



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:00 pm BST

PDB ID : 2LCY  
Title : NMR Structure of the Complete Internal Fusion Loop from Ebolavirus GP2 at pH 5.5  
Authors : Gregory, S.M.; Harada, E.; Liang, B.; Tamm, L.K.  
Deposited on : 2011-05-12

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

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

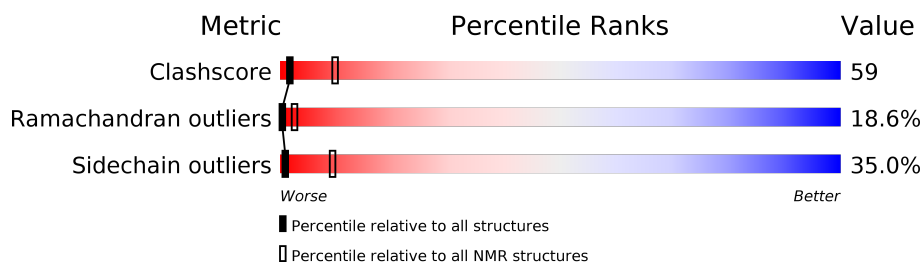
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

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	54	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:507-A:560 (54)	0.51	17

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 815 atoms, of which 396 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Virion spike glycoprotein.

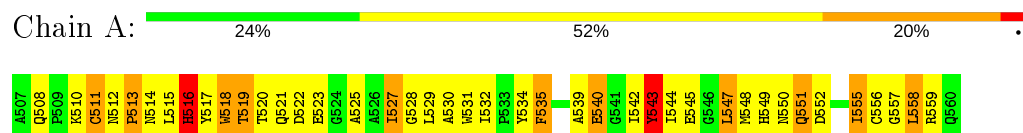
Mol	Chain	Residues	Atoms						Trace
1	A	54	Total	C	H	N	O	S	0
			815	268	396	71	77	3	

## 4 Residue-property plots [i](#)

### 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: Virion spike glycoprotein

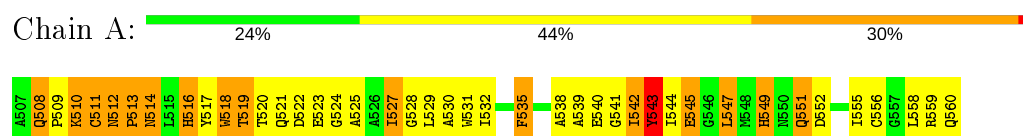


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

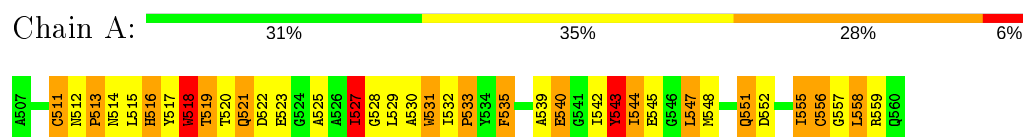
#### 4.2.1 Score per residue for model 1

- Molecule 1: Virion spike glycoprotein



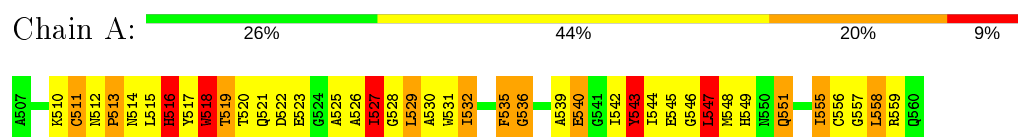
#### 4.2.2 Score per residue for model 2

- Molecule 1: Virion spike glycoprotein



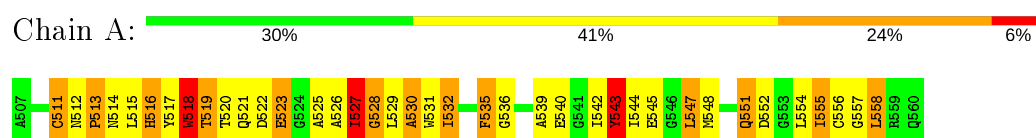
### 4.2.3 Score per residue for model 3

- Molecule 1: Virion spike glycoprotein



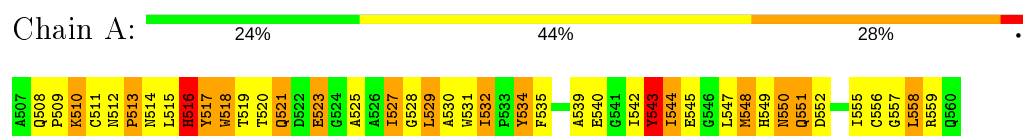
### 4.2.4 Score per residue for model 4

- Molecule 1: Virion spike glycoprotein



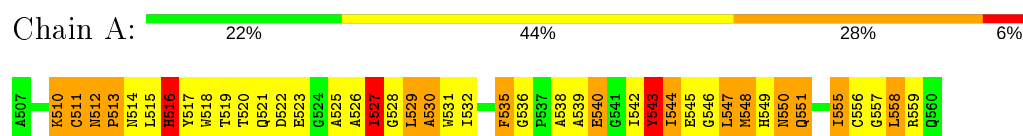
### 4.2.5 Score per residue for model 5

- Molecule 1: Virion spike glycoprotein



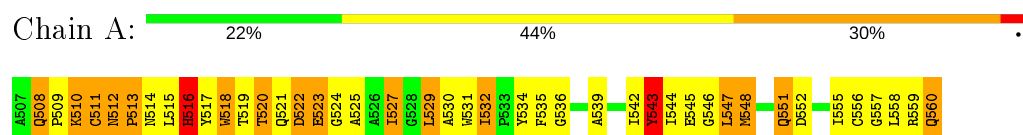
### 4.2.6 Score per residue for model 6

- Molecule 1: Virion spike glycoprotein



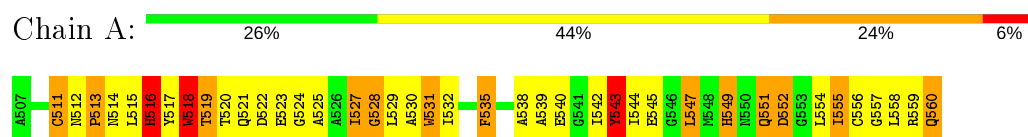
### 4.2.7 Score per residue for model 7

- Molecule 1: Virion spike glycoprotein



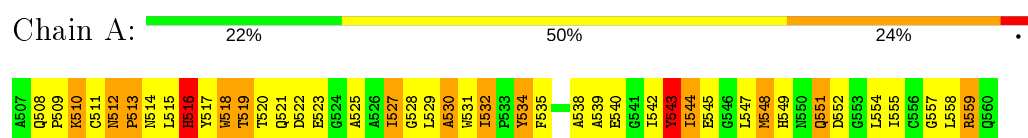
### 4.2.8 Score per residue for model 8

- Molecule 1: Virion spike glycoprotein



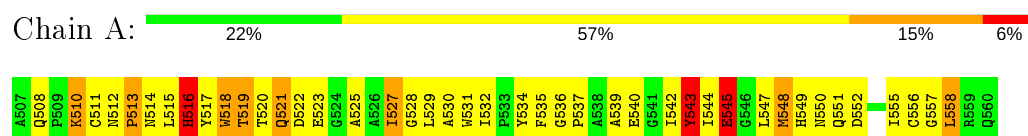
### 4.2.9 Score per residue for model 9

- Molecule 1: Virion spike glycoprotein



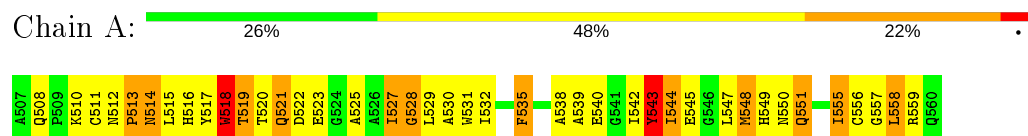
### 4.2.10 Score per residue for model 10

- Molecule 1: Virion spike glycoprotein



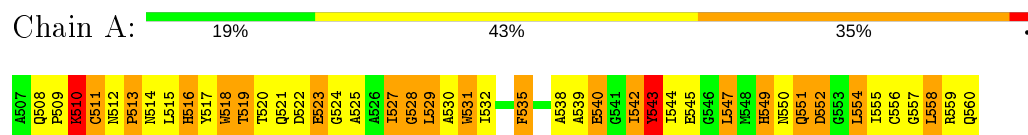
### 4.2.11 Score per residue for model 11

- Molecule 1: Virion spike glycoprotein



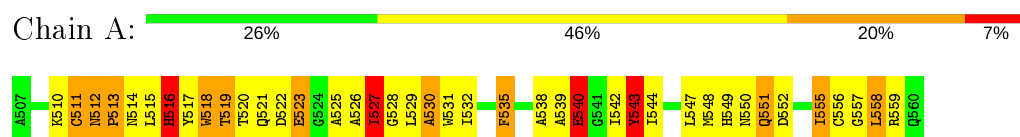
### 4.2.12 Score per residue for model 12

- Molecule 1: Virion spike glycoprotein



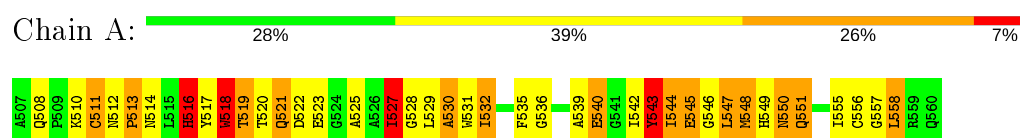
### 4.2.13 Score per residue for model 13

- Molecule 1: Virion spike glycoprotein



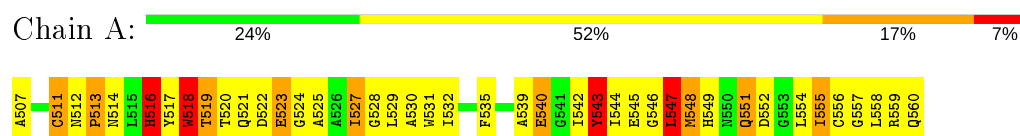
### 4.2.14 Score per residue for model 14

- Molecule 1: Virion spike glycoprotein



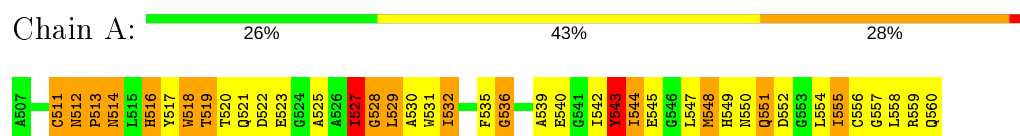
### 4.2.15 Score per residue for model 15

- Molecule 1: Virion spike glycoprotein



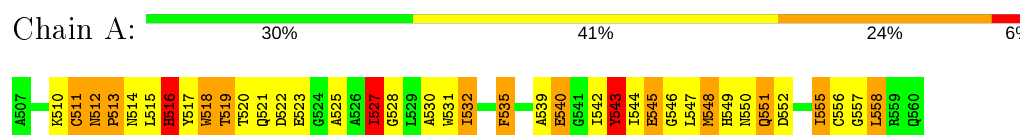
### 4.2.16 Score per residue for model 16

- Molecule 1: Virion spike glycoprotein



### 4.2.17 Score per residue for model 17 (medoid)

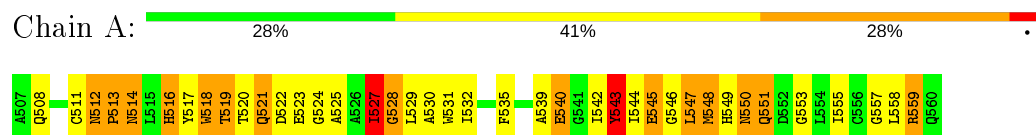
- Molecule 1: Virion spike glycoprotein





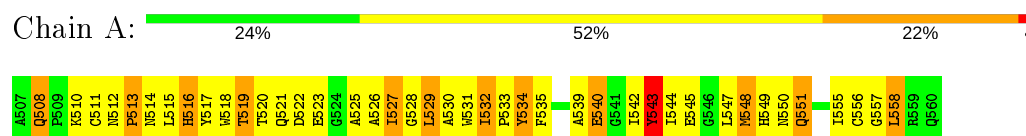
#### 4.2.18 Score per residue for model 18

- Molecule 1: Virion spike glycoprotein



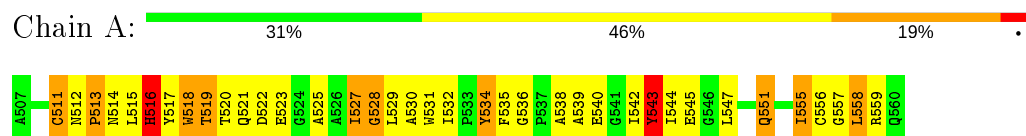
#### 4.2.19 Score per residue for model 19

- Molecule 1: Virion spike glycoprotein



#### 4.2.20 Score per residue for model 20

- Molecule 1: Virion spike glycoprotein



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *20 structures for lowest energy*.

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

Software name	Classification	Version
CNS	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	523
Number of shifts mapped to atoms	523
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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	419	396	391	47±6
All	All	8380	7920	7820	948

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 59.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:557:GLY:O	1:A:558:LEU:HD23	0.93	1.64	14	12
1:A:513:PRO:HB3	1:A:555:ILE:HD12	0.85	1.45	5	10
1:A:530:ALA:HB2	1:A:544:ILE:CG2	0.84	2.02	1	7
1:A:539:ALA:HA	1:A:542:ILE:HD12	0.82	1.51	20	17
1:A:557:GLY:C	1:A:558:LEU:HD23	0.81	1.96	12	5
1:A:512:ASN:N	1:A:513:PRO:HD3	0.80	1.91	5	19
1:A:530:ALA:CB	1:A:544:ILE:HG21	0.80	2.07	2	3
1:A:547:LEU:O	1:A:547:LEU:HD12	0.78	1.77	10	4
1:A:521:GLN:HA	1:A:525:ALA:HB3	0.76	1.55	5	20
1:A:535:PHE:HB2	1:A:538:ALA:HB3	0.76	1.57	11	7
1:A:539:ALA:O	1:A:542:ILE:HD12	0.76	1.81	18	5
1:A:539:ALA:HB3	1:A:545:GLU:HA	0.73	1.60	4	14
1:A:512:ASN:N	1:A:513:PRO:CD	0.73	2.52	12	20
1:A:530:ALA:HB2	1:A:544:ILE:HG21	0.72	1.62	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:516:HIS:O	1:A:519:THR:HG22	0.72	1.84	5	20
1:A:544:ILE:O	1:A:547:LEU:HD23	0.72	1.85	3	6
1:A:529:LEU:O	1:A:544:ILE:HG21	0.72	1.83	5	5
1:A:525:ALA:CB	1:A:547:LEU:HD11	0.71	2.16	12	5
1:A:528:GLY:C	1:A:529:LEU:HD23	0.71	2.06	12	1
1:A:557:GLY:C	1:A:558:LEU:HD12	0.69	2.08	7	3
1:A:528:GLY:C	1:A:529:LEU:HD12	0.67	2.10	9	2
1:A:525:ALA:HA	1:A:530:ALA:HB2	0.67	1.64	5	7
1:A:547:LEU:HD12	1:A:547:LEU:O	0.66	1.90	16	8
1:A:513:PRO:HD2	1:A:515:LEU:HD23	0.65	1.66	11	2
1:A:529:LEU:HD22	1:A:535:PHE:CZ	0.65	2.27	4	1
1:A:525:ALA:HB2	1:A:544:ILE:HG23	0.64	1.69	17	2
1:A:539:ALA:HB1	1:A:542:ILE:HD11	0.64	1.70	2	1
1:A:544:ILE:O	1:A:547:LEU:HD21	0.63	1.94	6	8
1:A:521:GLN:HA	1:A:525:ALA:CB	0.62	2.24	18	19
1:A:511:CYS:HA	1:A:556:CYS:HA	0.61	1.72	11	13
1:A:528:GLY:O	1:A:529:LEU:HD12	0.61	1.94	11	6
1:A:539:ALA:CA	1:A:542:ILE:HD12	0.61	2.25	20	14
1:A:546:GLY:O	1:A:548:MET:N	0.61	2.34	15	2
1:A:514:ASN:O	1:A:515:LEU:HD13	0.60	1.96	12	1
1:A:542:ILE:HD13	1:A:542:ILE:N	0.60	2.12	1	1
1:A:532:ILE:HB	1:A:534:TYR:CE2	0.60	2.32	19	1
1:A:544:ILE:HG22	1:A:547:LEU:HG	0.60	1.72	17	1
1:A:521:GLN:CA	1:A:525:ALA:HB3	0.60	2.27	5	19
1:A:510:LYS:HB2	1:A:555:ILE:HG22	0.59	1.75	11	4
1:A:529:LEU:O	1:A:530:ALA:CB	0.59	2.51	13	5
1:A:544:ILE:O	1:A:547:LEU:HG	0.59	1.97	20	2
1:A:524:GLY:O	1:A:544:ILE:HG23	0.58	1.98	12	4
1:A:514:ASN:HB3	1:A:552:ASP:HA	0.58	1.75	7	8
1:A:558:LEU:HD12	1:A:558:LEU:N	0.58	2.13	16	1
1:A:535:PHE:CD2	1:A:539:ALA:HB2	0.58	2.34	12	7
1:A:530:ALA:HA	1:A:544:ILE:HG21	0.58	1.76	3	5
1:A:529:LEU:HB2	1:A:544:ILE:HD13	0.58	1.75	13	1
1:A:528:GLY:O	1:A:529:LEU:HD23	0.58	1.99	20	2
1:A:508:GLN:HG3	1:A:555:ILE:HG23	0.57	1.73	12	8
1:A:558:LEU:N	1:A:558:LEU:HD12	0.57	2.15	15	1
1:A:525:ALA:HB1	1:A:547:LEU:HD11	0.57	1.77	1	4
1:A:513:PRO:CB	1:A:555:ILE:HD12	0.57	2.29	10	9
1:A:511:CYS:HA	1:A:556:CYS:CA	0.57	2.30	10	18
1:A:515:LEU:HD22	1:A:515:LEU:N	0.57	2.15	13	4
1:A:514:ASN:HA	1:A:517:TYR:CD1	0.57	2.34	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:529:LEU:HD23	1:A:532:ILE:CD1	0.57	2.29	4	1
1:A:547:LEU:CD1	1:A:547:LEU:O	0.56	2.53	10	8
1:A:529:LEU:O	1:A:530:ALA:HB3	0.56	2.01	14	2
1:A:539:ALA:CB	1:A:542:ILE:HD11	0.56	2.31	2	1
1:A:555:ILE:N	1:A:555:ILE:HD13	0.56	2.16	3	5
1:A:508:GLN:HB2	1:A:555:ILE:HG23	0.56	1.77	7	1
1:A:520:THR:HG21	1:A:543:TYR:O	0.55	2.02	14	2
1:A:555:ILE:HD13	1:A:555:ILE:N	0.55	2.16	4	5
1:A:529:LEU:O	1:A:530:ALA:HB2	0.55	2.02	9	3
1:A:532:ILE:H	1:A:532:ILE:HD13	0.55	1.61	9	3
1:A:532:ILE:HG23	1:A:532:ILE:O	0.55	2.02	15	4
1:A:532:ILE:HD11	1:A:535:PHE:HB2	0.54	1.77	14	4
1:A:530:ALA:N	1:A:544:ILE:HG21	0.54	2.18	12	2
1:A:535:PHE:CZ	1:A:544:ILE:HD13	0.54	2.37	10	1
1:A:532:ILE:O	1:A:532:ILE:HG23	0.54	2.03	18	4
1:A:515:LEU:N	1:A:515:LEU:HD22	0.54	2.18	10	8
1:A:510:LYS:HB2	1:A:555:ILE:HG21	0.53	1.81	7	2
1:A:547:LEU:O	1:A:547:LEU:CD1	0.53	2.56	5	1
1:A:529:LEU:HG	1:A:532:ILE:HG21	0.53	1.79	8	3
1:A:519:THR:HG23	1:A:520:THR:N	0.53	2.19	7	19
1:A:547:LEU:C	1:A:547:LEU:HD12	0.53	2.23	2	7
1:A:552:ASP:OD1	1:A:554:LEU:HD21	0.53	2.03	4	1
1:A:521:GLN:O	1:A:525:ALA:HB3	0.52	2.05	6	18
1:A:523:GLU:HA	1:A:527:ILE:HD11	0.52	1.80	4	19
1:A:510:LYS:HB2	1:A:555:ILE:CG2	0.52	2.35	14	3
1:A:544:ILE:O	1:A:547:LEU:CD2	0.52	2.57	14	13
1:A:529:LEU:CG	1:A:532:ILE:HG21	0.52	2.34	1	1
1:A:532:ILE:HG12	1:A:532:ILE:O	0.52	2.04	9	1
1:A:525:ALA:HB2	1:A:547:LEU:HD11	0.52	1.82	13	4
1:A:513:PRO:C	1:A:551:GLN:HB3	0.52	2.25	4	16
1:A:535:PHE:CD1	1:A:535:PHE:N	0.52	2.77	13	5
1:A:508:GLN:CB	1:A:555:ILE:HG23	0.51	2.36	7	1
1:A:543:TYR:CD1	1:A:543:TYR:N	0.51	2.78	18	11
1:A:552:ASP:OD2	1:A:554:LEU:HD21	0.51	2.04	9	1
1:A:510:LYS:O	1:A:511:CYS:HB2	0.51	2.06	12	9
1:A:529:LEU:HD23	1:A:532:ILE:HD12	0.51	1.82	4	1
1:A:511:CYS:CA	1:A:556:CYS:HA	0.51	2.36	5	4
1:A:550:ASN:O	1:A:551:GLN:CB	0.50	2.59	5	6
1:A:543:TYR:N	1:A:543:TYR:CD1	0.50	2.78	9	9
1:A:557:GLY:HA3	1:A:560:GLN:NE2	0.50	2.20	7	4
1:A:543:TYR:CD1	1:A:544:ILE:HD12	0.50	2.41	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:529:LEU:HB3	1:A:532:ILE:HD11	0.50	1.82	9	1
1:A:532:ILE:HD13	1:A:532:ILE:N	0.50	2.21	9	1
1:A:513:PRO:CA	1:A:555:ILE:HD12	0.50	2.37	10	3
1:A:529:LEU:C	1:A:544:ILE:HG21	0.50	2.27	12	1
1:A:532:ILE:O	1:A:532:ILE:CG1	0.50	2.59	19	2
1:A:547:LEU:HD12	1:A:547:LEU:C	0.50	2.27	18	6
1:A:509:PRO:O	1:A:510:LYS:HG3	0.49	2.07	9	3
1:A:513:PRO:CD	1:A:556:CYS:HB2	0.49	2.37	8	4
1:A:535:PHE:CB	1:A:538:ALA:HB3	0.49	2.33	11	3
1:A:523:GLU:CA	1:A:527:ILE:HD11	0.49	2.38	7	1
1:A:530:ALA:CA	1:A:544:ILE:HG21	0.49	2.38	15	2
1:A:547:LEU:HD12	1:A:548:MET:H	0.49	1.65	15	1
1:A:511:CYS:HA	1:A:556:CYS:CB	0.48	2.38	10	13
1:A:513:PRO:CA	1:A:551:GLN:HB3	0.48	2.39	12	1
1:A:549:HIS:O	1:A:550:ASN:HB2	0.48	2.08	17	2
1:A:512:ASN:N	1:A:513:PRO:HD2	0.48	2.23	12	1
1:A:529:LEU:HD23	1:A:529:LEU:N	0.48	2.22	12	1
1:A:534:TYR:CG	1:A:535:PHE:N	0.48	2.81	9	1
1:A:514:ASN:OD1	1:A:553:GLY:N	0.48	2.47	18	1
1:A:554:LEU:HB2	1:A:555:ILE:HD13	0.48	1.84	16	4
1:A:516:HIS:O	1:A:519:THR:CG2	0.48	2.61	5	2
1:A:509:PRO:O	1:A:510:LYS:CG	0.48	2.62	12	2
1:A:535:PHE:HD2	1:A:539:ALA:HB2	0.48	1.66	19	3
1:A:539:ALA:O	1:A:540:GLU:C	0.47	2.52	13	1
1:A:532:ILE:O	1:A:532:ILE:HG12	0.47	2.10	19	2
1:A:529:LEU:CD2	1:A:535:PHE:CE1	0.47	2.97	4	1
1:A:511:CYS:N	1:A:556:CYS:HA	0.47	2.23	12	1
1:A:558:LEU:HD12	1:A:558:LEU:H	0.47	1.70	16	3
1:A:535:PHE:N	1:A:535:PHE:CD1	0.47	2.82	6	2
1:A:542:ILE:HG22	1:A:543:TYR:CE2	0.47	2.44	14	2
1:A:532:ILE:CG1	1:A:535:PHE:CZ	0.47	2.98	17	1
1:A:520:THR:O	1:A:524:GLY:N	0.46	2.48	7	1
1:A:508:GLN:CG	1:A:555:ILE:HG23	0.46	2.41	7	1
1:A:535:PHE:CD1	1:A:539:ALA:HB2	0.46	2.45	3	1
1:A:547:LEU:O	1:A:547:LEU:HG	0.46	2.10	20	2
1:A:529:LEU:HB3	1:A:532:ILE:HG23	0.46	1.88	10	1
1:A:529:LEU:CD1	1:A:535:PHE:CZ	0.46	2.98	14	1
1:A:534:TYR:CD1	1:A:535:PHE:N	0.46	2.84	9	2
1:A:540:GLU:HA	1:A:545:GLU:CG	0.46	2.41	6	5
1:A:552:ASP:CG	1:A:554:LEU:HD21	0.46	2.31	9	1
1:A:512:ASN:O	1:A:512:ASN:ND2	0.46	2.48	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:547:LEU:CB	1:A:549:HIS:CE1	0.46	2.99	8	3
1:A:519:THR:HG23	1:A:520:THR:H	0.46	1.70	17	18
1:A:530:ALA:CB	1:A:544:ILE:CG2	0.46	2.88	12	3
1:A:513:PRO:HB3	1:A:555:ILE:CD1	0.45	2.41	12	1
1:A:547:LEU:O	1:A:548:MET:HE3	0.45	2.10	3	1
1:A:514:ASN:ND2	1:A:551:GLN:O	0.45	2.49	11	1
1:A:547:LEU:CA	1:A:549:HIS:CE1	0.45	2.99	12	3
1:A:529:LEU:HB3	1:A:532:ILE:CG2	0.45	2.41	2	3
1:A:519:THR:CG2	1:A:520:THR:N	0.45	2.79	7	1
1:A:547:LEU:C	1:A:549:HIS:H	0.45	2.14	19	9
1:A:547:LEU:HA	1:A:549:HIS:CE1	0.45	2.47	12	3
1:A:532:ILE:HD11	1:A:535:PHE:CZ	0.45	2.47	17	1
1:A:539:ALA:HA	1:A:542:ILE:CD1	0.45	2.42	17	7
1:A:547:LEU:HD12	1:A:548:MET:N	0.45	2.27	15	1
1:A:547:LEU:O	1:A:549:HIS:N	0.45	2.49	14	7
1:A:540:GLU:O	1:A:540:GLU:CG	0.45	2.65	16	4
1:A:518:TRP:CD1	1:A:518:TRP:O	0.45	2.70	11	6
1:A:529:LEU:CD2	1:A:535:PHE:CZ	0.45	3.00	4	1
1:A:533:PRO:O	1:A:534:TYR:CD1	0.45	2.70	19	1
1:A:550:ASN:O	1:A:551:GLN:HB2	0.44	2.12	5	4
1:A:517:TYR:CG	1:A:518:TRP:N	0.44	2.86	4	4
1:A:526:ALA:C	1:A:527:ILE:HD13	0.44	2.32	4	5
1:A:540:GLU:CG	1:A:540:GLU:O	0.44	2.65	4	6
1:A:532:ILE:N	1:A:532:ILE:CD1	0.44	2.81	5	2
1:A:517:TYR:O	1:A:521:GLN:CG	0.44	2.66	11	1
1:A:525:ALA:CA	1:A:530:ALA:HB2	0.44	2.38	5	1
1:A:530:ALA:HB2	1:A:544:ILE:HG22	0.44	1.83	12	3
1:A:507:ALA:CB	1:A:558:LEU:HD23	0.44	2.43	15	1
1:A:514:ASN:O	1:A:517:TYR:CE1	0.44	2.70	6	16
1:A:508:GLN:O	1:A:555:ILE:HG23	0.44	2.12	9	1
1:A:532:ILE:CG1	1:A:532:ILE:O	0.44	2.66	20	2
1:A:540:GLU:HA	1:A:545:GLU:HG2	0.43	1.90	14	2
1:A:517:TYR:HB2	1:A:521:GLN:HG2	0.43	1.90	2	5
1:A:529:LEU:O	1:A:544:ILE:CB	0.43	2.67	6	1
1:A:521:GLN:O	1:A:522:ASP:CB	0.43	2.65	7	1
1:A:560:GLN:NE2	1:A:560:GLN:N	0.43	2.65	1	1
1:A:539:ALA:C	1:A:542:ILE:HD12	0.43	2.34	19	3
1:A:544:ILE:C	1:A:545:GLU:HG3	0.43	2.33	6	3
1:A:530:ALA:HB2	1:A:544:ILE:HG23	0.43	1.88	11	1
1:A:529:LEU:HB3	1:A:532:ILE:HG21	0.43	1.90	12	1
1:A:544:ILE:O	1:A:545:GLU:CB	0.43	2.67	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:524:GLY:O	1:A:544:ILE:HG12	0.43	2.12	18	2
1:A:523:GLU:O	1:A:527:ILE:CG1	0.43	2.67	14	8
1:A:547:LEU:O	1:A:547:LEU:CG	0.43	2.66	20	2
1:A:532:ILE:N	1:A:532:ILE:HD13	0.43	2.28	5	1
1:A:535:PHE:O	1:A:538:ALA:HB3	0.43	2.14	9	1
1:A:518:TRP:CD1	1:A:518:TRP:N	0.43	2.84	4	7
1:A:511:CYS:C	1:A:513:PRO:HD3	0.43	2.33	5	1
1:A:532:ILE:HD13	1:A:532:ILE:H	0.43	1.73	17	1
1:A:535:PHE:CE2	1:A:539:ALA:HB2	0.43	2.49	5	1
1:A:555:ILE:HD12	1:A:555:ILE:H	0.43	1.73	12	1
1:A:549:HIS:C	1:A:551:GLN:H	0.42	2.17	19	4
1:A:546:GLY:O	1:A:548:MET:HE2	0.42	2.14	17	2
1:A:535:PHE:O	1:A:536:GLY:O	0.42	2.37	16	2
1:A:542:ILE:C	1:A:543:TYR:CG	0.42	2.93	13	4
1:A:529:LEU:CB	1:A:544:ILE:HD13	0.42	2.45	4	1
1:A:555:ILE:CD1	1:A:555:ILE:N	0.42	2.81	3	2
1:A:514:ASN:O	1:A:517:TYR:CD1	0.42	2.72	8	10
1:A:539:ALA:CB	1:A:542:ILE:HD12	0.42	2.45	13	1
1:A:521:GLN:NE2	1:A:522:ASP:N	0.42	2.67	7	1
1:A:529:LEU:HD22	1:A:532:ILE:HG21	0.42	1.90	10	1
1:A:539:ALA:HB3	1:A:545:GLU:H	0.42	1.75	20	1
1:A:521:GLN:CD	1:A:521:GLN:C	0.42	2.79	2	1
1:A:560:GLN:N	1:A:560:GLN:NE2	0.42	2.68	7	1
1:A:530:ALA:HA	1:A:544:ILE:CG2	0.42	2.45	20	1
1:A:546:GLY:O	1:A:547:LEU:HG	0.42	2.14	3	1
1:A:535:PHE:HZ	1:A:544:ILE:HD13	0.42	1.74	5	1
1:A:518:TRP:O	1:A:518:TRP:CD1	0.42	2.73	1	5
1:A:530:ALA:HB1	1:A:544:ILE:HG21	0.42	1.92	17	2
1:A:539:ALA:HB1	1:A:542:ILE:HD12	0.42	1.92	13	1
1:A:520:THR:HG1	1:A:543:TYR:C	0.42	2.17	3	1
1:A:529:LEU:O	1:A:532:ILE:CD1	0.41	2.68	7	2
1:A:528:GLY:O	1:A:531:TRP:CZ2	0.41	2.73	8	2
1:A:518:TRP:N	1:A:518:TRP:CD1	0.41	2.88	3	2
1:A:521:GLN:O	1:A:522:ASP:HB2	0.41	2.15	7	1
1:A:524:GLY:O	1:A:544:ILE:CG1	0.41	2.68	8	1
1:A:547:LEU:HB2	1:A:549:HIS:CE1	0.41	2.50	12	3
1:A:532:ILE:HG13	1:A:535:PHE:CD1	0.41	2.50	4	1
1:A:547:LEU:HG	1:A:547:LEU:O	0.41	2.15	4	1
1:A:555:ILE:N	1:A:555:ILE:CD1	0.41	2.81	4	2
1:A:534:TYR:CD2	1:A:535:PHE:HD1	0.41	2.34	20	1
1:A:517:TYR:CD2	1:A:521:GLN:HG2	0.41	2.51	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:539:ALA:HB3	1:A:545:GLU:CA	0.41	2.44	16	2
1:A:531:TRP:O	1:A:533:PRO:HD3	0.41	2.14	2	1
1:A:547:LEU:CG	1:A:547:LEU:O	0.41	2.69	13	1
1:A:517:TYR:CD2	1:A:550:ASN:O	0.41	2.73	10	2
1:A:532:ILE:HB	1:A:534:TYR:CZ	0.41	2.50	19	1
1:A:520:THR:O	1:A:525:ALA:N	0.41	2.53	5	1
1:A:515:LEU:O	1:A:516:HIS:CG	0.41	2.74	7	1
1:A:514:ASN:C	1:A:515:LEU:HD13	0.41	2.35	12	1
1:A:546:GLY:C	1:A:547:LEU:HG	0.41	2.36	15	1
1:A:517:TYR:HB2	1:A:550:ASN:O	0.41	2.15	5	1
1:A:536:GLY:N	1:A:537:PRO:HD2	0.41	2.31	10	1
1:A:532:ILE:HD13	1:A:532:ILE:O	0.41	2.15	19	1
1:A:534:TYR:CD1	1:A:534:TYR:C	0.40	2.94	20	1
1:A:549:HIS:O	1:A:551:GLN:N	0.40	2.50	5	1
1:A:554:LEU:CD2	1:A:554:LEU:N	0.40	2.84	12	1
1:A:524:GLY:O	1:A:544:ILE:CG2	0.40	2.70	18	1
1:A:532:ILE:HG13	1:A:534:TYR:CE1	0.40	2.51	7	1
1:A:539:ALA:O	1:A:541:GLY:N	0.40	2.55	1	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	52/54 (96%)	24±2 (47±4%)	18±2 (35±4%)	10±2 (19±4%)	0	2
All	All	1040/1080 (96%)	484 (47%)	363 (35%)	193 (19%)	0	2

All 22 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	543	TYR	20
1	A	513	PRO	20
1	A	551	GLN	20
1	A	516	HIS	18

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Mol	Chain	Res	Type	Models (Total)
1	A	528	GLY	17
1	A	519	THR	17
1	A	540	GLU	13
1	A	548	MET	9
1	A	527	ILE	9
1	A	518	TRP	8
1	A	536	GLY	7
1	A	547	LEU	5
1	A	545	GLU	5
1	A	530	ALA	5
1	A	544	ILE	4
1	A	510	LYS	4
1	A	546	GLY	3
1	A	534	TYR	3
1	A	509	PRO	2
1	A	559	ARG	2
1	A	533	PRO	1
1	A	511	CYS	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	41/41 (100%)	27±2 (65±6%)	14±2 (35±6%)	<b>1</b> <b>9</b>
All	All	820/820 (100%)	533 (65%)	287 (35%)	<b>1</b> <b>9</b>

All 34 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	TRP	20
1	A	531	TRP	20
1	A	527	ILE	20
1	A	543	TYR	20
1	A	522	ASP	19
1	A	548	MET	15
1	A	511	CYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	559	ARG	15
1	A	558	LEU	14
1	A	516	HIS	13
1	A	535	PHE	13
1	A	555	ILE	11
1	A	532	ILE	10
1	A	512	ASN	8
1	A	547	LEU	8
1	A	529	LEU	7
1	A	521	GLN	6
1	A	523	GLU	6
1	A	552	ASP	5
1	A	549	HIS	5
1	A	550	ASN	5
1	A	514	ASN	4
1	A	508	GLN	4
1	A	545	GLU	4
1	A	510	LYS	4
1	A	544	ILE	3
1	A	560	GLN	3
1	A	542	ILE	2
1	A	534	TYR	2
1	A	540	GLU	2
1	A	517	TYR	1
1	A	520	THR	1
1	A	556	CYS	1
1	A	554	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 carbohydrates 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 76% for the well-defined parts and 76% 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	523
Number of shifts mapped to atoms	523
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
$^{13}\text{C}_\alpha$	54	$0.01 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	43	$-0.07 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	48	$0.65 \pm 0.22$	Should be applied

#### 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 76%, i.e. 486 atoms were assigned a chemical shift out of a possible 640. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	205/262 (78%)	103/104 (99%)	54/108 (50%)	48/50 (96%)
Sidechain	223/305 (73%)	163/180 (91%)	60/114 (53%)	0/11 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	58/73 (79%)	31/37 (84%)	27/30 (90%)	0/6 (0%)
Overall	486/640 (76%)	297/321 (93%)	141/252 (56%)	48/67 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 76%, i.e. 486 atoms were assigned a chemical shift out of a possible 640. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	205/262 (78%)	103/104 (99%)	54/108 (50%)	48/50 (96%)
Sidechain	223/305 (73%)	163/180 (91%)	60/114 (53%)	0/11 (0%)
Aromatic	58/73 (79%)	31/37 (84%)	27/30 (90%)	0/6 (0%)
Overall	486/640 (76%)	297/321 (93%)	141/252 (56%)	48/67 (72%)

#### 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:

