA	1:A:377:LEU:HD23	0.57	1.75	9	1
1:A:390:ILE:O	1:A:394:SER:N	0.57	2.38	7	3
1:A:398:PRO:O	1:A:401:VAL:HG22	0.57	2.00	5	3
1:A:391:ALA:HB1	1:A:397:SER:CA	0.56	2.30	3	8
1:A:410:THR:O	1:A:413:ASN:N	0.56	2.39	6	7
1:A:371:MET:CG	1:A:376:LEU:HD11	0.56	2.31	3	1
1:A:318:LEU:HD23	1:A:408:TYR:CZ	0.56	2.36	2	1
1:A:318:LEU:HD13	1:A:376:LEU:O	0.55	2.01	2	2
1:A:391:ALA:HB1	1:A:397:SER:HA	0.54	1.78	9	6
1:A:364:PHE:CZ	1:A:404:LEU:HD11	0.54	2.37	1	4
1:A:396:THR:O	1:A:397:SER:CB	0.54	2.54	4	1
1:A:396:THR:HG21	1:A:400:GLU:OE1	0.53	2.03	5	1
1:A:363:LYS:O	1:A:367:ILE:HD12	0.53	2.04	5	1
1:A:408:TYR:O	1:A:411:MET:HB2	0.52	2.05	2	1
1:A:364:PHE:CE1	1:A:404:LEU:CD1	0.52	2.93	1	1
1:A:316:PHE:CD2	1:A:316:PHE:O	0.52	2.63	9	1
1:A:410:THR:O	1:A:413:ASN:CB	0.51	2.59	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:408:TYR:O	1:A:411:MET:CB	0.51	2.58	10	9
1:A:407:TYR:O	1:A:410:THR:CB	0.51	2.58	6	2
1:A:387:ILE:HA	1:A:390:ILE:HD12	0.50	1.81	8	1
1:A:317:THR:HG21	1:A:377:LEU:HA	0.50	1.82	8	2
1:A:318:LEU:HD23	1:A:408:TYR:CE2	0.50	2.42	2	1
1:A:370:SER:O	1:A:371:MET:O	0.49	2.31	6	3
1:A:318:LEU:CB	1:A:376:LEU:HD22	0.49	2.38	10	1
1:A:391:ALA:O	1:A:395:GLY:N	0.49	2.46	4	7
1:A:400:GLU:O	1:A:404:LEU:HD23	0.49	2.07	6	2
1:A:409:LYS:O	1:A:412:LYS:N	0.48	2.44	6	6
1:A:316:PHE:CD2	1:A:317:THR:O	0.48	2.66	3	1
1:A:395:GLY:O	1:A:396:THR:HG23	0.48	2.07	3	1
1:A:387:ILE:HG23	1:A:401:VAL:CB	0.48	2.38	10	1
1:A:377:LEU:CD1	1:A:377:LEU:N	0.48	2.76	4	1
1:A:371:MET:O	1:A:372:THR:CB	0.48	2.60	5	1
1:A:360:LYS:O	1:A:364:PHE:CD1	0.48	2.66	6	1
1:A:406:ASN:O	1:A:409:LYS:CB	0.48	2.62	1	5
1:A:318:LEU:N	1:A:318:LEU:CD1	0.48	2.76	9	1
1:A:318:LEU:CD2	1:A:408:TYR:CE2	0.48	2.97	3	2
1:A:367:ILE:HD12	1:A:394:SER:CB	0.47	2.39	7	1
1:A:406:ASN:O	1:A:409:LYS:HB3	0.47	2.10	3	5
1:A:372:THR:O	1:A:376:LEU:HD12	0.47	2.10	8	1
1:A:371:MET:HG2	1:A:376:LEU:HD21	0.47	1.85	5	1
1:A:321:ILE:CD1	1:A:408:TYR:CE1	0.46	2.94	3	1
1:A:398:PRO:O	1:A:401:VAL:CG2	0.46	2.64	8	3
1:A:325:ILE:HG21	1:A:365:ARG:HB2	0.46	1.86	3	1
1:A:374:GLU:HA	1:A:377:LEU:CD2	0.46	2.40	9	1
1:A:325:ILE:HG23	1:A:361:MET:SD	0.46	2.51	2	1
1:A:387:ILE:HD11	1:A:401:VAL:CG1	0.46	2.41	2	1
1:A:370:SER:O	1:A:390:ILE:CG1	0.46	2.64	2	4
1:A:364:PHE:CE2	1:A:404:LEU:CD1	0.45	2.95	8	1
1:A:408:TYR:CD1	1:A:411:MET:SD	0.45	3.10	8	1
1:A:325:ILE:HG23	1:A:361:MET:CG	0.45	2.41	6	2
1:A:391:ALA:HA	1:A:395:GLY:O	0.45	2.11	10	1
1:A:317:THR:O	1:A:318:LEU:HD12	0.45	2.11	7	1
1:A:373:GLU:CG	1:A:374:GLU:N	0.45	2.80	9	2
1:A:325:ILE:HD12	1:A:364:PHE:CD1	0.45	2.47	10	1
1:A:322:TYR:CE2	1:A:365:ARG:HG3	0.45	2.47	6	1
1:A:367:ILE:HD12	1:A:394:SER:HB2	0.45	1.88	7	1
1:A:408:TYR:CZ	1:A:411:MET:SD	0.44	3.10	6	1
1:A:371:MET:SD	1:A:376:LEU:HD11	0.44	2.51	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:391:ALA:HB1	1:A:397:SER:N	0.44	2.27	3	1
1:A:316:PHE:O	1:A:317:THR:O	0.44	2.35	6	1
1:A:371:MET:HG2	1:A:376:LEU:HD11	0.44	1.89	3	2
1:A:396:THR:O	1:A:400:GLU:CG	0.44	2.66	4	1
1:A:325:ILE:HG21	1:A:364:PHE:HB3	0.44	1.89	8	1
1:A:371:MET:SD	1:A:376:LEU:HD21	0.44	2.52	2	2
1:A:326:GLU:OE2	1:A:365:ARG:NH2	0.44	2.51	7	1
1:A:403:GLU:O	1:A:406:ASN:HB3	0.44	2.13	3	3
1:A:363:LYS:CE	1:A:394:SER:O	0.44	2.66	2	1
1:A:399:GLN:CG	1:A:400:GLU:N	0.43	2.82	2	1
1:A:320:ASP:OD1	1:A:321:ILE:HG23	0.43	2.13	6	1
1:A:384:SER:O	1:A:387:ILE:HG22	0.43	2.12	4	1
1:A:367:ILE:HG22	1:A:371:MET:HG3	0.43	1.89	7	1
1:A:377:LEU:N	1:A:377:LEU:HD12	0.43	2.28	4	1
1:A:407:TYR:O	1:A:410:THR:N	0.43	2.50	6	1
1:A:410:THR:O	1:A:411:MET:C	0.43	2.57	7	3
1:A:409:LYS:O	1:A:412:LYS:CB	0.43	2.67	6	2
1:A:409:LYS:O	1:A:412:LYS:HB3	0.43	2.14	9	1
1:A:367:ILE:HG12	1:A:394:SER:CB	0.43	2.44	5	1
1:A:396:THR:CG2	1:A:400:GLU:OE1	0.43	2.66	5	1
1:A:378:ASN:OD1	1:A:378:ASN:N	0.43	2.52	10	1
1:A:369:ASP:OD1	1:A:370:SER:N	0.43	2.52	1	3
1:A:408:TYR:O	1:A:408:TYR:CD1	0.43	2.72	5	1
1:A:322:TYR:CD1	1:A:368:MET:HB3	0.43	2.48	10	1
1:A:387:ILE:HG13	1:A:388:ARG:N	0.43	2.29	5	1
1:A:372:THR:O	1:A:376:LEU:CD1	0.42	2.67	3	1
1:A:372:THR:HG23	1:A:375:GLU:H	0.42	1.73	4	1
1:A:401:VAL:O	1:A:405:LEU:CD1	0.42	2.67	5	1
1:A:408:TYR:O	1:A:411:MET:N	0.42	2.52	6	1
1:A:371:MET:CE	1:A:401:VAL:HG13	0.42	2.44	10	1
1:A:370:SER:O	1:A:390:ILE:HG12	0.42	2.15	2	1
1:A:322:TYR:O	1:A:325:ILE:HG22	0.42	2.14	3	1
1:A:371:MET:HE1	1:A:401:VAL:HG11	0.42	1.91	1	1
1:A:408:TYR:O	1:A:411:MET:HB3	0.42	2.14	3	5
1:A:396:THR:CB	1:A:400:GLU:OE1	0.42	2.67	5	1
1:A:362:LYS:O	1:A:366:VAL:HG23	0.42	2.14	6	1
1:A:408:TYR:CE1	1:A:411:MET:SD	0.42	3.13	8	1
1:A:320:ASP:OD1	1:A:321:ILE:N	0.42	2.52	5	1
1:A:376:LEU:HD12	1:A:376:LEU:H	0.42	1.75	8	1
1:A:376:LEU:HD12	1:A:376:LEU:N	0.42	2.28	9	1
1:A:391:ALA:O	1:A:395:GLY:O	0.42	2.37	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:390:ILE:HG22	1:A:391:ALA:N	0.42	2.29	10	1
1:A:375:GLU:OE2	1:A:386:ARG:CD	0.42	2.67	5	1
1:A:387:ILE:HG21	1:A:401:VAL:HB	0.42	1.92	3	1
1:A:375:GLU:OE2	1:A:386:ARG:NH2	0.42	2.52	10	1
1:A:325:ILE:HG23	1:A:361:MET:HB2	0.41	1.91	1	1
1:A:375:GLU:O	1:A:378:ASN:O	0.41	2.38	2	1
1:A:391:ALA:CB	1:A:397:SER:CA	0.41	2.97	3	2
1:A:322:TYR:CE1	1:A:365:ARG:HA	0.41	2.50	4	1
1:A:322:TYR:CE1	1:A:368:MET:HB2	0.41	2.51	4	1
1:A:363:LYS:HB3	1:A:396:THR:HG23	0.41	1.91	4	1
1:A:372:THR:CG2	1:A:375:GLU:HG3	0.41	2.46	4	1
1:A:386:ARG:O	1:A:390:ILE:CD1	0.41	2.66	10	1
1:A:378:ASN:O	1:A:378:ASN:OD1	0.41	2.39	8	1
1:A:408:TYR:CD2	1:A:411:MET:SD	0.41	3.13	1	1
1:A:363:LYS:NZ	1:A:394:SER:O	0.41	2.52	2	1
1:A:391:ALA:CA	1:A:395:GLY:O	0.41	2.69	7	2
1:A:371:MET:CG	1:A:375:GLU:OE2	0.41	2.69	1	1
1:A:370:SER:OG	1:A:390:ILE:HA	0.41	2.16	3	1
1:A:387:ILE:HG23	1:A:388:ARG:N	0.41	2.30	7	1
1:A:318:LEU:HB3	1:A:321:ILE:HD12	0.41	1.93	9	1
1:A:360:LYS:HE2	1:A:404:LEU:HD11	0.40	1.91	2	1
1:A:367:ILE:N	1:A:367:ILE:HD13	0.40	2.31	7	1
1:A:322:TYR:CD1	1:A:368:MET:HG2	0.40	2.51	9	1
1:A:318:LEU:HB2	1:A:376:LEU:HD22	0.40	1.93	10	1
1:A:373:GLU:HG3	1:A:374:GLU:N	0.40	2.31	4	1
1:A:320:ASP:OD1	1:A:320:ASP:N	0.40	2.54	6	1
1:A:407:TYR:O	1:A:410:THR:HB	0.40	2.16	6	1
1:A:374:GLU:O	1:A:377:LEU:CD2	0.40	2.69	9	1
1:A:370:SER:O	1:A:390:ILE:HG13	0.40	2.15	3	1
1:A:408:TYR:O	1:A:409:LYS:C	0.40	2.59	8	1
1:A:375:GLU:HB2	1:A:386:ARG:HD2	0.40	1.93	10	1
1:A:316:PHE:O	1:A:317:THR:OG1	0.40	2.39	3	1
1:A:367:ILE:HD11	1:A:396:THR:CG2	0.40	2.41	10	1
1:A:387:ILE:CG2	1:A:401:VAL:HB	0.40	2.46	3	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	61/119 (51%)	55±1 (90±2%)	4±1 (7±2%)	2±1 (3±2%)	8 44
All	All	610/1190 (51%)	550 (90%)	44 (7%)	16 (3%)	8 44

All 7 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	317	THR	7
1	A	371	MET	3
1	A	316	PHE	2
1	A	370	SER	1
1	A	396	THR	1
1	A	397	SER	1
1	A	372	THR	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	57/109 (52%)	53±1 (93±2%)	4±1 (7±2%)	20 68
All	All	570/1090 (52%)	532 (93%)	38 (7%)	20 68

All 18 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	390	ILE	7
1	A	397	SER	6
1	A	317	THR	5
1	A	375	GLU	3
1	A	364	PHE	3
1	A	378	ASN	2
1	A	405	LEU	1
1	A	318	LEU	1
1	A	323	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	396	THR	1
1	A	363	LYS	1
1	A	408	TYR	1
1	A	409	LYS	1
1	A	322	TYR	1
1	A	372	THR	1
1	A	411	MET	1
1	A	389	ARG	1
1	A	377	LEU	1

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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1084
Number of shifts mapped to atoms	562
Number of unparsed shifts	0
Number of shifts with mapping errors	522
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

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

- No matching atom found in the structure. All 522 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	311	MET	HA	4.47	0.03	1
1	A	312	GLU	H	8.41	0.03	1
1	A	312	GLU	HA	4.33	0.03	1
1	A	312	GLU	HB2	1.79	0.03	2
1	A	312	GLU	HB3	1.84	0.03	2
1	A	313	LYS	H	8.42	0.03	1
1	A	313	LYS	HA	4.29	0.03	1
1	A	313	LYS	HB2	1.9	0.03	2
1	A	313	LYS	HB3	1.9	0.03	2
1	A	313	LYS	HE2	3.0	0.03	2
1	A	313	LYS	HE3	3.0	0.03	2
1	A	314	GLY	H	8.54	0.03	1
1	A	314	GLY	HA2	4.0	0.03	2
1	A	314	GLY	HA3	4.03	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	315	THR	H	7.97	0.03	1
1	A	315	THR	HA	4.42	0.03	1
1	A	315	THR	HB	4.19	0.03	1
1	A	316	PHE	H	8.49	0.03	1
1	A	316	PHE	HA	5.05	0.03	1
1	A	316	PHE	HB2	2.98	0.03	2
1	A	316	PHE	HB3	3.1	0.03	2
1	A	316	PHE	HD1	6.74	0.03	3
1	A	316	PHE	HD2	6.73	0.03	3
1	A	316	PHE	HE1	7.13	0.03	3
1	A	316	PHE	HE2	7.13	0.03	3
1	A	317	THR	H	9.77	0.03	1
1	A	317	THR	HA	4.73	0.03	1
1	A	317	THR	HB	5.01	0.03	1
1	A	318	LEU	H	7.8	0.03	1
1	A	318	LEU	HA	3.95	0.03	1
1	A	318	LEU	HB2	2.03	0.03	2
1	A	318	LEU	HB3	1.61	0.03	2
1	A	318	LEU	HD11	0.7	0.03	2
1	A	318	LEU	HD12	0.7	0.03	2
1	A	318	LEU	HD13	0.7	0.03	2
1	A	318	LEU	HD21	0.69	0.03	2
1	A	318	LEU	HD22	0.69	0.03	2
1	A	318	LEU	HD23	0.69	0.03	2
1	A	318	LEU	HG	1.0	0.03	1
1	A	319	LYS	H	7.95	0.03	1
1	A	319	LYS	HA	3.88	0.03	1
1	A	319	LYS	HB2	1.55	0.03	2
1	A	319	LYS	HB3	1.74	0.03	2
1	A	319	LYS	HE2	2.89	0.03	2
1	A	319	LYS	HE3	2.89	0.03	2
1	A	320	ASP	H	7.17	0.03	1
1	A	320	ASP	HA	4.35	0.03	1
1	A	320	ASP	HB2	2.49	0.03	2
1	A	320	ASP	HB3	2.42	0.03	2
1	A	321	ILE	H	7.0	0.03	1
1	A	321	ILE	HA	3.97	0.03	1
1	A	321	ILE	HB	2.36	0.03	1
1	A	321	ILE	HD11	1.13	0.03	1
1	A	321	ILE	HD12	1.13	0.03	1
1	A	321	ILE	HD13	1.13	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	322	TYR	HD1	7.15	0.03	3
1	A	322	TYR	HD2	7.15	0.03	3
1	A	322	TYR	HE1	6.83	0.03	3
1	A	322	TYR	HE2	6.83	0.03	3
1	A	323	LYS	H	8.07	0.03	1
1	A	323	LYS	HA	4.22	0.03	1
1	A	323	LYS	HB2	1.99	0.03	2
1	A	323	LYS	HB3	1.99	0.03	2
1	A	323	LYS	HE2	2.83	0.03	1
1	A	324	GLN	H	7.77	0.03	1
1	A	324	GLN	HA	4.13	0.03	1
1	A	324	GLN	HB2	2.31	0.03	2
1	A	324	GLN	HB3	2.31	0.03	2
1	A	325	ILE	H	8.25	0.03	1
1	A	325	ILE	HA	3.72	0.03	1
1	A	325	ILE	HB	1.87	0.03	1
1	A	325	ILE	HD11	0.86	0.03	1
1	A	325	ILE	HD12	0.86	0.03	1
1	A	325	ILE	HD13	0.86	0.03	1
1	A	326	GLU	H	8.19	0.03	1
1	A	326	GLU	HA	3.97	0.03	1
1	A	326	GLU	HB2	2.05	0.03	2
1	A	326	GLU	HB3	2.05	0.03	2
1	A	326	GLU	HG2	2.35	0.03	1
1	A	326	GLU	HG3	2.64	0.03	1
1	A	327	ALA	H	7.81	0.03	1
1	A	327	ALA	HA	4.16	0.03	1
1	A	327	ALA	HB1	1.52	0.03	1
1	A	327	ALA	HB2	1.52	0.03	1
1	A	327	ALA	HB3	1.52	0.03	1
1	A	342	PRO	HA	4.53	0.03	1
1	A	342	PRO	HB2	2.15	0.03	1
1	A	342	PRO	HB3	2.35	0.03	1
1	A	342	PRO	HD2	3.56	0.03	1
1	A	342	PRO	HD3	3.46	0.03	1
1	A	342	PRO	HG2	1.9	0.03	1
1	A	342	PRO	HG3	1.85	0.03	1
1	A	343	PHE	H	7.95	0.03	1
1	A	343	PHE	HA	3.99	0.03	1
1	A	343	PHE	HB2	1.82	0.03	2
1	A	343	PHE	HB3	1.82	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	344	GLY	HA2	3.93	0.03	2
1	A	344	GLY	HA3	3.93	0.03	2
1	A	345	LEU	H	8.06	0.03	1
1	A	345	LEU	HA	4.32	0.03	1
1	A	345	LEU	HB2	1.51	0.03	1
1	A	345	LEU	HD21	0.83	0.03	2
1	A	345	LEU	HD11	0.83	0.03	2
1	A	345	LEU	HD12	0.83	0.03	2
1	A	345	LEU	HD13	0.83	0.03	2
1	A	345	LEU	HD22	0.83	0.03	2
1	A	345	LEU	HD23	0.83	0.03	2
1	A	348	LYS	H	7.98	0.03	1
1	A	348	LYS	HA	4.26	0.03	1
1	A	348	LYS	HB2	1.8	0.03	2
1	A	348	LYS	HB3	1.8	0.03	2
1	A	348	LYS	HG2	1.42	0.03	2
1	A	348	LYS	HG3	1.42	0.03	2
1	A	349	VAL	H	8.18	0.03	1
1	A	349	VAL	HA	4.12	0.03	1
1	A	349	VAL	HB	2.0	0.03	1
1	A	350	ASP	H	8.34	0.03	1
1	A	350	ASP	HA	4.58	0.03	1
1	A	350	ASP	HB2	2.69	0.03	2
1	A	350	ASP	HB3	2.69	0.03	2
1	A	351	ASN	H	8.36	0.03	1
1	A	351	ASN	HA	4.76	0.03	1
1	A	351	ASN	HB2	2.76	0.03	2
1	A	351	ASN	HB3	3.24	0.03	2
1	A	352	ASP	H	8.4	0.03	1
1	A	352	ASP	HA	4.54	0.03	1
1	A	357	THR	HA	4.33	0.03	1
1	A	357	THR	HB	4.21	0.03	1
1	A	358	GLN	HA	3.93	0.03	1
1	A	358	GLN	HB2	2.07	0.03	2
1	A	358	GLN	HB3	2.07	0.03	2
1	A	358	GLN	HE21	7.5	0.03	1
1	A	358	GLN	HE22	6.9	0.03	1
1	A	358	GLN	HG2	2.39	0.03	2
1	A	358	GLN	HG3	2.39	0.03	2
1	A	360	LYS	HA	3.63	0.03	1
1	A	360	LYS	HB2	1.27	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	360	LYS	HB3	1.27	0.03	2
1	A	360	LYS	HD2	1.57	0.03	2
1	A	360	LYS	HD3	1.57	0.03	2
1	A	360	LYS	HE2	2.86	0.03	1
1	A	360	LYS	HG2	1.47	0.03	2
1	A	360	LYS	HG3	1.47	0.03	2
1	A	361	MET	H	7.91	0.03	1
1	A	361	MET	HA	3.65	0.03	1
1	A	361	MET	HB2	1.89	0.03	2
1	A	361	MET	HB3	1.89	0.03	2
1	A	361	MET	HE1	2.09	0.03	1
1	A	361	MET	HE2	2.09	0.03	1
1	A	361	MET	HE3	2.09	0.03	1
1	A	361	MET	HG2	2.52	0.03	1
1	A	361	MET	HG3	2.33	0.03	1
1	A	362	LYS	H	7.67	0.03	1
1	A	362	LYS	HA	3.91	0.03	1
1	A	362	LYS	HB2	1.87	0.03	2
1	A	362	LYS	HB3	1.87	0.03	2
1	A	362	LYS	HD2	1.63	0.03	2
1	A	362	LYS	HD3	1.63	0.03	2
1	A	362	LYS	HE2	2.91	0.03	2
1	A	362	LYS	HE3	2.91	0.03	2
1	A	363	LYS	H	7.61	0.03	1
1	A	363	LYS	HA	4.04	0.03	1
1	A	363	LYS	HB2	1.79	0.03	2
1	A	363	LYS	HB3	1.93	0.03	2
1	A	363	LYS	HE2	2.96	0.03	2
1	A	363	LYS	HE3	2.96	0.03	2
1	A	364	PHE	H	8.71	0.03	1
1	A	364	PHE	HA	4.47	0.03	1
1	A	364	PHE	HB2	2.88	0.03	2
1	A	364	PHE	HB3	3.45	0.03	2
1	A	365	ARG	H	7.85	0.03	1
1	A	365	ARG	HA	3.75	0.03	1
1	A	365	ARG	HB2	1.74	0.03	1
1	A	365	ARG	HB3	2.02	0.03	1
1	A	365	ARG	HD2	2.99	0.03	2
1	A	365	ARG	HD3	2.99	0.03	2
1	A	365	ARG	HG2	1.43	0.03	1
1	A	365	ARG	HG3	1.43	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	366	VAL	H	7.71	0.03	1
1	A	366	VAL	HA	3.92	0.03	1
1	A	366	VAL	HB	2.28	0.03	1
1	A	367	ILE	H	8.29	0.03	1
1	A	367	ILE	HA	3.53	0.03	1
1	A	367	ILE	HB	2.0	0.03	1
1	A	367	ILE	HD11	0.79	0.03	1
1	A	367	ILE	HD12	0.79	0.03	1
1	A	367	ILE	HD13	0.79	0.03	1
1	A	368	MET	H	8.03	0.03	1
1	A	368	MET	HA	4.22	0.03	1
1	A	368	MET	HB2	2.02	0.03	2
1	A	368	MET	HB3	2.49	0.03	2
1	A	369	ASP	H	8.47	0.03	1
1	A	369	ASP	HA	4.64	0.03	1
1	A	369	ASP	HB2	2.81	0.03	2
1	A	369	ASP	HB3	2.93	0.03	2
1	A	370	SER	H	7.64	0.03	1
1	A	370	SER	HA	4.63	0.03	1
1	A	370	SER	HB2	3.92	0.03	2
1	A	370	SER	HB3	4.13	0.03	2
1	A	371	MET	H	7.5	0.03	1
1	A	371	MET	HA	4.37	0.03	1
1	A	371	MET	HB2	2.15	0.03	2
1	A	371	MET	HB3	2.1	0.03	2
1	A	371	MET	HE1	1.77	0.03	1
1	A	371	MET	HE2	1.77	0.03	1
1	A	371	MET	HE3	1.77	0.03	1
1	A	372	THR	H	9.07	0.03	1
1	A	372	THR	HA	4.41	0.03	1
1	A	372	THR	HB	4.63	0.03	1
1	A	373	GLU	H	8.67	0.03	1
1	A	373	GLU	HA	3.88	0.03	1
1	A	373	GLU	HB2	1.92	0.03	2
1	A	373	GLU	HB3	1.99	0.03	2
1	A	373	GLU	HG2	2.23	0.03	2
1	A	373	GLU	HG3	2.23	0.03	2
1	A	374	GLU	H	8.05	0.03	1
1	A	374	GLU	HA	3.84	0.03	1
1	A	374	GLU	HB2	1.84	0.03	2
1	A	374	GLU	HB3	1.96	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	375	GLU	H	7.25	0.03	1
1	A	375	GLU	HA	3.51	0.03	1
1	A	375	GLU	HB2	1.64	0.03	2
1	A	375	GLU	HB3	2.37	0.03	2
1	A	375	GLU	HG2	2.25	0.03	2
1	A	375	GLU	HG3	2.38	0.03	2
1	A	376	LEU	H	7.73	0.03	1
1	A	376	LEU	HA	3.91	0.03	1
1	A	376	LEU	HB2	1.87	0.03	2
1	A	376	LEU	HB3	1.0	0.03	2
1	A	376	LEU	HD11	0.65	0.03	2
1	A	376	LEU	HD12	0.65	0.03	2
1	A	376	LEU	HD13	0.65	0.03	2
1	A	376	LEU	HD21	0.76	0.03	2
1	A	376	LEU	HD22	0.76	0.03	2
1	A	376	LEU	HD23	0.76	0.03	2
1	A	376	LEU	HG	1.67	0.03	1
1	A	377	LEU	H	7.79	0.03	1
1	A	377	LEU	HA	4.17	0.03	1
1	A	377	LEU	HB2	1.47	0.03	2
1	A	377	LEU	HB3	1.77	0.03	2
1	A	377	LEU	HD11	0.84	0.03	2
1	A	377	LEU	HD12	0.84	0.03	2
1	A	377	LEU	HD13	0.84	0.03	2
1	A	377	LEU	HD21	0.86	0.03	2
1	A	377	LEU	HD22	0.86	0.03	2
1	A	377	LEU	HD23	0.86	0.03	2
1	A	377	LEU	HG	1.72	0.03	1
1	A	378	ASN	H	7.71	0.03	1
1	A	378	ASN	HA	5.06	0.03	1
1	A	378	ASN	HB2	2.65	0.03	1
1	A	378	ASN	HB3	2.91	0.03	1
1	A	378	ASN	HD21	7.74	0.03	1
1	A	378	ASN	HD22	6.93	0.03	1
1	A	379	PRO	HA	4.45	0.03	1
1	A	379	PRO	HB2	1.68	0.03	2
1	A	379	PRO	HB3	1.93	0.03	2
1	A	379	PRO	HD2	3.59	0.03	1
1	A	379	PRO	HD3	3.41	0.03	1
1	A	379	PRO	HG2	1.37	0.03	2
1	A	379	PRO	HG3	1.48	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	380	LYS	H	7.73	0.03	1
1	A	380	LYS	HA	4.14	0.03	1
1	A	380	LYS	HB2	1.84	0.03	1
1	A	380	LYS	HB3	1.93	0.03	1
1	A	380	LYS	HE2	3.02	0.03	2
1	A	381	ILE	H	7.83	0.03	1
1	A	381	ILE	HA	4.21	0.03	1
1	A	381	ILE	HB	2.06	0.03	1
1	A	381	ILE	HD11	0.67	0.03	1
1	A	381	ILE	HD12	0.67	0.03	1
1	A	381	ILE	HD13	0.67	0.03	1
1	A	382	ILE	H	7.45	0.03	1
1	A	382	ILE	HA	3.49	0.03	1
1	A	382	ILE	HB	1.95	0.03	1
1	A	382	ILE	HD11	0.79	0.03	1
1	A	382	ILE	HD12	0.79	0.03	1
1	A	382	ILE	HD13	0.79	0.03	1
1	A	383	ASP	H	7.58	0.03	1
1	A	383	ASP	HA	4.8	0.03	1
1	A	383	ASP	HB2	2.76	0.03	1
1	A	383	ASP	HB3	3.25	0.03	1
1	A	384	SER	H	8.61	0.03	1
1	A	384	SER	HA	5.09	0.03	1
1	A	384	SER	HB2	3.94	0.03	2
1	A	384	SER	HB3	3.94	0.03	2
1	A	385	SER	HA	4.25	0.03	1
1	A	385	SER	HB2	3.72	0.03	2
1	A	386	ARG	H	8.09	0.03	1
1	A	386	ARG	HA	4.16	0.03	1
1	A	386	ARG	HB2	1.76	0.03	1
1	A	386	ARG	HB3	1.99	0.03	1
1	A	386	ARG	HD2	3.4	0.03	2
1	A	386	ARG	HD3	3.4	0.03	2
1	A	386	ARG	HG2	1.61	0.03	2
1	A	387	ILE	H	8.76	0.03	1
1	A	387	ILE	HA	3.38	0.03	1
1	A	387	ILE	HB	1.9	0.03	1
1	A	387	ILE	HD11	0.66	0.03	1
1	A	387	ILE	HD12	0.66	0.03	1
1	A	387	ILE	HD13	0.66	0.03	1
1	A	388	ARG	H	7.56	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	388	ARG	HA	3.87	0.03	1
1	A	388	ARG	HB2	1.95	0.03	2
1	A	388	ARG	HB3	1.95	0.03	2
1	A	388	ARG	HD2	3.23	0.03	2
1	A	388	ARG	HD3	3.23	0.03	2
1	A	388	ARG	HG2	1.6	0.03	2
1	A	388	ARG	HG3	1.6	0.03	2
1	A	389	ARG	H	7.4	0.03	1
1	A	389	ARG	HA	3.85	0.03	1
1	A	389	ARG	HB2	2.06	0.03	2
1	A	389	ARG	HB3	2.06	0.03	2
1	A	390	ILE	H	8.88	0.03	1
1	A	390	ILE	HA	3.55	0.03	1
1	A	390	ILE	HB	1.7	0.03	1
1	A	390	ILE	HD11	0.72	0.03	1
1	A	390	ILE	HD12	0.72	0.03	1
1	A	390	ILE	HD13	0.72	0.03	1
1	A	391	ALA	H	8.85	0.03	1
1	A	391	ALA	HA	3.77	0.03	1
1	A	391	ALA	HB1	1.29	0.03	1
1	A	391	ALA	HB2	1.29	0.03	1
1	A	391	ALA	HB3	1.29	0.03	1
1	A	392	ILE	H	8.05	0.03	1
1	A	392	ILE	HA	3.83	0.03	1
1	A	392	ILE	HB	1.87	0.03	1
1	A	392	ILE	HD11	0.86	0.03	1
1	A	392	ILE	HD12	0.86	0.03	1
1	A	392	ILE	HD13	0.86	0.03	1
1	A	393	GLY	H	8.58	0.03	1
1	A	393	GLY	HA2	3.88	0.03	2
1	A	393	GLY	HA3	3.88	0.03	2
1	A	394	SER	H	7.99	0.03	1
1	A	394	SER	HA	4.45	0.03	1
1	A	394	SER	HB2	3.94	0.03	2
1	A	394	SER	HB3	3.94	0.03	2
1	A	395	GLY	H	7.8	0.03	1
1	A	395	GLY	HA2	3.99	0.03	2
1	A	395	GLY	HA3	3.99	0.03	2
1	A	396	THR	H	8.33	0.03	1
1	A	396	THR	HA	4.63	0.03	1
1	A	396	THR	HB	4.34	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	397	SER	H	8.55	0.03	1
1	A	397	SER	HA	5.04	0.03	1
1	A	397	SER	HB2	3.99	0.03	1
1	A	397	SER	HB3	4.23	0.03	1
1	A	398	PRO	HA	4.52	0.03	1
1	A	398	PRO	HD2	3.95	0.03	2
1	A	398	PRO	HD3	3.88	0.03	2
1	A	398	PRO	HG2	2.27	0.03	2
1	A	398	PRO	HG3	1.76	0.03	2
1	A	399	GLN	H	8.44	0.03	1
1	A	399	GLN	HA	3.94	0.03	1
1	A	399	GLN	HB2	1.99	0.03	2
1	A	399	GLN	HB3	2.15	0.03	2
1	A	399	GLN	HE21	7.63	0.03	1
1	A	399	GLN	HE22	6.86	0.03	1
1	A	399	GLN	HG2	2.41	0.03	1
1	A	399	GLN	HG3	2.51	0.03	1
1	A	400	GLU	H	7.84	0.03	1
1	A	400	GLU	HA	4.14	0.03	1
1	A	400	GLU	HB2	2.0	0.03	2
1	A	400	GLU	HB3	2.41	0.03	2
1	A	400	GLU	HG2	2.29	0.03	2
1	A	400	GLU	HG3	2.29	0.03	2
1	A	401	VAL	H	7.68	0.03	1
1	A	401	VAL	HA	3.59	0.03	1
1	A	401	VAL	HB	2.26	0.03	1
1	A	402	LYS	H	8.31	0.03	1
1	A	402	LYS	HA	3.82	0.03	1
1	A	402	LYS	HB2	1.9	0.03	2
1	A	402	LYS	HB3	1.9	0.03	2
1	A	402	LYS	HD2	1.63	0.03	2
1	A	402	LYS	HE2	2.88	0.03	2
1	A	402	LYS	HG2	1.42	0.03	2
1	A	403	GLU	H	8.07	0.03	1
1	A	403	GLU	HA	4.14	0.03	1
1	A	403	GLU	HB2	2.33	0.03	1
1	A	403	GLU	HB3	2.4	0.03	1
1	A	403	GLU	HG2	2.62	0.03	2
1	A	403	GLU	HG3	2.35	0.03	2
1	A	404	LEU	H	7.34	0.03	1
1	A	404	LEU	HA	3.45	0.03	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	404	LEU	HB2	2.02	0.03	2
1	A	404	LEU	HB3	0.88	0.03	2
1	A	404	LEU	HD11	0.41	0.03	2
1	A	404	LEU	HD12	0.41	0.03	2
1	A	404	LEU	HD13	0.41	0.03	2
1	A	404	LEU	HD21	0.79	0.03	2
1	A	404	LEU	HD22	0.79	0.03	2
1	A	404	LEU	HD23	0.79	0.03	2
1	A	404	LEU	HG	1.18	0.03	1
1	A	405	LEU	H	7.88	0.03	1
1	A	405	LEU	HA	4.03	0.03	1
1	A	405	LEU	HB2	1.58	0.03	2
1	A	405	LEU	HB3	1.99	0.03	2
1	A	405	LEU	HD11	0.85	0.03	2
1	A	405	LEU	HD12	0.85	0.03	2
1	A	405	LEU	HD13	0.85	0.03	2
1	A	405	LEU	HD21	0.77	0.03	2
1	A	405	LEU	HD22	0.77	0.03	2
1	A	405	LEU	HD23	0.77	0.03	2
1	A	405	LEU	HG	1.85	0.03	1
1	A	406	ASN	H	8.78	0.03	1
1	A	406	ASN	HA	4.6	0.03	1
1	A	406	ASN	HB2	2.94	0.03	2
1	A	406	ASN	HB3	2.94	0.03	2
1	A	406	ASN	HD21	7.76	0.03	1
1	A	406	ASN	HD22	6.95	0.03	1
1	A	407	TYR	H	8.48	0.03	1
1	A	407	TYR	HA	4.24	0.03	1
1	A	407	TYR	HB2	3.34	0.03	1
1	A	407	TYR	HB3	3.28	0.03	1
1	A	407	TYR	HD1	6.95	0.03	3
1	A	407	TYR	HD2	6.95	0.03	3
1	A	407	TYR	HE1	6.91	0.03	3
1	A	407	TYR	HE2	6.91	0.03	3
1	A	408	TYR	H	8.63	0.03	1
1	A	408	TYR	HA	3.98	0.03	1
1	A	408	TYR	HB2	3.27	0.03	2
1	A	408	TYR	HB3	3.07	0.03	2
1	A	408	TYR	HD1	6.84	0.03	3
1	A	408	TYR	HD2	6.84	0.03	3
1	A	408	TYR	HE1	6.54	0.03	3

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	408	TYR	HE2	6.54	0.03	3
1	A	409	LYS	H	8.15	0.03	1
1	A	409	LYS	HA	3.43	0.03	1
1	A	409	LYS	HB2	1.94	0.03	2
1	A	409	LYS	HB3	1.98	0.03	2
1	A	409	LYS	HD2	1.72	0.03	1
1	A	409	LYS	HD3	1.68	0.03	1
1	A	409	LYS	HE2	2.98	0.03	2
1	A	409	LYS	HE3	2.98	0.03	2
1	A	409	LYS	HG2	1.41	0.03	1
1	A	409	LYS	HG3	1.41	0.03	1
1	A	410	THR	H	8.2	0.03	1
1	A	410	THR	HA	3.85	0.03	1
1	A	410	THR	HB	4.22	0.03	1
1	A	411	MET	H	8.29	0.03	1
1	A	411	MET	HA	4.07	0.03	1
1	A	411	MET	HB2	1.65	0.03	1
1	A	411	MET	HB3	1.93	0.03	1
1	A	412	LYS	H	8.56	0.03	1
1	A	412	LYS	HA	3.3	0.03	1
1	A	412	LYS	HB2	1.36	0.03	1
1	A	412	LYS	HB3	1.6	0.03	1
1	A	412	LYS	HE2	2.96	0.03	2
1	A	412	LYS	HE3	3.0	0.03	2
1	A	412	LYS	HG2	1.23	0.03	2
1	A	412	LYS	HG3	1.23	0.03	2
1	A	413	ASN	H	7.64	0.03	1
1	A	413	ASN	HA	4.4	0.03	1
1	A	413	ASN	HB2	2.76	0.03	1
1	A	413	ASN	HB3	2.85	0.03	1
1	A	413	ASN	HD21	7.64	0.03	1
1	A	413	ASN	HD22	6.95	0.03	1
1	A	414	LEU	H	7.93	0.03	1
1	A	414	LEU	HA	4.0	0.03	1
1	A	414	LEU	HB2	1.51	0.03	1
1	A	414	LEU	HB3	1.74	0.03	1
1	A	414	LEU	HD11	0.82	0.03	2
1	A	414	LEU	HD12	0.82	0.03	2
1	A	414	LEU	HD13	0.82	0.03	2
1	A	414	LEU	HD21	0.79	0.03	2
1	A	414	LEU	HD22	0.79	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	414	LEU	HD23	0.79	0.03	2
1	A	415	MET	H	8.05	0.03	1
1	A	415	MET	HA	4.04	0.03	1
1	A	415	MET	HB2	2.09	0.03	2
1	A	415	MET	HB3	2.09	0.03	2
1	A	415	MET	HG2	2.2	0.03	2
1	A	415	MET	HG3	2.2	0.03	2
1	A	416	LYS	H	7.52	0.03	1
1	A	416	LYS	HA	4.03	0.03	1
1	A	416	LYS	HB2	1.87	0.03	2
1	A	416	LYS	HB3	1.87	0.03	2
1	A	417	LYS	H	7.66	0.03	1
1	A	417	LYS	HA	4.13	0.03	1
1	A	417	LYS	HB2	1.9	0.03	2
1	A	417	LYS	HB3	1.9	0.03	2
1	A	418	MET	H	7.83	0.03	1
1	A	418	MET	HA	4.29	0.03	1
1	A	418	MET	HB2	2.06	0.03	2
1	A	418	MET	HB3	2.02	0.03	2
1	A	419	LYS	H	7.95	0.03	1
1	A	419	LYS	HA	4.18	0.03	1
1	A	419	LYS	HB2	1.84	0.03	2
1	A	419	LYS	HB3	1.84	0.03	2
1	A	420	LYS	H	8.09	0.03	1
1	A	420	LYS	HA	4.29	0.03	1
1	A	421	ASN	H	8.27	0.03	1
1	A	421	ASN	HA	4.64	0.03	1
1	A	421	ASN	HB2	2.74	0.03	1
1	A	421	ASN	HB3	2.81	0.03	1
1	A	421	ASN	HD21	7.58	0.03	1
1	A	421	ASN	HD22	6.91	0.03	1
1	A	422	LYS	H	8.07	0.03	1
1	A	422	LYS	HA	4.31	0.03	1
1	A	423	LEU	H	8.23	0.03	1
1	A	423	LEU	HA	4.59	0.03	1
1	A	423	LEU	HB2	1.52	0.03	1
1	A	423	LEU	HB3	1.63	0.03	1
1	A	423	LEU	HD11	0.94	0.03	2
1	A	423	LEU	HD12	0.94	0.03	2
1	A	423	LEU	HD13	0.94	0.03	2
1	A	423	LEU	HD21	0.9	0.03	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	423	LEU	HD22	0.9	0.03	2
1	A	423	LEU	HD23	0.9	0.03	2
1	A	423	LEU	HG	1.65	0.03	1
1	A	424	PRO	HA	4.47	0.03	1
1	A	424	PRO	HB2	2.19	0.03	2
1	A	424	PRO	HB3	2.19	0.03	2
1	A	424	PRO	HD2	3.79	0.03	1
1	A	424	PRO	HD3	3.61	0.03	1
1	A	424	PRO	HG2	1.99	0.03	2
1	A	424	PRO	HG3	1.99	0.03	2
1	A	425	ILE	H	7.57	0.03	1
1	A	425	ILE	HA	4.05	0.03	1
1	A	425	ILE	HB	1.8	0.03	1
1	A	425	ILE	HD11	0.85	0.03	1
1	A	425	ILE	HD12	0.85	0.03	1
1	A	425	ILE	HD13	0.85	0.03	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	93	-0.47 ± 0.19	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	88	0.11 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	81	-0.33 ± 0.11	None needed (< 0.5 ppm)
^{15}N	84	0.24 ± 0.26	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 82%, i.e. 729 atoms were assigned a chemical shift out of a possible 893. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	291/305 (95%)	119/123 (97%)	115/122 (94%)	57/60 (95%)
Sidechain	416/541 (77%)	274/349 (79%)	138/167 (83%)	4/25 (16%)
Aromatic	22/47 (47%)	16/22 (73%)	6/25 (24%)	0/0 (—%)
Overall	729/893 (82%)	409/494 (83%)	259/314 (82%)	61/85 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure.

The overall completeness is 65%, i.e. 1084 atoms were assigned a chemical shift out of a possible 1679. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	438/571 (77%)	180/231 (78%)	174/230 (76%)	84/110 (76%)
Sidechain	624/1041 (60%)	401/674 (59%)	217/325 (67%)	6/42 (14%)
Aromatic	22/67 (33%)	16/32 (50%)	6/35 (17%)	0/0 (—%)
Overall	1084/1679 (65%)	597/937 (64%)	397/590 (67%)	90/152 (59%)

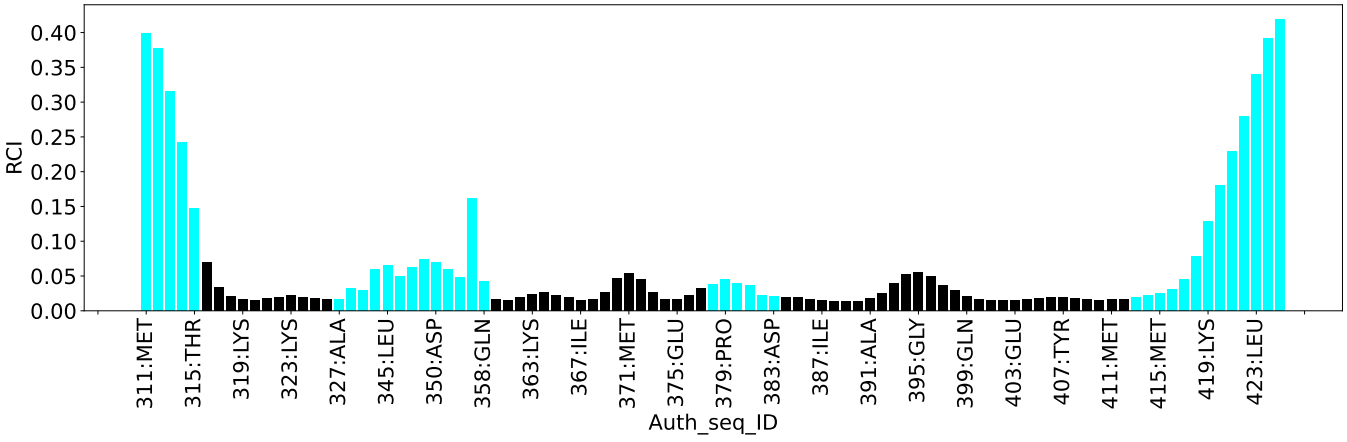
7.1.4 Statistically unusual chemical shifts (i)

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	1122
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	518
Medium range (|i-j|>1 and |i-j|<5)	430
Long range (|i-j|≥5)	174
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	1118
Number of restraints per residue	9.4
Number of long range restraints per residue[1]	1.5

[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

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.There are no distance violations

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis (i)

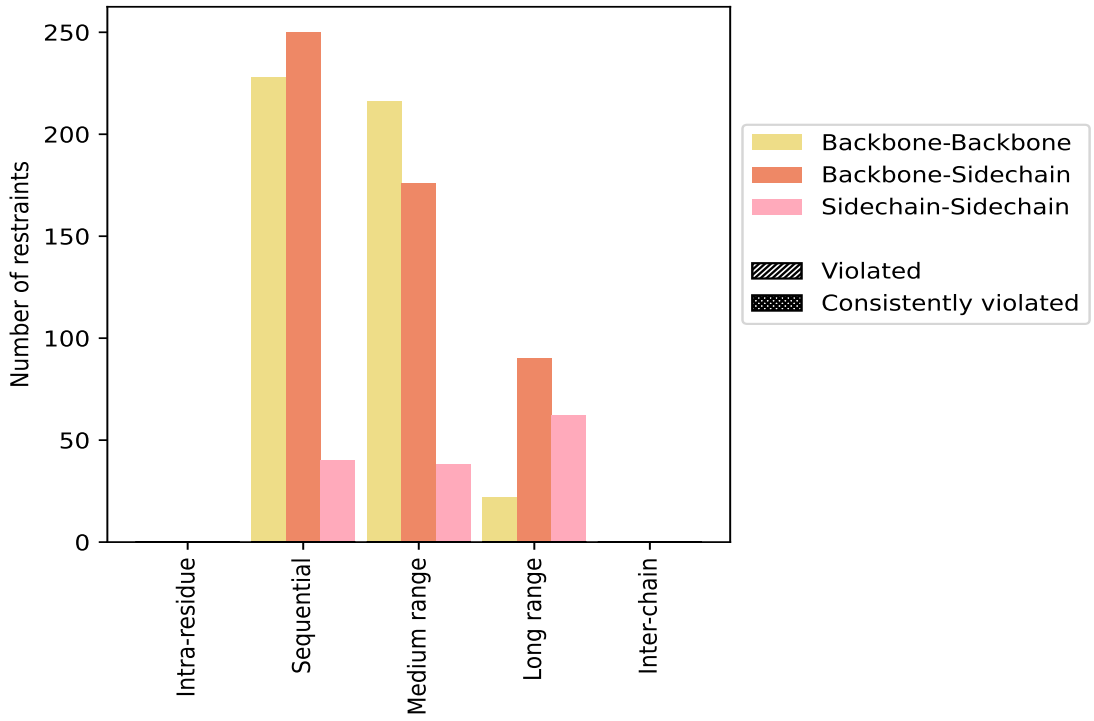
9.1 Summary of distance violations (i)

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)	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)	518	46.2	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	228	20.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	250	22.3	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	40	3.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	430	38.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	216	19.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	176	15.7	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	38	3.4	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	174	15.5	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	22	2.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	90	8.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	62	5.5	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	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	1122	100.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	466	41.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	516	46.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	140	12.5	0	0.0	0.0	0	0.0	0.0

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

9.1.1 Bar chart : Distribution of distance restraints and violations



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

No violations found

9.3 Distance violation statistics for the ensemble

No violations found

9.4 Most violated distance restraints in the ensemble

No violations found

9.5 All violated distance restraints

No violations found

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found