



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:29 pm BST

PDB ID : 2M2V  
Title : African Swine Fever Virus Pol X in the ternary complex with MgdGTP and DNA  
Authors : Wu, W.; Su, M.; Tsai, M.  
Deposited on : 2013-01-03

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

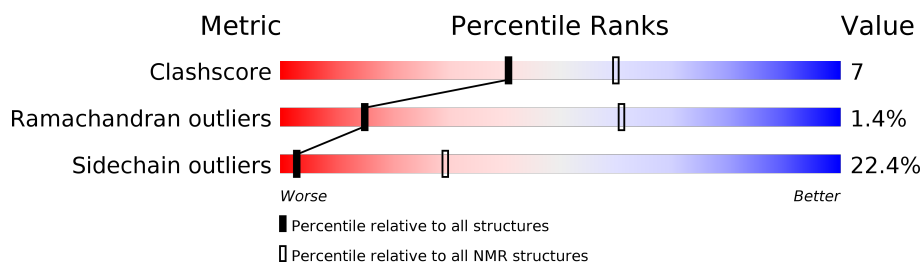
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 44%.

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	174	 66% 30% . .

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 13 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:1-A:80, A:85-A:173 (169)	0.39	13

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 and 2 single-model clusters were found.

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

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

There is only 1 type of molecule in this entry. The entry contains 3006 atoms, of which 1572 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Repair DNA polymerase X.

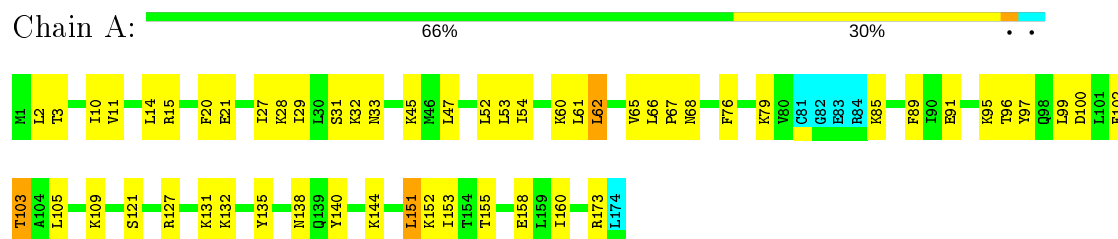
Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			3006	943	1572	248	239	4	

## 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: Repair DNA polymerase X

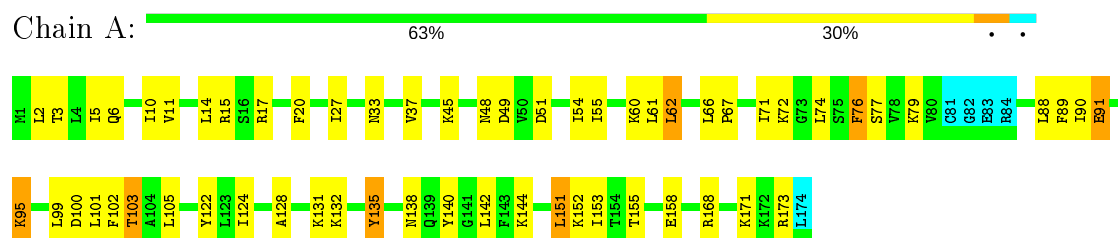


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

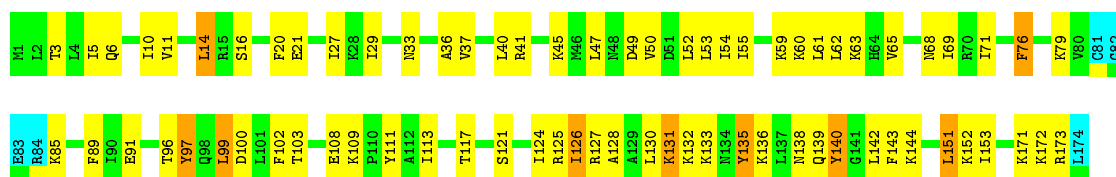
- Molecule 1: Repair DNA polymerase X



#### 4.2.2 Score per residue for model 2

- Molecule 1: Repair DNA polymerase X

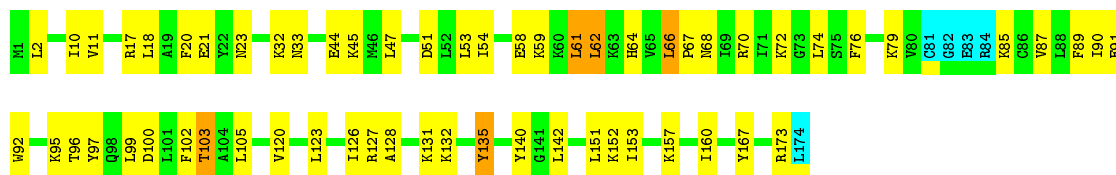




### 4.2.3 Score per residue for model 3

- Molecule 1: Repair DNA polymerase X

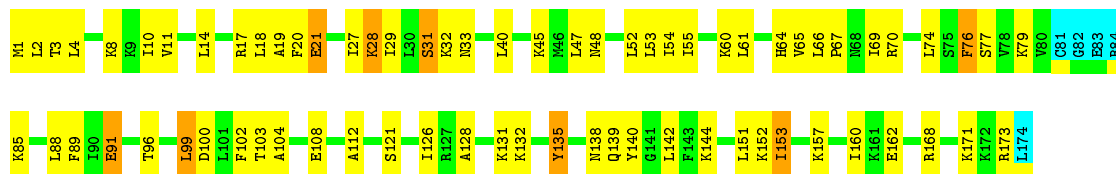
Chain A: 63% 32%



### 4.2.4 Score per residue for model 4

- Molecule 1: Repair DNA polymerase X

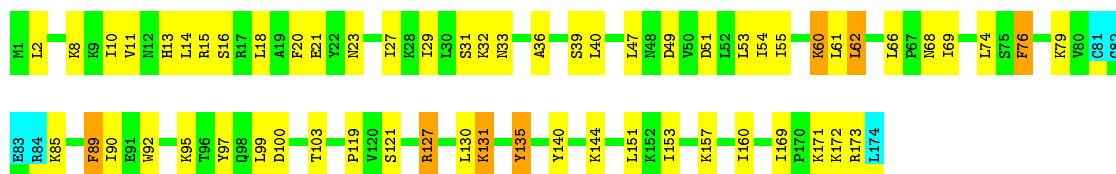
Chain A: 56% 36% 5%



### 4.2.5 Score per residue for model 5

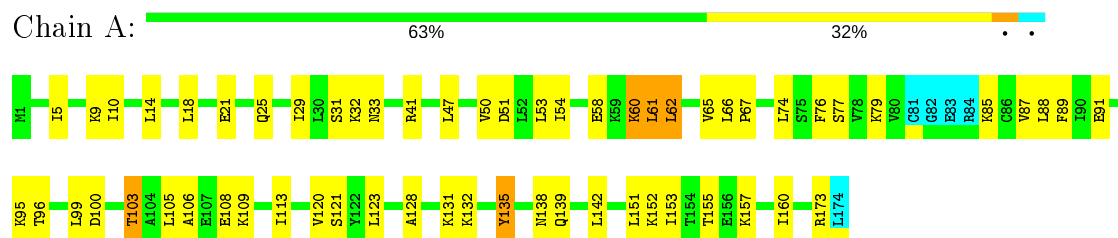
- Molecule 1: Repair DNA polymerase X

Chain A: 63% 30%



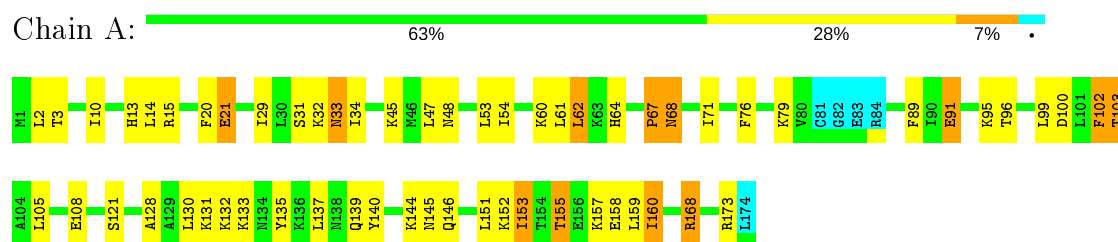
### 4.2.6 Score per residue for model 6

- Molecule 1: Repair DNA polymerase X



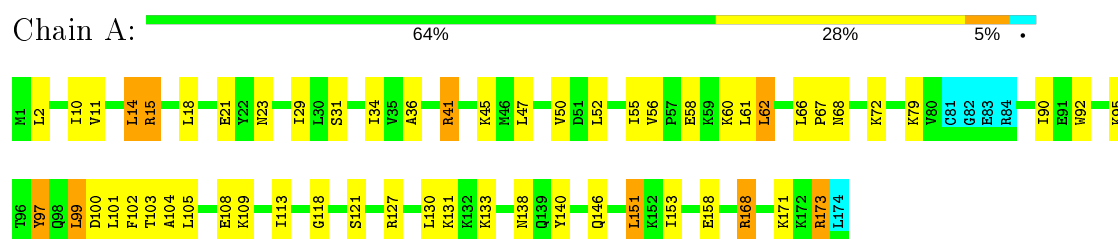
#### 4.2.7 Score per residue for model 7

- Molecule 1: Repair DNA polymerase X



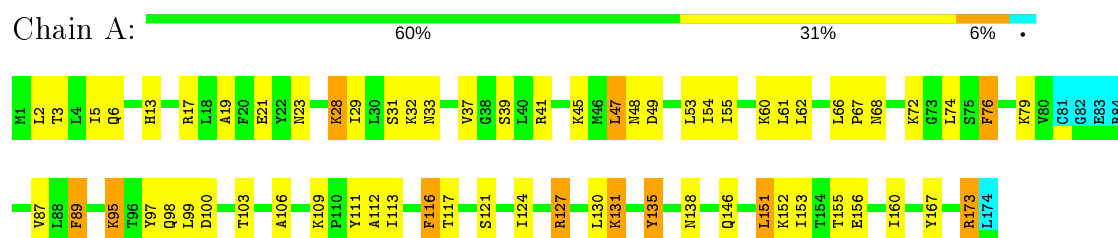
#### 4.2.8 Score per residue for model 8

- Molecule 1: Repair DNA polymerase X



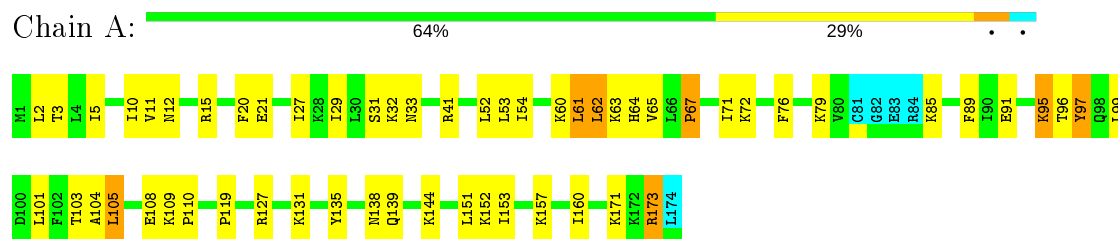
#### 4.2.9 Score per residue for model 9

- Molecule 1: Repair DNA polymerase X



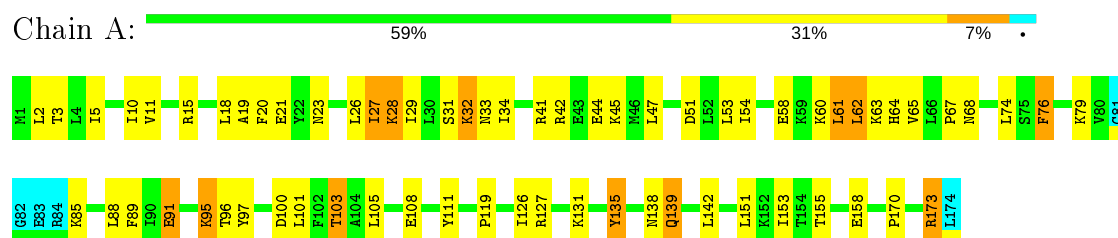
### 4.2.10 Score per residue for model 10

- Molecule 1: Repair DNA polymerase X



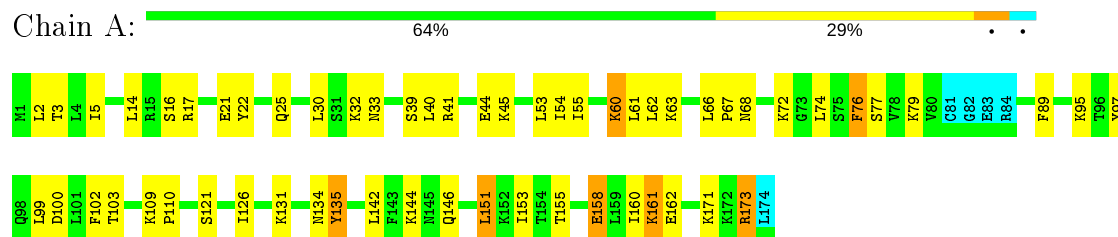
### 4.2.11 Score per residue for model 11

- Molecule 1: Repair DNA polymerase X



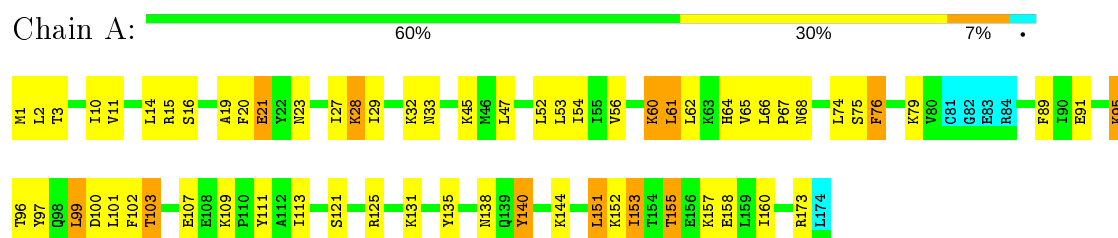
### 4.2.12 Score per residue for model 12

- Molecule 1: Repair DNA polymerase X



### 4.2.13 Score per residue for model 13 (medoid)

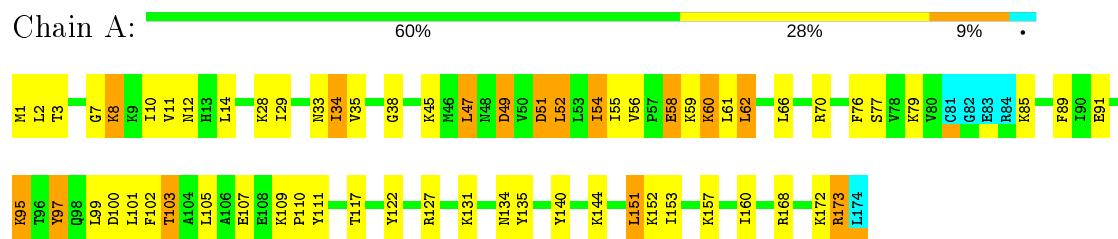
- Molecule 1: Repair DNA polymerase X





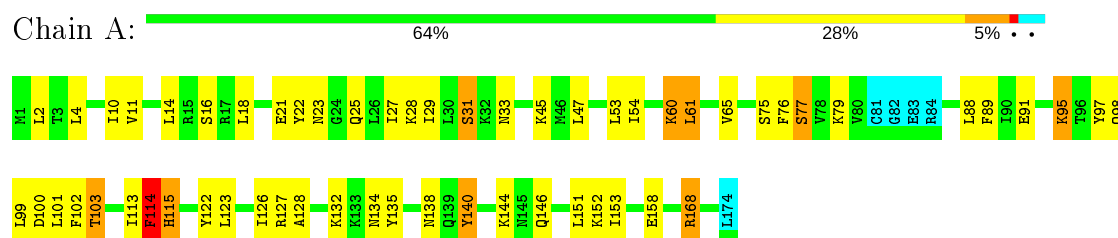
### 4.2.14 Score per residue for model 14

- Molecule 1: Repair DNA polymerase X



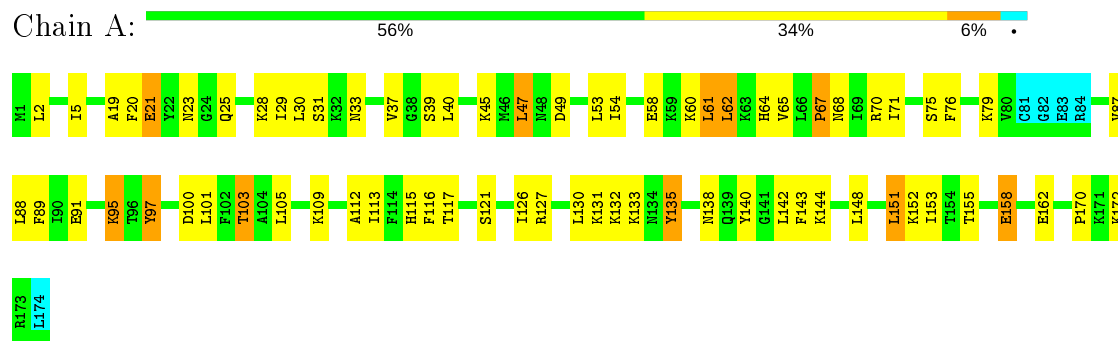
### 4.2.15 Score per residue for model 15

- Molecule 1: Repair DNA polymerase X



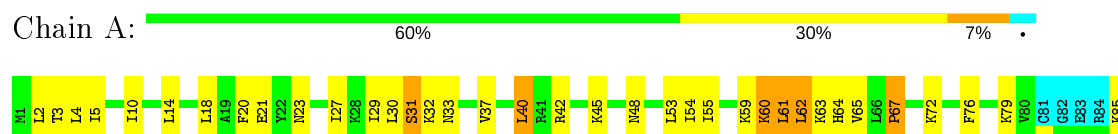
### 4.2.16 Score per residue for model 16

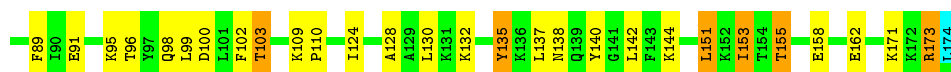
- Molecule 1: Repair DNA polymerase X



### 4.2.17 Score per residue for model 17

- Molecule 1: Repair DNA polymerase X

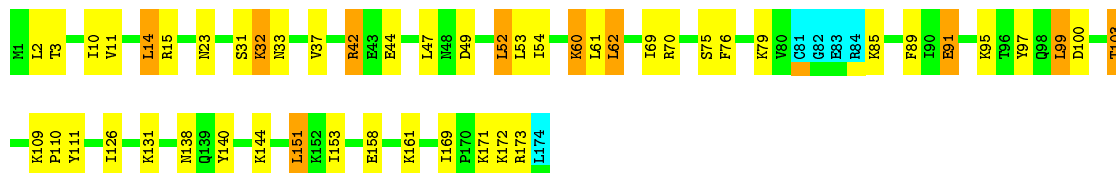




#### 4.2.18 Score per residue for model 18

- Molecule 1: Repair DNA polymerase X

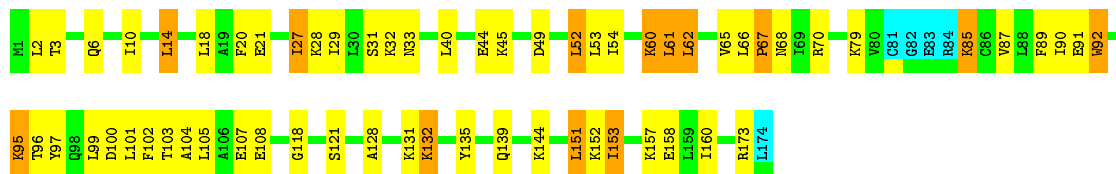
Chain A: 68% 23% 6% .



#### 4.2.19 Score per residue for model 19

- Molecule 1: Repair DNA polymerase X

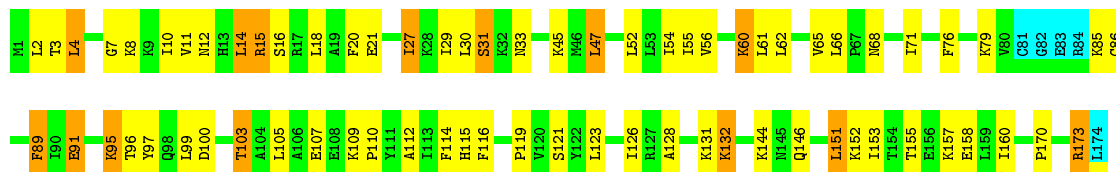
Chain A: 61% 29% 7% .



#### 4.2.20 Score per residue for model 20

- Molecule 1: Repair DNA polymerase X

Chain A: 57% 32% 8% .



## 5 Refinement protocol and experimental data overview

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

Of the 2000 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
CYANA	structure solution	
Haddock	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	1212
Number of shifts mapped to atoms	1212
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	44%

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	1395	1534	1531	22±5
All	All	27900	30680	30620	436

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:GLU:HB2	1:A:96:THR:HG22	0.74	1.58	6	8
1:A:119:PRO:O	1:A:123:LEU:HG	0.69	1.88	20	1
1:A:76:PHE:HA	1:A:89:PHE:O	0.69	1.88	15	18
1:A:91:GLU:HG2	1:A:96:THR:HG22	0.68	1.66	3	2
1:A:33:ASN:O	1:A:54:ILE:HA	0.68	1.88	15	14
1:A:122:TYR:CE1	1:A:168:ARG:HG3	0.66	2.25	15	1
1:A:124:ILE:C	1:A:126:ILE:H	0.64	1.96	2	1
1:A:128:ALA:O	1:A:132:LYS:HG2	0.61	1.95	20	10
1:A:157:LYS:O	1:A:160:ILE:HG13	0.61	1.96	19	10
1:A:61:LEU:O	1:A:65:VAL:HG23	0.61	1.96	15	9
1:A:62:LEU:HD13	1:A:105:LEU:HG	0.60	1.74	11	8
1:A:35:VAL:HG23	1:A:55:ILE:HD11	0.60	1.72	14	1
1:A:170:PRO:O	1:A:173:ARG:HG2	0.59	1.97	11	1
1:A:109:LYS:O	1:A:113:ILE:HG12	0.58	1.99	9	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:HD2	1:A:60:LYS:N	0.58	2.14	20	2
1:A:130:LEU:HB3	1:A:135:TYR:CD1	0.58	2.34	2	1
1:A:111:TYR:OH	1:A:151:LEU:HB3	0.58	1.98	11	5
1:A:135:TYR:CD1	1:A:142:LEU:HD12	0.57	2.34	4	4
1:A:20:PHE:HD1	1:A:21:GLU:O	0.57	1.83	4	9
1:A:52:LEU:HD12	1:A:99:LEU:HD11	0.57	1.75	4	2
1:A:77:SER:O	1:A:88:LEU:HA	0.56	1.99	15	4
1:A:153:ILE:HD12	1:A:159:LEU:HA	0.56	1.76	7	1
1:A:11:VAL:O	1:A:15:ARG:HB2	0.56	2.01	11	1
1:A:104:ALA:HB1	1:A:108:GLU:CD	0.56	2.20	10	4
1:A:131:LYS:HA	1:A:135:TYR:O	0.56	1.99	5	2
1:A:69:ILE:O	1:A:70:ARG:HG3	0.56	2.01	18	1
1:A:112:ALA:HA	1:A:115:HIS:CE1	0.55	2.37	20	1
1:A:54:ILE:HG22	1:A:55:ILE:H	0.55	1.62	20	1
1:A:108:GLU:OE1	1:A:139:GLN:HB3	0.54	2.03	11	3
1:A:130:LEU:O	1:A:133:LYS:HG2	0.54	2.03	7	2
1:A:21:GLU:HB2	1:A:68:ASN:CB	0.54	2.33	19	6
1:A:36:ALA:HB1	1:A:40:LEU:HD11	0.53	1.78	5	1
1:A:95:LYS:HB3	1:A:97:TYR:CE1	0.53	2.38	13	8
1:A:31:SER:C	1:A:33:ASN:H	0.53	2.07	10	9
1:A:71:ILE:HG12	1:A:72:LYS:N	0.53	2.18	10	1
1:A:158:GLU:O	1:A:161:LYS:HG2	0.53	2.04	18	2
1:A:52:LEU:O	1:A:101:LEU:HA	0.53	2.04	14	2
1:A:53:LEU:HD12	1:A:102:PHE:O	0.53	2.04	7	2
1:A:124:ILE:O	1:A:126:ILE:N	0.52	2.42	2	1
1:A:41:ARG:NE	1:A:41:ARG:HA	0.52	2.20	8	1
1:A:169:ILE:HD11	1:A:172:LYS:HD3	0.52	1.80	5	2
1:A:63:LYS:O	1:A:67:PRO:HD3	0.52	2.05	17	4
1:A:42:ARG:HD2	1:A:44:GLU:OE1	0.52	2.03	18	1
1:A:91:GLU:HB3	1:A:96:THR:HG22	0.52	1.81	17	1
1:A:21:GLU:HA	1:A:25:GLN:O	0.52	2.05	15	3
1:A:117:THR:O	1:A:170:PRO:HD3	0.51	2.05	16	1
1:A:108:GLU:HG2	1:A:139:GLN:O	0.51	2.06	6	2
1:A:130:LEU:O	1:A:133:LYS:HG3	0.51	2.06	8	1
1:A:22:TYR:HB3	1:A:27:ILE:HD11	0.51	1.82	15	1
1:A:54:ILE:O	1:A:103:THR:HA	0.51	2.06	15	10
1:A:21:GLU:HB3	1:A:68:ASN:HB3	0.51	1.81	12	2
1:A:104:ALA:HB1	1:A:108:GLU:CG	0.51	2.36	19	1
1:A:92:TRP:CZ3	1:A:95:LYS:HB3	0.51	2.41	19	1
1:A:8:LYS:O	1:A:12:ASN:HB2	0.51	2.06	14	2
1:A:64:HIS:C	1:A:67:PRO:HD2	0.50	2.26	10	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:N	1:A:67:PRO:HD2	0.50	2.20	1	7
1:A:62:LEU:HD22	1:A:105:LEU:HD21	0.50	1.82	19	2
1:A:2:LEU:HD21	1:A:97:TYR:CE2	0.50	2.41	15	1
1:A:127:ARG:O	1:A:131:LYS:HB2	0.50	2.07	2	1
1:A:89:PHE:HB2	1:A:98:GLN:OE1	0.50	2.07	9	1
1:A:54:ILE:HD12	1:A:103:THR:HG23	0.50	1.83	14	1
1:A:33:ASN:O	1:A:54:ILE:HG23	0.50	2.07	11	3
1:A:135:TYR:HE2	1:A:142:LEU:HD13	0.50	1.65	2	1
1:A:173:ARG:O	1:A:173:ARG:HD3	0.50	2.06	12	1
1:A:111:TYR:CZ	1:A:151:LEU:HD13	0.49	2.42	11	1
1:A:124:ILE:C	1:A:126:ILE:N	0.49	2.66	2	1
1:A:135:TYR:CE1	1:A:142:LEU:HB3	0.49	2.42	3	4
1:A:41:ARG:HA	1:A:41:ARG:NE	0.49	2.22	6	1
1:A:11:VAL:O	1:A:15:ARG:HG3	0.49	2.08	20	1
1:A:10:ILE:HG13	1:A:11:VAL:N	0.48	2.23	3	12
1:A:138:ASN:HB3	1:A:140:TYR:CD2	0.48	2.44	15	3
1:A:22:TYR:HB3	1:A:27:ILE:CD1	0.48	2.38	15	1
1:A:135:TYR:HD1	1:A:142:LEU:HD12	0.48	1.68	4	1
1:A:88:LEU:HD13	1:A:101:LEU:HD21	0.48	1.84	11	4
1:A:54:ILE:HB	1:A:103:THR:HA	0.48	1.86	20	1
1:A:61:LEU:HA	1:A:64:HIS:HB2	0.48	1.86	3	2
1:A:113:ILE:HG21	1:A:156:GLU:HG2	0.48	1.85	9	1
1:A:10:ILE:O	1:A:14:LEU:N	0.48	2.47	17	13
1:A:55:ILE:CG2	1:A:106:ALA:HA	0.48	2.39	9	1
1:A:151:LEU:HD13	1:A:151:LEU:N	0.48	2.24	16	3
1:A:41:ARG:HD3	1:A:117:THR:HG23	0.48	1.84	2	1
1:A:20:PHE:CZ	1:A:27:ILE:HB	0.48	2.44	17	4
1:A:116:PHE:C	1:A:116:PHE:CD1	0.47	2.87	9	1
1:A:111:TYR:CZ	1:A:151:LEU:HD12	0.47	2.45	9	1
1:A:151:LEU:N	1:A:151:LEU:HD13	0.47	2.24	20	4
1:A:95:LYS:HB3	1:A:97:TYR:CZ	0.47	2.44	14	1
1:A:92:TRP:CE3	1:A:97:TYR:CD1	0.47	3.03	5	2
1:A:38:GLY:HA3	1:A:51:ASP:OD1	0.47	2.10	14	1
1:A:21:GLU:HB2	1:A:68:ASN:HB2	0.47	1.87	19	1
1:A:45:LYS:N	1:A:45:LYS:HD3	0.47	2.25	13	1
1:A:91:GLU:HA	1:A:95:LYS:O	0.47	2.10	1	1
1:A:70:ARG:HB2	1:A:76:PHE:CZ	0.47	2.45	16	1
1:A:120:VAL:O	1:A:123:LEU:HB2	0.46	2.10	6	2
1:A:39:SER:HB2	1:A:47:LEU:HB3	0.46	1.88	9	1
1:A:112:ALA:HA	1:A:115:HIS:ND1	0.46	2.26	16	1
1:A:105:LEU:HB3	1:A:107:GLU:OE1	0.46	2.11	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:20:PHE:CD1	1:A:21:GLU:O	0.46	2.68	4	6
1:A:122:TYR:CE2	1:A:168:ARG:HG3	0.46	2.45	1	1
1:A:37:VAL:HB	1:A:51:ASP:HB2	0.46	1.88	1	1
1:A:112:ALA:O	1:A:116:PHE:HB3	0.46	2.10	9	1
1:A:143:PHE:CE1	1:A:148:LEU:HD13	0.46	2.45	16	1
1:A:5:ILE:O	1:A:9:LYS:HG3	0.46	2.11	6	1
1:A:11:VAL:HG13	1:A:15:ARG:HD2	0.46	1.87	8	1
1:A:130:LEU:HD13	1:A:135:TYR:CE1	0.45	2.46	2	1
1:A:58:GLU:OE1	1:A:60:LYS:HE3	0.45	2.11	14	1
1:A:20:PHE:HB2	1:A:68:ASN:O	0.45	2.10	2	1
1:A:19:ALA:HA	1:A:28:LYS:HA	0.45	1.88	9	5
1:A:118:GLY:HA3	1:A:168:ARG:CZ	0.45	2.41	8	1
1:A:12:ASN:O	1:A:15:ARG:HG2	0.45	2.11	10	1
1:A:135:TYR:CE1	1:A:142:LEU:HD12	0.45	2.46	11	1
1:A:172:LYS:O	1:A:173:ARG:HB2	0.45	2.10	14	1
1:A:36:ALA:HA	1:A:52:LEU:HD23	0.45	1.87	8	2
1:A:168:ARG:HD2	1:A:168:ARG:C	0.45	2.31	8	1
1:A:39:SER:CB	1:A:47:LEU:HD22	0.45	2.42	16	1
1:A:36:ALA:HB1	1:A:40:LEU:HG	0.45	1.89	2	1
1:A:155:THR:HB	1:A:158:GLU:HB2	0.44	1.89	11	5
1:A:115:HIS:HA	1:A:123:LEU:HD21	0.44	1.88	15	1
1:A:50:VAL:HB	1:A:99:LEU:CD2	0.44	2.42	2	3
1:A:124:ILE:O	1:A:127:ARG:N	0.44	2.51	9	1
1:A:153:ILE:HG22	1:A:158:GLU:HG2	0.44	1.88	17	2
1:A:26:LEU:C	1:A:27:ILE:HD13	0.44	2.33	11	1
1:A:7:GLY:O	1:A:10:ILE:HG12	0.44	2.13	14	2
1:A:33:ASN:HB3	1:A:55:ILE:O	0.44	2.13	14	1
1:A:113:ILE:C	1:A:115:HIS:H	0.44	2.16	15	1
1:A:107:GLU:O	1:A:151:LEU:HD11	0.44	2.13	19	1
1:A:5:ILE:HG13	1:A:6:GLN:N	0.44	2.28	2	2
1:A:54:ILE:O	1:A:55:ILE:HG13	0.44	2.13	20	1
1:A:17:ARG:NE	1:A:17:ARG:HA	0.44	2.28	4	2
1:A:56:VAL:HG21	1:A:62:LEU:HA	0.44	1.90	13	2
1:A:136:LYS:HB3	1:A:143:PHE:HB2	0.44	1.88	2	1
1:A:21:GLU:HB2	1:A:68:ASN:HB3	0.44	1.89	2	1
1:A:20:PHE:HA	1:A:68:ASN:O	0.44	2.12	3	1
1:A:75:SER:HB2	1:A:91:GLU:O	0.43	2.12	18	3
1:A:127:ARG:HA	1:A:130:LEU:HD12	0.43	1.88	5	1
1:A:97:TYR:CD1	1:A:97:TYR:N	0.43	2.85	16	7
1:A:170:PRO:O	1:A:173:ARG:HB3	0.43	2.13	20	1
1:A:4:LEU:HA	1:A:47:LEU:HD21	0.43	1.90	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:LYS:HB3	1:A:110:PRO:CD	0.43	2.43	12	5
1:A:52:LEU:HD13	1:A:99:LEU:HD11	0.43	1.88	18	1
1:A:65:VAL:O	1:A:69:ILE:HB	0.43	2.13	2	1
1:A:60:LYS:C	1:A:62:LEU:N	0.43	2.72	19	7
1:A:21:GLU:HB3	1:A:68:ASN:CB	0.43	2.44	9	1
1:A:119:PRO:HG3	1:A:173:ARG:HB2	0.43	1.91	10	1
1:A:127:ARG:O	1:A:127:ARG:HG3	0.43	2.13	2	1
1:A:33:ASN:O	1:A:34:ILE:HD12	0.43	2.14	14	1
1:A:106:ALA:O	1:A:109:LYS:HB2	0.43	2.14	6	1
1:A:168:ARG:O	1:A:168:ARG:HD2	0.42	2.14	7	1
1:A:60:LYS:N	1:A:60:LYS:HD2	0.42	2.28	15	2
1:A:106:ALA:O	1:A:109:LYS:HG3	0.42	2.14	9	1
1:A:63:LYS:HA	1:A:66:LEU:HD12	0.42	1.91	12	1
1:A:47:LEU:HD12	1:A:49:ASP:O	0.42	2.14	14	1
1:A:151:LEU:HD22	1:A:151:LEU:H	0.42	1.74	16	1
1:A:10:ILE:O	1:A:14:LEU:HB2	0.42	2.15	20	1
1:A:151:LEU:H	1:A:151:LEU:CD2	0.42	2.27	11	1
1:A:97:TYR:N	1:A:97:TYR:CD1	0.42	2.88	2	2
1:A:109:LYS:N	1:A:110:PRO:HD2	0.42	2.30	14	1
1:A:153:ILE:HB	1:A:158:GLU:HB3	0.42	1.91	19	1
1:A:60:LYS:HD2	1:A:60:LYS:H	0.42	1.73	20	1
1:A:4:LEU:CD1	1:A:40:LEU:HA	0.42	2.45	17	1
1:A:71:ILE:HG22	1:A:72:LYS:H	0.42	1.74	1	1
1:A:62:LEU:HD22	1:A:105:LEU:CG	0.42	2.44	6	1
1:A:151:LEU:H	1:A:151:LEU:HD22	0.42	1.75	8	1
1:A:56:VAL:HG11	1:A:61:LEU:C	0.42	2.35	20	1
1:A:41:ARG:HD3	1:A:117:THR:CG2	0.41	2.45	2	1
1:A:62:LEU:O	1:A:65:VAL:HG22	0.41	2.15	2	1
1:A:20:PHE:CD2	1:A:65:VAL:HG22	0.41	2.50	19	1
1:A:65:VAL:CG1	1:A:69:ILE:HD12	0.41	2.45	4	1
1:A:30:LEU:O	1:A:33:ASN:HB2	0.41	2.16	16	1
1:A:151:LEU:HD13	1:A:151:LEU:H	0.41	1.76	17	1
1:A:20:PHE:CE1	1:A:27:ILE:HB	0.41	2.51	1	2
1:A:108:GLU:OE2	1:A:139:GLN:HB3	0.41	2.15	2	1
1:A:59:LYS:N	1:A:59:LYS:HD2	0.41	2.31	2	1
1:A:60:LYS:O	1:A:63:LYS:N	0.41	2.53	2	1
1:A:53:LEU:HD11	1:A:112:ALA:HB1	0.41	1.92	4	1
1:A:151:LEU:H	1:A:151:LEU:HD13	0.41	1.75	2	1
1:A:21:GLU:HB3	1:A:68:ASN:HB2	0.41	1.93	9	1
1:A:114:PHE:O	1:A:114:PHE:CG	0.41	2.74	15	1
1:A:151:LEU:HD23	1:A:151:LEU:H	0.41	1.76	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:ILE:HD12	1:A:162:GLU:HG2	0.41	1.93	4	1
1:A:69:ILE:O	1:A:69:ILE:HG23	0.41	2.16	5	1
1:A:134:ASN:O	1:A:144:LYS:HD3	0.41	2.15	12	2
1:A:13:HIS:O	1:A:17:ARG:HG2	0.40	2.16	9	1
1:A:62:LEU:HD22	1:A:105:LEU:HG	0.40	1.93	6	1
1:A:30:LEU:HG	1:A:31:SER:H	0.40	1.76	20	1
1:A:145:ASN:O	1:A:146:GLN:HB2	0.40	2.16	7	1
1:A:107:GLU:HB2	1:A:151:LEU:HD21	0.40	1.94	20	1
1:A:1:MET:HB3	1:A:48:ASN:HA	0.40	1.92	4	1
1:A:15:ARG:CZ	1:A:52:LEU:HD13	0.40	2.47	13	1
1:A:108:GLU:HB2	1:A:139:GLN:O	0.40	2.17	19	1
1:A:58:GLU:OE1	1:A:61:LEU:HG	0.40	2.17	6	1
1:A:111:TYR:CD1	1:A:111:TYR:N	0.40	2.90	9	1
1:A:11:VAL:O	1:A:15:ARG:HG2	0.40	2.16	18	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	168/174 (97%)	152±2 (91±1%)	13±2 (8±1%)	2±1 (1±1%)	15	61
All	All	3360/3480 (97%)	3046 (91%)	267 (8%)	47 (1%)	15	61

All 9 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	61	LEU	19
1	A	173	ARG	11
1	A	67	PRO	5
1	A	32	LYS	4
1	A	132	LYS	3
1	A	114	PHE	2
1	A	125	ARG	1
1	A	134	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	118	GLY	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	155/159 (97%)	120±5 (78±3%)	35±5 (22±3%)	3	29
All	All	3100/3180 (97%)	2406 (78%)	694 (22%)	3	29

All 105 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	79	LYS	20
1	A	153	ILE	20
1	A	103	THR	20
1	A	100	ASP	19
1	A	151	LEU	18
1	A	131	LYS	18
1	A	135	TYR	17
1	A	95	LYS	17
1	A	2	LEU	17
1	A	60	LYS	17
1	A	99	LEU	17
1	A	29	ILE	16
1	A	62	LEU	15
1	A	45	LYS	15
1	A	47	LEU	15
1	A	3	THR	14
1	A	152	LYS	14
1	A	144	LYS	13
1	A	140	TYR	13
1	A	53	LEU	13
1	A	32	LYS	11
1	A	102	PHE	11
1	A	121	SER	11
1	A	138	ASN	10

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ASN	10
1	A	18	LEU	10
1	A	126	ILE	9
1	A	74	LEU	9
1	A	171	LYS	9
1	A	127	ARG	9
1	A	31	SER	9
1	A	173	ARG	9
1	A	49	ASP	8
1	A	155	THR	8
1	A	76	PHE	8
1	A	91	GLU	7
1	A	28	LYS	7
1	A	14	LEU	7
1	A	55	ILE	7
1	A	5	ILE	6
1	A	16	SER	6
1	A	158	GLU	6
1	A	97	TYR	6
1	A	27	ILE	6
1	A	58	GLU	5
1	A	72	LYS	5
1	A	15	ARG	5
1	A	52	LEU	5
1	A	21	GLU	5
1	A	40	LEU	5
1	A	146	GLN	5
1	A	90	ILE	5
1	A	51	ASP	5
1	A	66	LEU	5
1	A	41	ARG	5
1	A	37	VAL	5
1	A	70	ARG	4
1	A	48	ASN	4
1	A	34	ILE	4
1	A	71	ILE	4
1	A	89	PHE	4
1	A	168	ARG	4
1	A	44	GLU	4
1	A	8	LYS	3
1	A	116	PHE	3
1	A	77	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	101	LEU	3
1	A	162	GLU	3
1	A	4	LEU	3
1	A	42	ARG	3
1	A	59	LYS	3
1	A	160	ILE	3
1	A	139	GLN	3
1	A	85	LYS	2
1	A	130	LEU	2
1	A	172	LYS	2
1	A	68	ASN	2
1	A	98	GLN	2
1	A	124	ILE	2
1	A	137	LEU	2
1	A	13	HIS	2
1	A	6	GLN	2
1	A	92	TRP	2
1	A	39	SER	2
1	A	117	THR	2
1	A	1	MET	2
1	A	167	TYR	2
1	A	107	GLU	2
1	A	17	ARG	2
1	A	30	LEU	2
1	A	125	ARG	1
1	A	54	ILE	1
1	A	133	LYS	1
1	A	114	PHE	1
1	A	115	HIS	1
1	A	33	ASN	1
1	A	105	LEU	1
1	A	86	CYS	1
1	A	75	SER	1
1	A	122	TYR	1
1	A	25	GLN	1
1	A	161	LYS	1
1	A	87	VAL	1
1	A	56	VAL	1
1	A	22	TYR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no 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 44% for the well-defined parts and 44% 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	1212
Number of shifts mapped to atoms	1212
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
$^{13}\text{C}_\alpha$	165	$0.27 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	157	$1.09 \pm 0.09$	Should be applied
$^{13}\text{C}'$	161	$0.12 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	165	$1.36 \pm 0.59$	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 44%, i.e. 1009 atoms were assigned a chemical shift out of a possible 2304. 34 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	636/833 (76%)	160/332 (48%)	316/338 (93%)	160/163 (98%)
Sidechain	348/1307 (27%)	109/767 (14%)	239/476 (50%)	0/64 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	25/164 (15%)	25/86 (29%)	0/71 (0%)	0/7 (0%)
Overall	1009/2304 (44%)	294/1185 (25%)	555/885 (63%)	160/234 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 1036 atoms were assigned a chemical shift out of a possible 2366. 35 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	656/858 (76%)	165/342 (48%)	326/348 (94%)	165/168 (98%)
Sidechain	355/1344 (26%)	110/789 (14%)	245/488 (50%)	0/67 (0%)
Aromatic	25/164 (15%)	25/86 (29%)	0/71 (0%)	0/7 (0%)
Overall	1036/2366 (44%)	300/1217 (25%)	571/907 (63%)	165/242 (68%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots ⓘ

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:

