



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 09:53 pm BST

PDB ID : 2GG1  
Title : NMR solution structure of domain III of the E-protein of tick-borne Langat flavivirus (includes RDC restraints)  
Authors : Mukherjee, M.; Dutta, K.; White, M.A.; Cowburn, D.; Fox, R.O.  
Deposited on : 2006-03-23

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

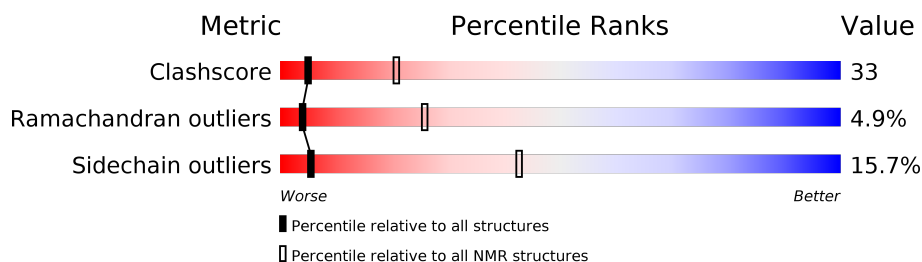
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 81%.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	102	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:303-A:364, A:368-A:395 (90)	0.30	1

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

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

The models can be grouped into 5 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1427 atoms, of which 704 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms						Trace
1	A	93	Total	C	H	N	O	S	0
			1427	457	704	126	134	6	

There are 6 discrepancies between the modelled and reference sequences:

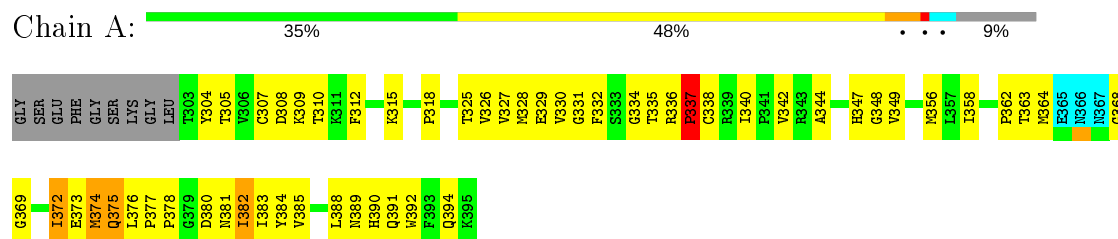
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	GLY	-	cloning artifact	UNP P29838
A	295	SER	-	cloning artifact	UNP P29838
A	296	GLU	-	cloning artifact	UNP P29838
A	297	PHE	-	cloning artifact	UNP P29838
A	298	GLY	-	cloning artifact	UNP P29838
A	299	SER	-	cloning artifact	UNP P29838

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Genome polyprotein

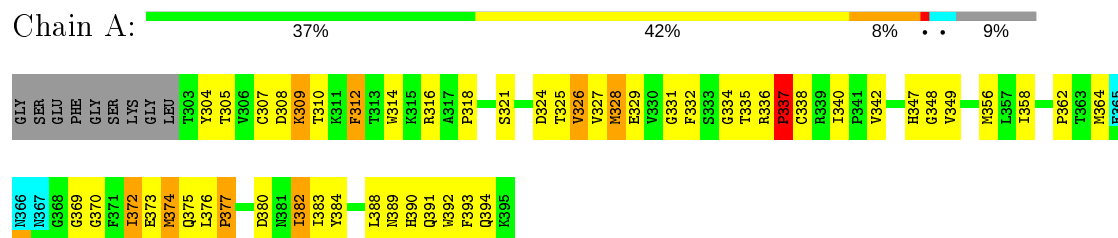


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Genome polyprotein

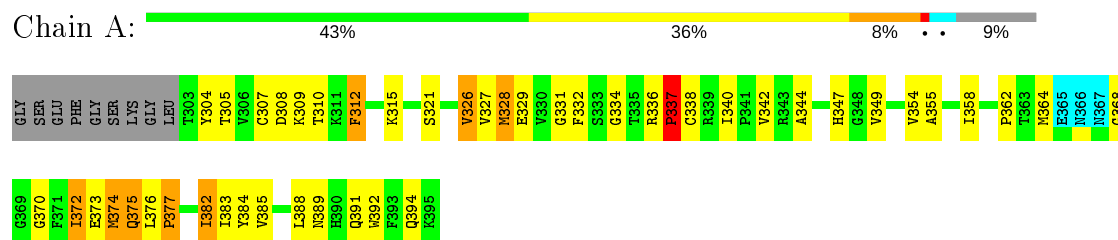


#### 4.2.2 Score per residue for model 2

- Molecule 1: Genome polyprotein

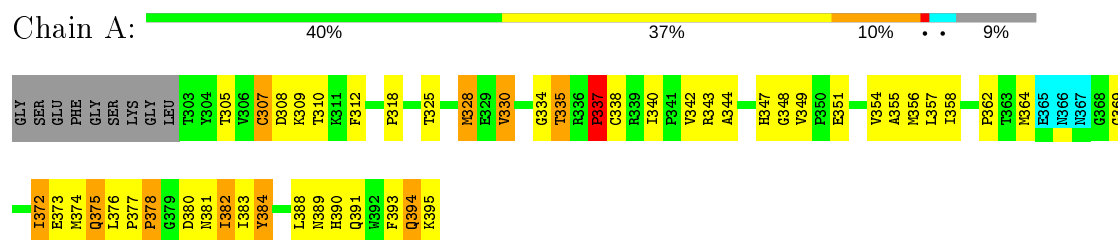






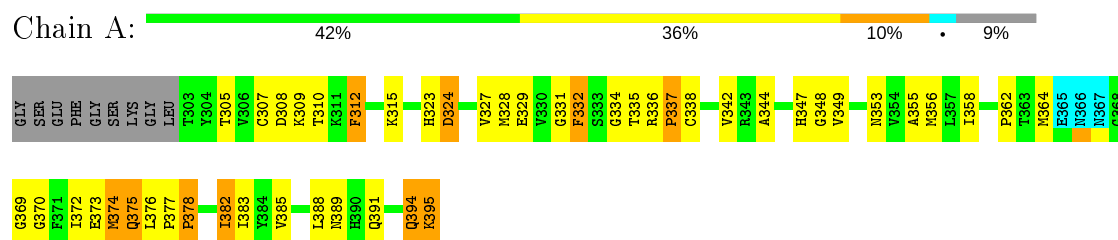
#### 4.2.7 Score per residue for model 7

- Molecule 1: Genome polyprotein



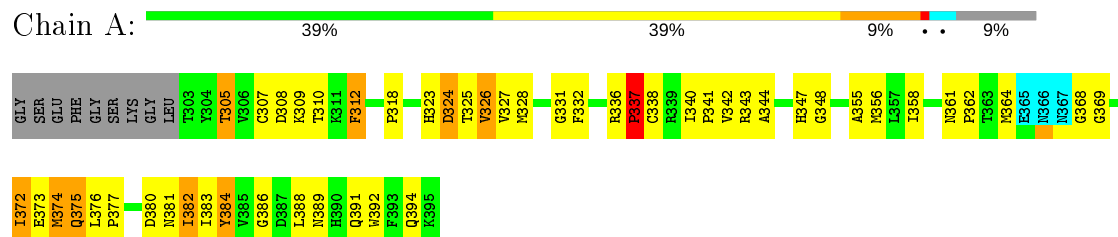
#### 4.2.8 Score per residue for model 8

- Molecule 1: Genome polyprotein



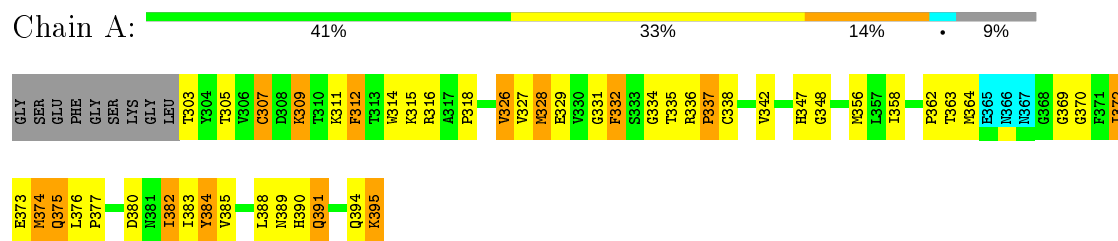
#### 4.2.9 Score per residue for model 9

- Molecule 1: Genome polyprotein



### 4.2.10 Score per residue for model 10

- Molecule 1: Genome polyprotein



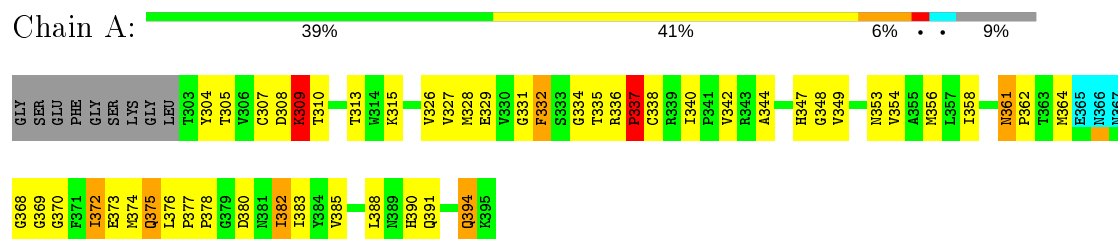
### 4.2.11 Score per residue for model 11

- Molecule 1: Genome polyprotein



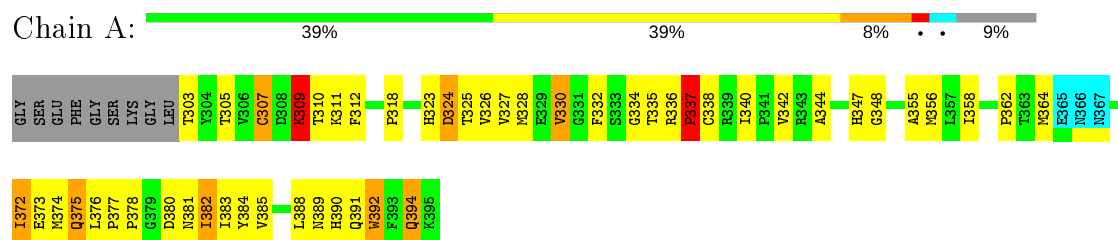
### 4.2.12 Score per residue for model 12

- Molecule 1: Genome polyprotein



### 4.2.13 Score per residue for model 13

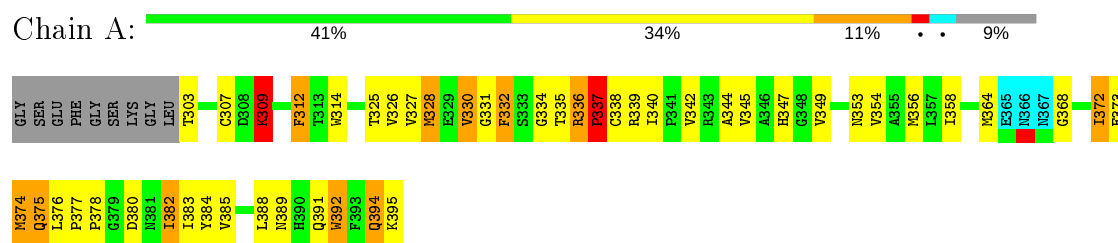
- Molecule 1: Genome polyprotein





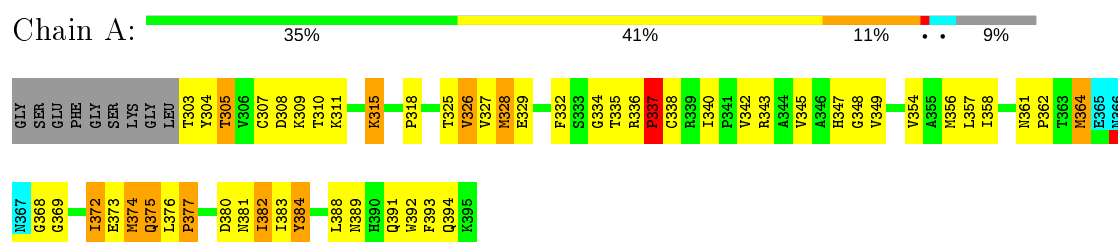
#### 4.2.14 Score per residue for model 14

- Molecule 1: Genome polyprotein



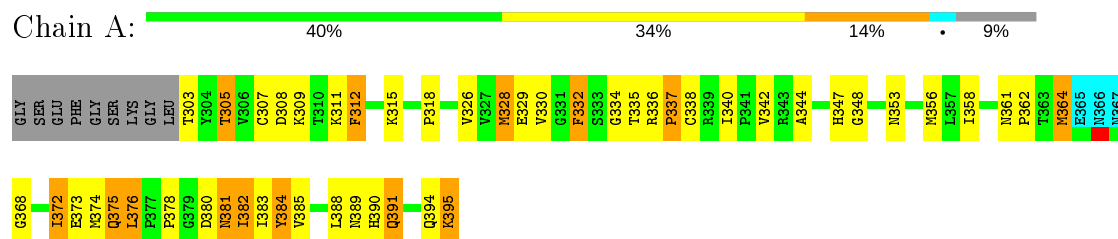
#### 4.2.15 Score per residue for model 15

- Molecule 1: Genome polypotein



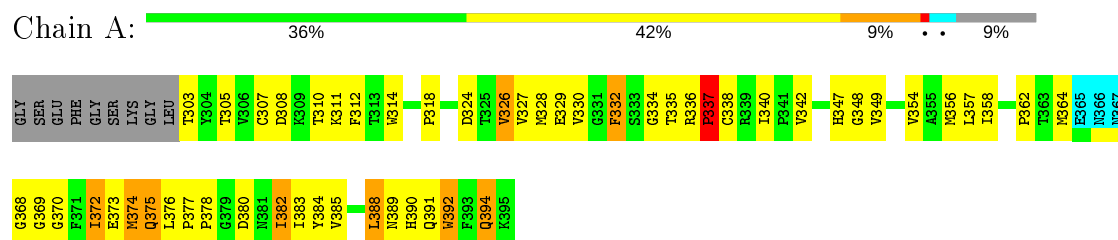
#### 4.2.16 Score per residue for model 16

- Molecule 1: Genome polypprotein



#### 4.2.17 Score per residue for model 17

- Molecule 1: Genome polypeptide





## 5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	2.2
CNS	refinement	1.1

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1048
Number of shifts mapped to atoms	1048
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts ⓘ

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	698	686	682	45±5
All	All	13960	13720	13640	906

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:382:ILE:HB	1:A:391:GLN:HA	1.09	1.20	7	20
1:A:376:LEU:HG	1:A:377:PRO:HD2	1.00	1.27	10	10
1:A:332:PHE:H	1:A:368:GLY:HA2	0.88	1.28	9	4
1:A:375:GLN:HE21	1:A:375:GLN:HA	0.86	1.31	16	7
1:A:307:CYS:HB3	1:A:335:THR:HG21	0.85	1.49	7	2
1:A:312:PHE:HZ	1:A:340:ILE:HD12	0.83	1.32	17	1
1:A:337:PRO:HA	1:A:364:MET:O	0.82	1.73	20	18
1:A:338:CYS:SG	1:A:364:MET:HG2	0.82	2.14	10	9
1:A:332:PHE:CZ	1:A:335:THR:HB	0.81	2.10	15	2
1:A:375:GLN:HA	1:A:375:GLN:HE21	0.80	1.35	3	4
1:A:326:VAL:HG23	1:A:375:GLN:HG2	0.79	1.51	20	7
1:A:332:PHE:HZ	1:A:335:THR:HB	0.78	1.38	15	1
1:A:375:GLN:HE22	1:A:394:GLN:HG3	0.78	1.36	16	10
1:A:362:PRO:HB3	1:A:372:ILE:HG23	0.77	1.56	5	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:375:GLN:HE22	1:A:394:GLN:HG2	0.77	1.40	17	8
1:A:374:MET:HG2	1:A:383:ILE:HD11	0.75	1.59	12	9
1:A:315:LYS:HD3	1:A:329:GLU:HG2	0.75	1.56	2	3
1:A:318:PRO:HD2	1:A:390:HIS:HB3	0.73	1.57	5	8
1:A:312:PHE:HD1	1:A:388:LEU:HD13	0.73	1.43	3	4
1:A:328:MET:SD	1:A:372:ILE:HB	0.73	2.23	16	4
1:A:336:ARG:HB2	1:A:337:PRO:HD2	0.72	1.59	15	19
1:A:340:ILE:HG22	1:A:342:VAL:HG13	0.72	1.61	11	11
1:A:382:ILE:HB	1:A:391:GLN:CA	0.72	2.13	14	18
1:A:325:THR:HA	1:A:375:GLN:HG3	0.71	1.61	19	7
1:A:347:HIS:HB2	1:A:380:ASP:HB2	0.71	1.62	12	5
1:A:378:PRO:HA	1:A:394:GLN:HE22	0.71	1.46	14	7
1:A:326:VAL:HG21	1:A:392:TRP:HZ2	0.70	1.46	13	2
1:A:340:ILE:HB	1:A:364:MET:SD	0.70	2.25	16	2
1:A:364:MET:HB3	1:A:369:GLY:CA	0.70	2.17	15	1
1:A:358:ILE:HD11	1:A:375:GLN:HB2	0.70	1.61	19	8
1:A:382:ILE:CB	1:A:391:GLN:HA	0.69	2.15	12	10
1:A:327:VAL:HG12	1:A:373:GLU:HG2	0.69	1.65	20	15
1:A:385:VAL:HB	1:A:388:LEU:HB2	0.68	1.65	8	5
1:A:318:PRO:HG3	1:A:383:ILE:HD12	0.68	1.65	17	1
1:A:332:PHE:CE2	1:A:335:THR:HB	0.67	2.25	8	1
1:A:376:LEU:HD22	1:A:377:PRO:HD2	0.67	1.67	18	8
1:A:332:PHE:CD1	1:A:368:GLY:HA2	0.67	2.25	18	4
1:A:326:VAL:HB	1:A:374:MET:HG2	0.67	1.67	2	1
1:A:340:ILE:HD12	1:A:362:PRO:HB2	0.67	1.64	5	4
1:A:364:MET:HB3	1:A:369:GLY:HA2	0.67	1.65	15	1
1:A:332:PHE:HB3	1:A:364:MET:SD	0.67	2.29	11	2
1:A:364:MET:HA	1:A:369:GLY:HA2	0.66	1.68	17	8
1:A:326:VAL:HB	1:A:374:MET:SD	0.66	2.30	6	1
1:A:357:LEU:HA	1:A:374:MET:HA	0.66	1.67	2	7
1:A:332:PHE:HE2	1:A:335:THR:HB	0.66	1.51	8	1
1:A:336:ARG:HH21	1:A:337:PRO:HB2	0.66	1.50	2	2
1:A:342:VAL:HG11	1:A:372:ILE:HD13	0.65	1.68	11	7
1:A:342:VAL:HG13	1:A:385:VAL:HG13	0.65	1.66	18	2
1:A:358:ILE:HB	1:A:373:GLU:CB	0.65	2.21	8	17
1:A:348:GLY:H	1:A:382:ILE:HG21	0.64	1.51	13	16
1:A:308:ASP:HB3	1:A:311:LYS:HG3	0.64	1.69	16	1
1:A:340:ILE:HD12	1:A:341:PRO:HD2	0.64	1.70	9	1
1:A:316:ARG:HB3	1:A:329:GLU:HB2	0.64	1.69	4	4
1:A:338:CYS:SG	1:A:364:MET:HE2	0.64	2.33	18	2
1:A:340:ILE:HG22	1:A:342:VAL:HG22	0.64	1.68	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:358:ILE:HB	1:A:373:GLU:HB3	0.63	1.70	19	19
1:A:383:ILE:O	1:A:389:ASN:HA	0.63	1.94	2	17
1:A:332:PHE:HB2	1:A:364:MET:SD	0.63	2.34	10	2
1:A:312:PHE:CD1	1:A:388:LEU:HD13	0.62	2.29	9	4
1:A:308:ASP:OD1	1:A:310:THR:HG22	0.62	1.95	6	8
1:A:331:GLY:HA2	1:A:368:GLY:HA3	0.62	1.71	14	5
1:A:315:LYS:HG2	1:A:329:GLU:HG2	0.61	1.72	15	1
1:A:375:GLN:HE21	1:A:376:LEU:H	0.61	1.39	18	3
1:A:347:HIS:HB3	1:A:380:ASP:CB	0.61	2.26	5	5
1:A:374:MET:HE3	1:A:383:ILE:HD11	0.61	1.72	14	1
1:A:376:LEU:HG	1:A:377:PRO:CD	0.61	2.24	2	8
1:A:342:VAL:HG12	1:A:385:VAL:HG22	0.61	1.70	18	2
1:A:340:ILE:HG23	1:A:342:VAL:HG22	0.61	1.71	16	2
1:A:375:GLN:NE2	1:A:394:GLN:HG2	0.61	2.11	14	2
1:A:315:LYS:HE3	1:A:315:LYS:HA	0.60	1.70	15	1
1:A:375:GLN:HE21	1:A:375:GLN:CA	0.60	2.06	16	4
1:A:375:GLN:HA	1:A:375:GLN:NE2	0.60	2.12	12	6
1:A:347:HIS:HB3	1:A:380:ASP:HB2	0.60	1.73	5	2
1:A:307:CYS:HB2	1:A:332:PHE:CZ	0.60	2.31	5	1
1:A:340:ILE:HG12	1:A:364:MET:HG2	0.60	1.72	5	1
1:A:335:THR:HB	1:A:364:MET:SD	0.60	2.37	1	3
1:A:340:ILE:HG12	1:A:364:MET:HG3	0.59	1.74	7	2
1:A:338:CYS:SG	1:A:364:MET:HB2	0.59	2.37	14	6
1:A:327:VAL:HG12	1:A:373:GLU:HG3	0.59	1.74	4	3
1:A:378:PRO:HA	1:A:394:GLN:NE2	0.59	2.12	13	9
1:A:325:THR:HA	1:A:375:GLN:CG	0.59	2.27	19	6
1:A:318:PRO:HG2	1:A:390:HIS:O	0.59	1.96	5	4
1:A:375:GLN:CA	1:A:375:GLN:HE21	0.59	2.09	3	7
1:A:374:MET:CE	1:A:383:ILE:HD11	0.58	2.28	14	1
1:A:326:VAL:HB	1:A:374:MET:HE2	0.58	1.74	14	1
1:A:326:VAL:HG21	1:A:392:TRP:CZ2	0.58	2.34	17	3
1:A:384:TYR:HA	1:A:388:LEU:O	0.57	1.98	18	9
1:A:315:LYS:CG	1:A:329:GLU:HG2	0.57	2.29	15	1
1:A:356:MET:HB3	1:A:375:GLN:O	0.57	2.00	10	12
1:A:348:GLY:H	1:A:382:ILE:CG2	0.57	2.11	13	8
1:A:363:THR:O	1:A:369:GLY:HA2	0.56	2.00	10	3
1:A:315:LYS:HB3	1:A:329:GLU:HG2	0.56	1.76	15	1
1:A:340:ILE:HD13	1:A:364:MET:HG3	0.56	1.77	9	1
1:A:374:MET:SD	1:A:383:ILE:HD11	0.56	2.41	6	1
1:A:375:GLN:NE2	1:A:375:GLN:HA	0.56	2.14	13	6
1:A:311:LYS:HE2	1:A:335:THR:OG1	0.56	2.00	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:375:GLN:NE2	1:A:394:GLN:HG3	0.56	2.16	4	2
1:A:332:PHE:HD1	1:A:368:GLY:HA2	0.56	1.60	14	3
1:A:354:VAL:HB	1:A:381:ASN:OD1	0.55	2.01	7	1
1:A:314:TRP:CE2	1:A:388:LEU:HG	0.55	2.36	1	5
1:A:342:VAL:CG2	1:A:362:PRO:HG3	0.55	2.31	13	3
1:A:308:ASP:OD2	1:A:310:THR:HG22	0.55	2.02	17	5
1:A:340:ILE:HB	1:A:362:PRO:HG2	0.55	1.77	2	4
1:A:312:PHE:HA	1:A:331:GLY:O	0.55	2.01	14	6
1:A:335:THR:HB	1:A:364:MET:CE	0.55	2.31	19	2
1:A:362:PRO:HB3	1:A:372:ILE:CG2	0.55	2.32	1	3
1:A:336:ARG:NH2	1:A:337:PRO:HB2	0.55	2.17	2	2
1:A:380:ASP:HB3	1:A:393:PHE:CD2	0.55	2.37	15	1
1:A:380:ASP:HA	1:A:393:PHE:HA	0.54	1.77	20	2
1:A:321:SER:HB3	1:A:327:VAL:HG13	0.54	1.78	11	3
1:A:340:ILE:HD11	1:A:364:MET:N	0.54	2.18	17	1
1:A:312:PHE:HD2	1:A:332:PHE:CZ	0.54	2.20	9	1
1:A:395:LYS:HD3	1:A:395:LYS:H	0.54	1.63	10	2
1:A:332:PHE:N	1:A:368:GLY:HA2	0.54	2.08	9	2
1:A:330:VAL:HG21	1:A:340:ILE:HD13	0.54	1.78	14	1
1:A:315:LYS:HD3	1:A:329:GLU:HB3	0.54	1.79	4	2
1:A:311:LYS:HB2	1:A:332:PHE:CE2	0.54	2.37	20	2
1:A:309:LYS:HA	1:A:312:PHE:CZ	0.53	2.38	2	2
1:A:323:HIS:O	1:A:324:ASP:HB3	0.53	2.03	8	1
1:A:312:PHE:HB3	1:A:364:MET:HE1	0.53	1.80	8	1
1:A:340:ILE:HG12	1:A:342:VAL:HG13	0.53	1.81	16	1
1:A:304:TYR:HB3	1:A:336:ARG:HG3	0.53	1.79	12	2
1:A:328:MET:SD	1:A:383:ILE:HG21	0.53	2.44	9	2
1:A:305:THR:O	1:A:338:CYS:HB2	0.53	2.04	9	12
1:A:327:VAL:HA	1:A:372:ILE:O	0.53	2.04	8	6
1:A:329:GLU:HA	1:A:370:GLY:O	0.52	2.04	12	6
1:A:338:CYS:SG	1:A:364:MET:HG3	0.52	2.44	18	3
1:A:304:TYR:HB2	1:A:337:PRO:O	0.52	2.05	6	1
1:A:332:PHE:CZ	1:A:364:MET:SD	0.52	3.02	16	1
1:A:326:VAL:HB	1:A:374:MET:HG3	0.52	1.80	1	2
1:A:328:MET:CG	1:A:372:ILE:HG13	0.52	2.35	4	1
1:A:330:VAL:HG22	1:A:372:ILE:HD11	0.52	1.79	16	1
1:A:330:VAL:CG2	1:A:372:ILE:HD11	0.52	2.34	16	1
1:A:344:ALA:O	1:A:353:ASN:HA	0.51	2.04	20	8
1:A:312:PHE:HZ	1:A:386:GLY:HA3	0.51	1.65	9	1
1:A:347:HIS:HB2	1:A:380:ASP:CB	0.51	2.35	7	4
1:A:328:MET:SD	1:A:383:ILE:HD13	0.51	2.44	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:343:ARG:HG2	1:A:384:TYR:O	0.51	2.05	9	3
1:A:315:LYS:CB	1:A:329:GLU:HG2	0.51	2.35	15	1
1:A:375:GLN:HE22	1:A:394:GLN:CG	0.51	2.18	11	3
1:A:312:PHE:CZ	1:A:340:ILE:HD12	0.51	2.25	17	1
1:A:340:ILE:HG13	1:A:342:VAL:HG13	0.51	1.83	9	1
1:A:361:ASN:N	1:A:362:PRO:HD3	0.51	2.21	16	3
1:A:342:VAL:CG1	1:A:385:VAL:HG22	0.51	2.35	18	2
1:A:358:ILE:HD11	1:A:375:GLN:HB3	0.51	1.81	5	2
1:A:326:VAL:HG23	1:A:374:MET:O	0.50	2.07	2	1
1:A:376:LEU:CG	1:A:377:PRO:HD2	0.50	2.32	2	3
1:A:344:ALA:N	1:A:355:ALA:HB2	0.50	2.21	11	8
1:A:328:MET:HG3	1:A:372:ILE:HG13	0.50	1.83	4	1
1:A:318:PRO:HB3	1:A:383:ILE:CD1	0.50	2.36	13	6
1:A:326:VAL:O	1:A:373:GLU:HA	0.50	2.06	9	1
1:A:326:VAL:HG11	1:A:392:TRP:CZ2	0.50	2.42	13	1
1:A:349:VAL:HG12	1:A:351:GLU:HG2	0.50	1.83	7	1
1:A:347:HIS:O	1:A:349:VAL:HG23	0.49	2.07	12	12
1:A:312:PHE:HB3	1:A:388:LEU:HD13	0.49	1.83	11	1
1:A:331:GLY:HA2	1:A:368:GLY:CA	0.49	2.37	14	2
1:A:312:PHE:HE2	1:A:385:VAL:O	0.49	1.90	16	2
1:A:330:VAL:HG11	1:A:385:VAL:HG11	0.49	1.84	13	2
1:A:354:VAL:HB	1:A:376:LEU:HG	0.49	1.84	17	2
1:A:354:VAL:HG12	1:A:376:LEU:HG	0.49	1.83	6	1
1:A:347:HIS:HB3	1:A:380:ASP:HB3	0.49	1.85	18	1
1:A:329:GLU:HG3	1:A:370:GLY:O	0.49	2.08	20	3
1:A:340:ILE:CG2	1:A:342:VAL:HG13	0.49	2.35	13	6
1:A:374:MET:O	1:A:375:GLN:HB2	0.49	2.08	10	6
1:A:312:PHE:HD2	1:A:332:PHE:HE1	0.48	1.50	5	1
1:A:342:VAL:HG12	1:A:385:VAL:HG13	0.48	1.83	10	3
1:A:323:HIS:O	1:A:324:ASP:HB2	0.48	2.08	13	1
1:A:342:VAL:HG21	1:A:362:PRO:HG3	0.48	1.85	1	1
1:A:374:MET:HG2	1:A:383:ILE:CD1	0.48	2.35	12	8
1:A:343:ARG:HG3	1:A:384:TYR:HB2	0.48	1.86	11	1
1:A:375:GLN:NE2	1:A:376:LEU:H	0.48	2.06	6	4
1:A:330:VAL:HG23	1:A:369:GLY:HA3	0.48	1.85	2	4
1:A:342:VAL:HG11	1:A:372:ILE:HD12	0.48	1.85	1	1
1:A:329:GLU:HG2	1:A:370:GLY:O	0.48	2.09	5	1
1:A:374:MET:N	1:A:374:MET:SD	0.48	2.87	14	3
1:A:326:VAL:CG2	1:A:375:GLN:HG2	0.47	2.38	15	1
1:A:312:PHE:HD2	1:A:330:VAL:HB	0.47	1.69	18	1
1:A:361:ASN:HD22	1:A:361:ASN:N	0.47	2.08	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:381:ASN:HB2	1:A:392:TRP:CH2	0.47	2.45	13	1
1:A:381:ASN:N	1:A:381:ASN:HD22	0.47	2.07	16	1
1:A:320:ASP:HB2	1:A:392:TRP:CZ2	0.47	2.45	5	1
1:A:385:VAL:O	1:A:388:LEU:HB2	0.47	2.09	10	2
1:A:340:ILE:HB	1:A:364:MET:HG2	0.47	1.86	9	1
1:A:328:MET:CE	1:A:372:ILE:HD12	0.47	2.40	12	1
1:A:380:ASP:C	1:A:381:ASN:HD22	0.46	2.14	3	2
1:A:340:ILE:CB	1:A:364:MET:SD	0.46	3.02	16	1
1:A:328:MET:HE2	1:A:372:ILE:HD12	0.46	1.88	8	1
1:A:340:ILE:CG1	1:A:364:MET:HG2	0.46	2.40	5	1
1:A:325:THR:HA	1:A:375:GLN:HG2	0.46	1.87	13	1
1:A:340:ILE:HD11	1:A:362:PRO:HB2	0.46	1.87	19	1
1:A:304:TYR:HB3	1:A:336:ARG:NE	0.46	2.26	2	4
1:A:354:VAL:HG12	1:A:376:LEU:HD22	0.46	1.88	2	2
1:A:311:LYS:HE2	1:A:332:PHE:CE1	0.46	2.45	15	1
1:A:309:LYS:HD2	1:A:310:THR:N	0.46	2.26	3	3
1:A:328:MET:CE	1:A:372:ILE:HB	0.46	2.41	6	1
1:A:338:CYS:O	1:A:363:THR:HG22	0.46	2.11	20	1
1:A:395:LYS:HA	1:A:395:LYS:HE2	0.46	1.87	16	1
1:A:312:PHE:HD2	1:A:364:MET:SD	0.45	2.33	3	1
1:A:392:TRP:NE1	1:A:394:GLN:HB3	0.45	2.27	13	1
1:A:345:VAL:HG22	1:A:382:ILE:HD12	0.45	1.87	15	2
1:A:335:THR:HB	1:A:364:MET:HE3	0.45	1.88	19	1
1:A:392:TRP:CD1	1:A:394:GLN:NE2	0.45	2.85	9	5
1:A:393:PHE:HD2	1:A:395:LYS:HE2	0.45	1.72	7	1
1:A:307:CYS:HB3	1:A:364:MET:HE1	0.45	1.88	13	1
1:A:326:VAL:CG2	1:A:375:GLN:HE21	0.45	2.24	15	3
1:A:385:VAL:HB	1:A:388:LEU:CB	0.45	2.38	8	1
1:A:307:CYS:HB2	1:A:332:PHE:HZ	0.45	1.68	5	1
1:A:328:MET:CE	1:A:383:ILE:HD13	0.45	2.42	9	1
1:A:332:PHE:N	1:A:332:PHE:CD1	0.45	2.85	16	1
1:A:332:PHE:CE1	1:A:335:THR:HB	0.45	2.47	20	1
1:A:304:TYR:HB3	1:A:336:ARG:HE	0.45	1.71	11	1
1:A:356:MET:HB2	1:A:375:GLN:O	0.45	2.12	12	1
1:A:336:ARG:CB	1:A:337:PRO:HD2	0.45	2.42	20	4
1:A:323:HIS:O	1:A:324:ASP:CB	0.45	2.65	9	1
1:A:303:THR:O	1:A:335:THR:HG23	0.45	2.11	15	2
1:A:340:ILE:HG21	1:A:362:PRO:HG2	0.44	1.87	16	1
1:A:340:ILE:HB	1:A:364:MET:CE	0.44	2.42	16	1
1:A:312:PHE:CD2	1:A:332:PHE:CE1	0.44	3.05	5	1
1:A:336:ARG:HB2	1:A:337:PRO:CD	0.44	2.37	5	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:375:GLN:CA	1:A:375:GLN:NE2	0.44	2.80	13	3
1:A:311:LYS:HE3	1:A:335:THR:OG1	0.44	2.12	17	1
1:A:354:VAL:HB	1:A:376:LEU:HD22	0.44	1.89	14	1
1:A:376:LEU:HD11	1:A:381:ASN:HD21	0.44	1.72	16	1
1:A:338:CYS:O	1:A:363:THR:HG23	0.44	2.12	5	2
1:A:347:HIS:HB2	1:A:380:ASP:OD1	0.44	2.12	14	1
1:A:312:PHE:HD2	1:A:332:PHE:CE1	0.44	2.30	5	1
1:A:382:ILE:HD13	1:A:382:ILE:C	0.44	2.33	12	1
1:A:381:ASN:HD22	1:A:394:GLN:HG2	0.44	1.73	9	2
1:A:340:ILE:CG1	1:A:364:MET:HG3	0.44	2.41	4	2
1:A:375:GLN:NE2	1:A:375:GLN:CA	0.44	2.79	9	2
1:A:328:MET:SD	1:A:330:VAL:HG13	0.44	2.53	7	3
1:A:315:LYS:HG2	1:A:329:GLU:OE1	0.44	2.12	6	1
1:A:307:CYS:SG	1:A:335:THR:HG21	0.44	2.52	10	1
1:A:312:PHE:CD1	1:A:330:VAL:HB	0.43	2.49	13	1
1:A:312:PHE:CE1	1:A:385:VAL:O	0.43	2.72	5	2
1:A:312:PHE:CD1	1:A:332:PHE:CE2	0.43	3.06	16	1
1:A:357:LEU:HA	1:A:373:GLU:O	0.43	2.12	2	1
1:A:336:ARG:HH11	1:A:337:PRO:HB2	0.43	1.74	4	1
1:A:309:LYS:O	1:A:312:PHE:CE1	0.43	2.71	5	1
1:A:364:MET:HG2	1:A:369:GLY:CA	0.43	2.42	7	1
1:A:374:MET:SD	1:A:374:MET:N	0.43	2.92	20	2
1:A:303:THR:HG23	1:A:335:THR:HG23	0.43	1.90	17	4
1:A:312:PHE:CZ	1:A:364:MET:SD	0.43	3.11	11	1
1:A:317:ALA:HB1	1:A:390:HIS:CG	0.43	2.49	5	1
1:A:364:MET:N	1:A:364:MET:HE3	0.43	2.28	16	1
1:A:364:MET:SD	1:A:364:MET:N	0.43	2.92	15	1
1:A:326:VAL:HB	1:A:374:MET:CG	0.43	2.44	18	1
1:A:342:VAL:HG11	1:A:372:ILE:CD1	0.43	2.44	6	2
1:A:328:MET:HE1	1:A:383:ILE:HG21	0.42	1.90	12	1
1:A:358:ILE:HD13	1:A:358:ILE:N	0.42	2.29	20	1
1:A:374:MET:SD	1:A:383:ILE:HG12	0.42	2.55	18	1
1:A:312:PHE:CD2	1:A:332:PHE:CZ	0.42	3.06	9	1
1:A:304:TYR:O	1:A:305:THR:HB	0.42	2.14	11	2
1:A:315:LYS:HB3	1:A:329:GLU:O	0.42	2.13	20	2
1:A:330:VAL:HG21	1:A:340:ILE:CD1	0.42	2.45	14	1
1:A:376:LEU:HD13	1:A:376:LEU:C	0.42	2.35	16	1
1:A:311:LYS:HE3	1:A:335:THR:H	0.42	1.73	13	1
1:A:382:ILE:C	1:A:382:ILE:HD13	0.42	2.36	20	2
1:A:312:PHE:CD2	1:A:332:PHE:HE1	0.42	2.31	5	1
1:A:315:LYS:HB3	1:A:329:GLU:HB3	0.42	1.91	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:312:PHE:CE2	1:A:385:VAL:O	0.42	2.73	16	1
1:A:345:VAL:O	1:A:382:ILE:HG23	0.41	2.15	15	1
1:A:317:ALA:HB1	1:A:318:PRO:HD2	0.41	1.92	2	1
1:A:312:PHE:CZ	1:A:386:GLY:HA3	0.41	2.48	9	1
1:A:313:THR:HG22	1:A:331:GLY:O	0.41	2.15	12	1
1:A:318:PRO:HD3	1:A:390:HIS:CD2	0.41	2.50	20	1
1:A:307:CYS:HB3	1:A:364:MET:CE	0.41	2.45	13	1
1:A:345:VAL:HB	1:A:350:PRO:HA	0.41	1.93	2	1
1:A:391:GLN:HG2	1:A:392:TRP:N	0.41	2.31	2	1
1:A:328:MET:CE	1:A:385:VAL:HG22	0.41	2.45	12	1
1:A:381:ASN:HB2	1:A:394:GLN:OE1	0.41	2.15	3	1
1:A:362:PRO:O	1:A:364:MET:HE2	0.41	2.16	16	1
1:A:326:VAL:HG13	1:A:394:GLN:HE22	0.41	1.75	10	2
1:A:384:TYR:CE1	1:A:389:ASN:HB3	0.41	2.51	17	1
1:A:325:THR:HB	1:A:358:ILE:HG13	0.41	1.93	3	2
1:A:354:VAL:CG1	1:A:376:LEU:HG	0.41	2.46	6	1
1:A:336:ARG:NE	1:A:337:PRO:HD2	0.41	2.31	1	1
1:A:336:ARG:O	1:A:337:PRO:C	0.41	2.59	20	3
1:A:358:ILE:HB	1:A:373:GLU:HB2	0.41	1.93	6	1
1:A:358:ILE:N	1:A:358:ILE:HD13	0.41	2.31	7	2
1:A:330:VAL:HG11	1:A:385:VAL:HG21	0.41	1.91	17	1
1:A:354:VAL:CG1	1:A:376:LEU:HD22	0.41	2.46	12	1
1:A:392:TRP:HD1	1:A:394:GLN:OE1	0.40	1.99	6	1
1:A:312:PHE:CZ	1:A:340:ILE:HG23	0.40	2.52	18	1
1:A:338:CYS:SG	1:A:364:MET:CG	0.40	3.01	10	1
1:A:328:MET:CG	1:A:372:ILE:HD12	0.40	2.47	14	1
1:A:316:ARG:HB3	1:A:329:GLU:HB3	0.40	1.93	1	1
1:A:318:PRO:HD3	1:A:328:MET:HE3	0.40	1.94	17	1
1:A:307:CYS:HB2	1:A:332:PHE:CE2	0.40	2.52	20	1
1:A:318:PRO:HB3	1:A:383:ILE:HD12	0.40	1.93	13	1
1:A:326:VAL:HG21	1:A:375:GLN:HE21	0.40	1.76	20	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

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	88/102 (86%)	72±2 (81±2%)	12±2 (14±2%)	4±1 (5±1%)	4	26
All	All	1760/2040 (86%)	1431 (81%)	243 (14%)	86 (5%)	4	26

All 12 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	337	PRO	20
1	A	334	GLY	16
1	A	309	LYS	14
1	A	305	THR	13
1	A	377	PRO	6
1	A	324	ASP	5
1	A	378	PRO	4
1	A	352	VAL	3
1	A	318	PRO	2
1	A	357	LEU	1
1	A	369	GLY	1
1	A	347	HIS	1

### 6.3.2 Protein sidechains ⓘ

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	77/86 (90%)	65±2 (84±3%)	12±2 (16±3%)	5	42
All	All	1540/1720 (90%)	1298 (84%)	242 (16%)	5	42

All 36 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	382	ILE	20
1	A	307	CYS	20
1	A	375	GLN	17
1	A	337	PRO	16
1	A	372	ILE	15
1	A	328	MET	14

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Mol	Chain	Res	Type	Models (Total)
1	A	326	VAL	14
1	A	312	PHE	14
1	A	332	PHE	13
1	A	374	MET	13
1	A	384	TYR	10
1	A	309	LYS	9
1	A	394	GLN	9
1	A	363	THR	6
1	A	330	VAL	6
1	A	395	LYS	5
1	A	356	MET	5
1	A	381	ASN	4
1	A	388	LEU	4
1	A	391	GLN	4
1	A	336	ARG	3
1	A	392	TRP	3
1	A	364	MET	2
1	A	390	HIS	2
1	A	342	VAL	2
1	A	304	TYR	2
1	A	320	ASP	1
1	A	361	ASN	1
1	A	325	THR	1
1	A	339	ARG	1
1	A	387	ASP	1
1	A	315	LYS	1
1	A	376	LEU	1
1	A	380	ASP	1
1	A	335	THR	1
1	A	318	PRO	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 [i](#)

There are no carbohydrates 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

The completeness of assignment taking into account all chemical shift lists is 81% for the well-defined parts and 81% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_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	1048
Number of shifts mapped to atoms	1048
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	100	$-0.11 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	88	$-0.08 \pm 0.18$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	92	$0.11 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	93	$0.03 \pm 0.43$	None needed ( $< 0.5$ ppm)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 81%, i.e. 872 atoms were assigned a chemical shift out of a possible 1082. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	414/434 (95%)	165/172 (96%)	168/180 (93%)	81/82 (99%)
Sidechain	424/548 (77%)	256/322 (80%)	158/203 (78%)	10/23 (43%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	34/100 (34%)	18/52 (35%)	14/40 (35%)	2/8 (25%)
Overall	872/1082 (81%)	439/546 (80%)	340/423 (80%)	93/113 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 905 atoms were assigned a chemical shift out of a possible 1118. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	429/449 (96%)	171/178 (96%)	174/186 (94%)	84/85 (99%)
Sidechain	442/569 (78%)	268/334 (80%)	162/210 (77%)	12/25 (48%)
Aromatic	34/100 (34%)	18/52 (35%)	14/40 (35%)	2/8 (25%)
Overall	905/1118 (81%)	457/564 (81%)	350/436 (80%)	98/118 (83%)

#### 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.

Random coil index (RCI) for chain A:

