



# Full wwPDB NMR Structure Validation Report ⓘ

Dec 5, 2016 – 12:05 PM EST

PDB ID : 5KNW  
Title : Solution NMR structure of human LARP7 xRRM2  
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Deposited on : 2016-06-28

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

<http://wwpdb.org/validation/2016/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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20028442  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

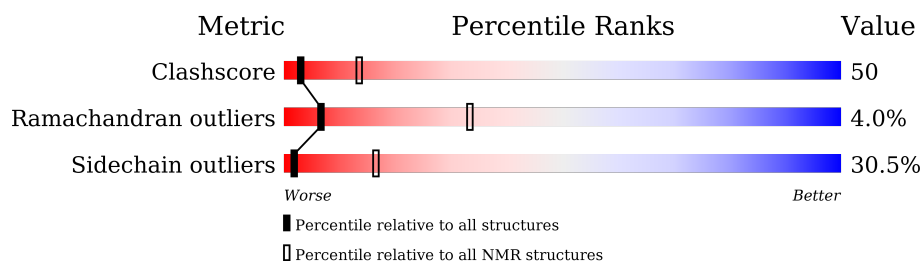
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 90%.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	125	<div> <div>18%</div> <div>41%</div> <div>10%</div> <div>•</div> <div>31%</div> </div>

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:455-A:540 (86)	0.31	3

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2042 atoms, of which 1029 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called La-related protein 7.

Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			2042	636	1029	189	185	3	

There are 8 discrepancies between the modelled and reference sequences:

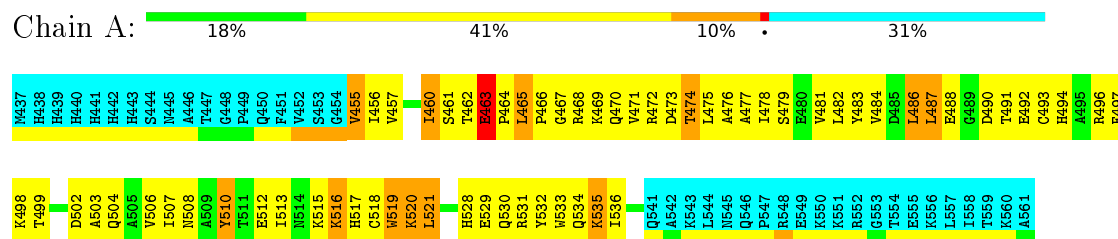
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	MET	-	initiating methionine	UNP Q4G0J3
A	438	HIS	-	expression tag	UNP Q4G0J3
A	439	HIS	-	expression tag	UNP Q4G0J3
A	440	HIS	-	expression tag	UNP Q4G0J3
A	441	HIS	-	expression tag	UNP Q4G0J3
A	442	HIS	-	expression tag	UNP Q4G0J3
A	443	HIS	-	expression tag	UNP Q4G0J3
A	444	SER	-	expression tag	UNP Q4G0J3

## 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: La-related protein 7

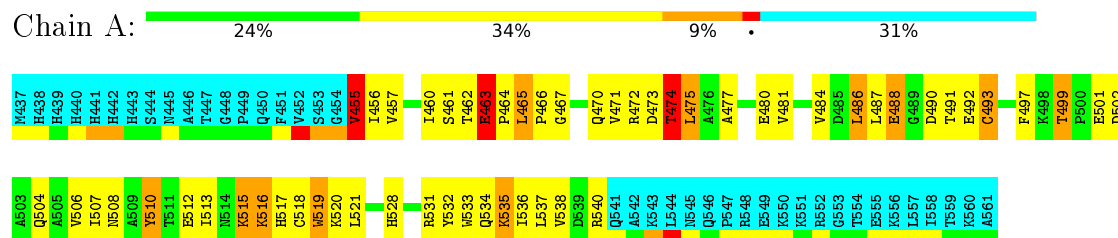


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

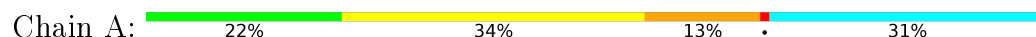
#### 4.2.1 Score per residue for model 1

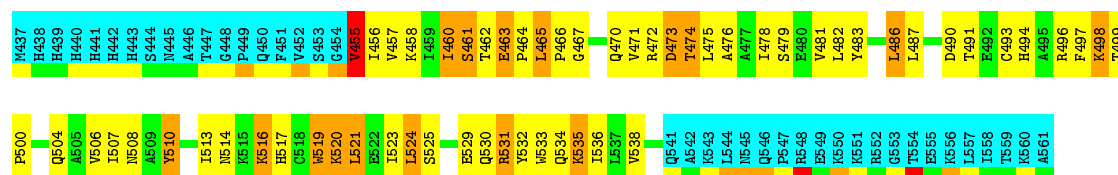
- Molecule 1: La-related protein 7



#### 4.2.2 Score per residue for model 2

- Molecule 1: La-related protein 7

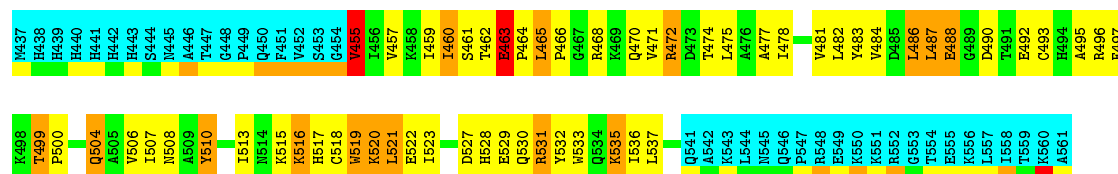




#### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: La-related protein 7

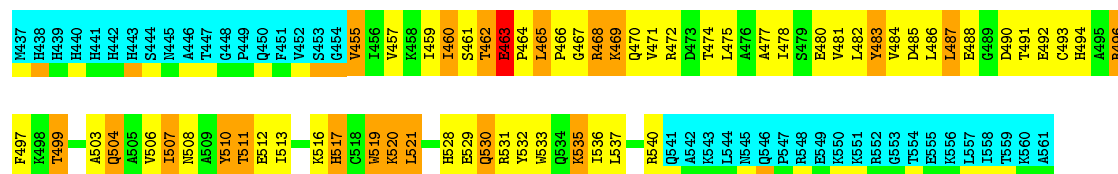
Chain A: 22% 33% 12% 31%



#### 4.2.4 Score per residue for model 4

- Molecule 1: La-related protein 7

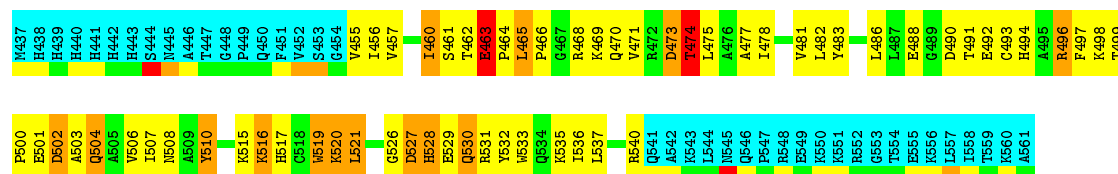
Chain A: 20% 32% 16% 31%



#### 4.2.5 Score per residue for model 5

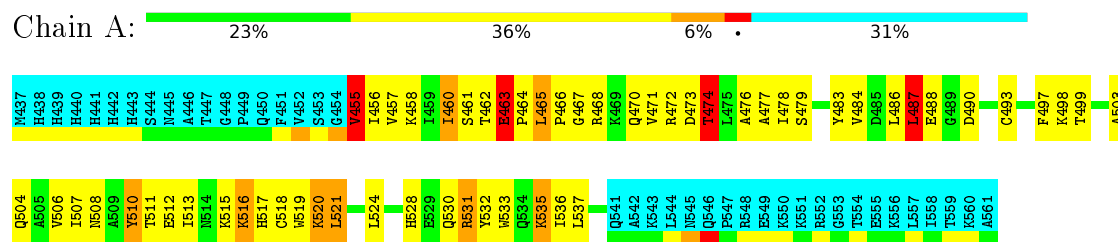
- Molecule 1: La-related protein 7

Chain A: 21% 35% 11% 31%



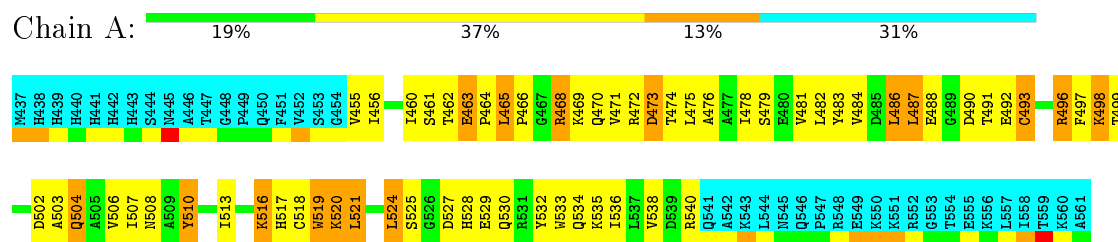
#### 4.2.6 Score per residue for model 6

- Molecule 1: La-related protein 7



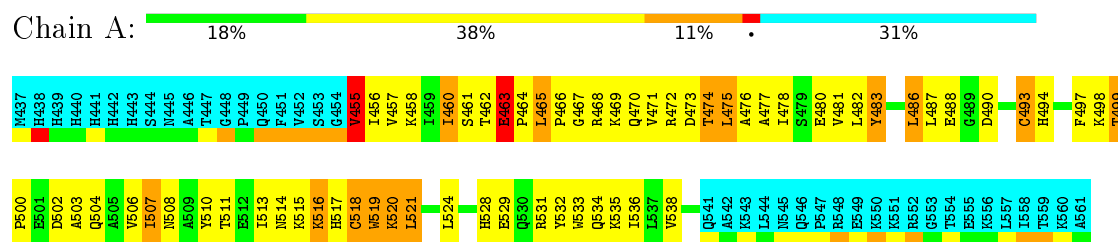
#### 4.2.7 Score per residue for model 7

- Molecule 1: La-related protein 7



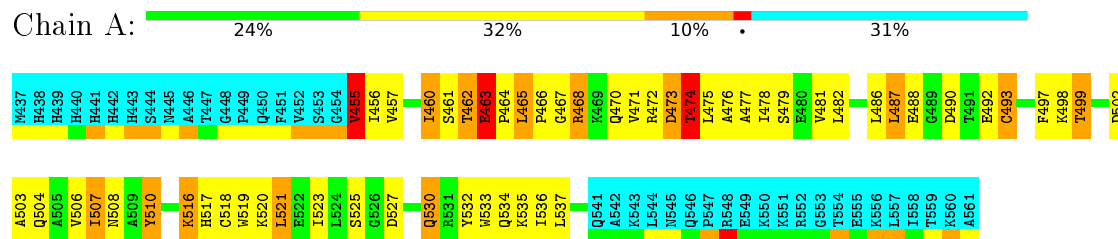
#### 4.2.8 Score per residue for model 8

- Molecule 1: La-related protein 7



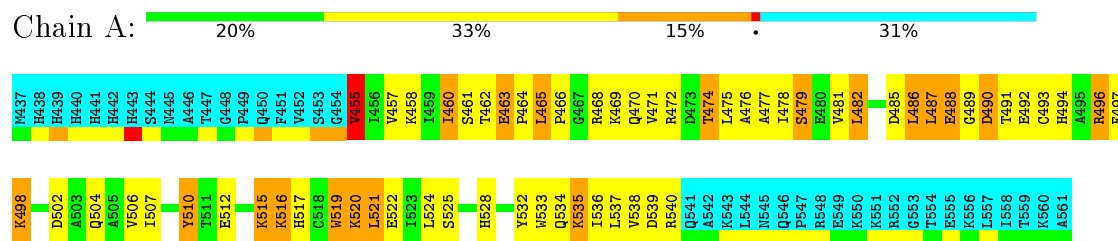
#### 4.2.9 Score per residue for model 9

- Molecule 1: La-related protein 7



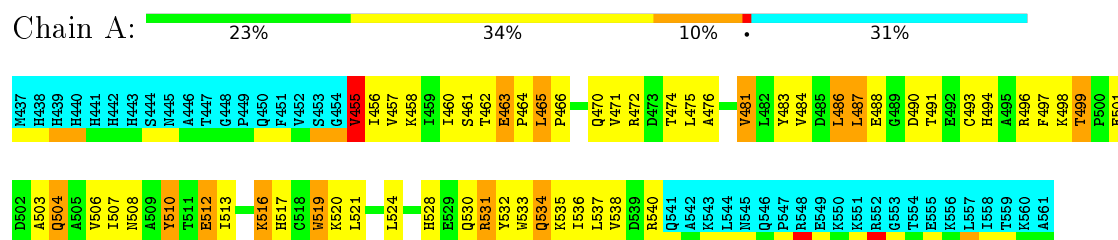
### 4.2.10 Score per residue for model 10

- Molecule 1: La-related protein 7



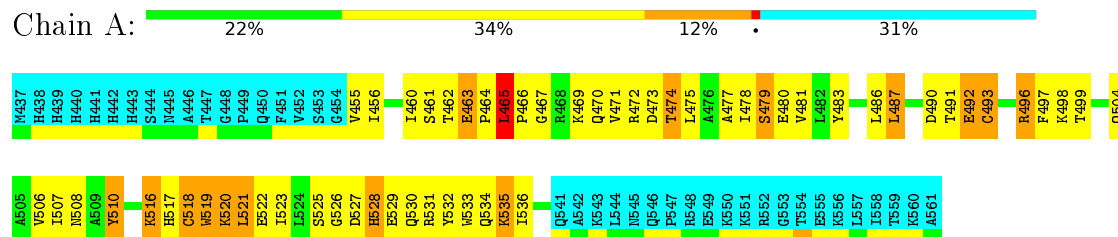
### 4.2.11 Score per residue for model 11

- Molecule 1: La-related protein 7



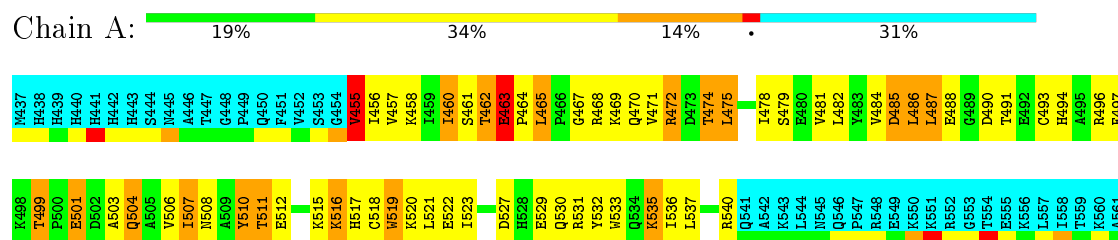
### 4.2.12 Score per residue for model 12

- Molecule 1: La-related protein 7



### 4.2.13 Score per residue for model 13

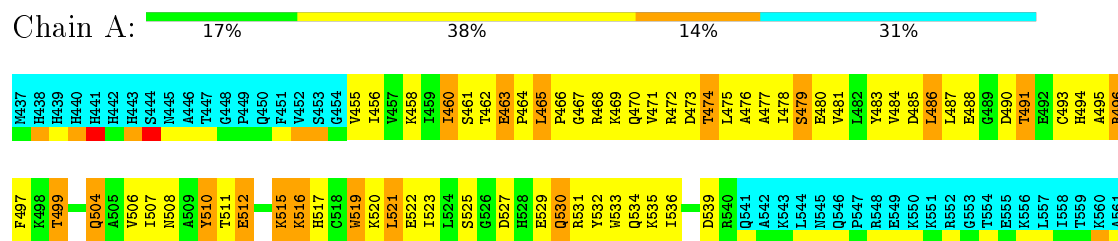
- Molecule 1: La-related protein 7





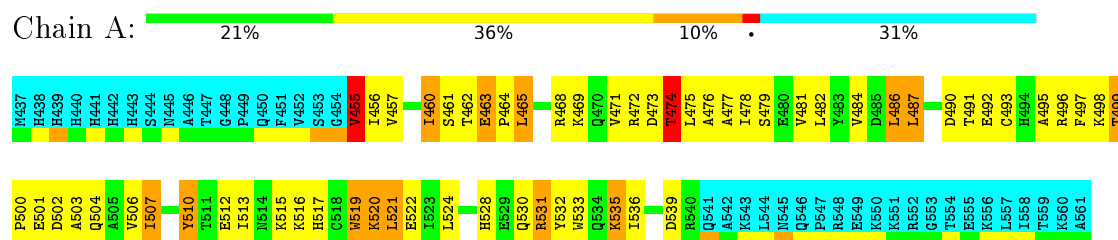
## 4.2.14 Score per residue for model 14

- Molecule 1: La-related protein 7



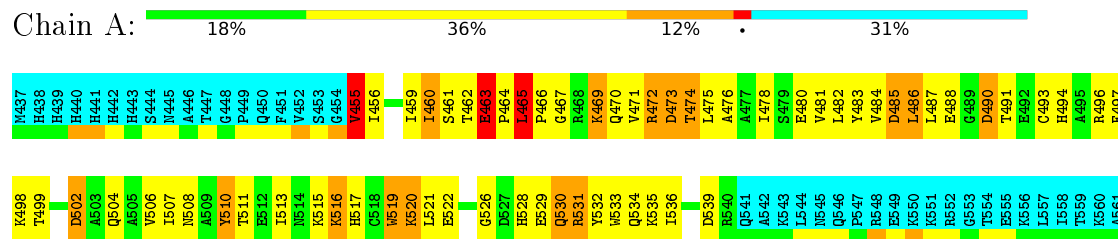
## 4.2.15 Score per residue for model 15

- Molecule 1: La-related protein 7



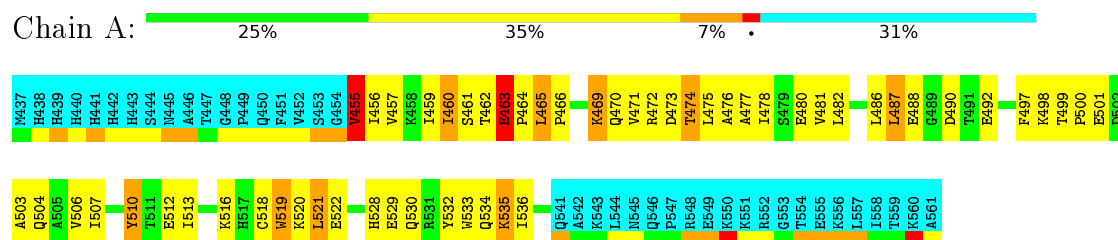
## 4.2.16 Score per residue for model 16

- Molecule 1: La-related protein 7



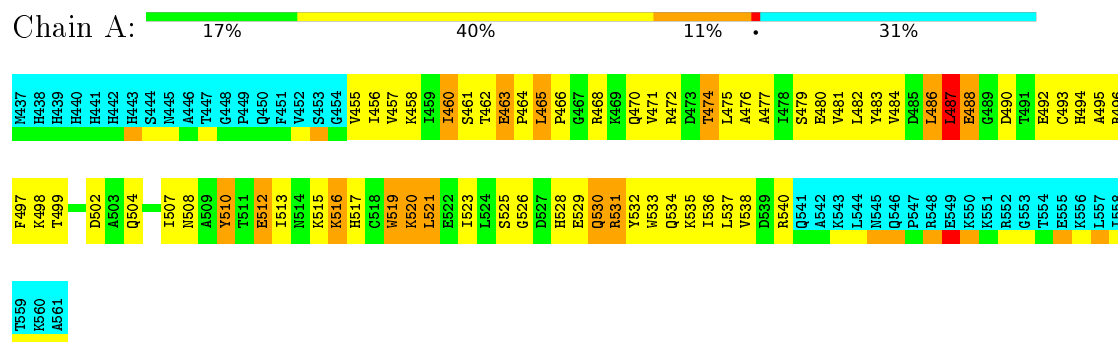
## 4.2.17 Score per residue for model 17

- Molecule 1: La-related protein 7



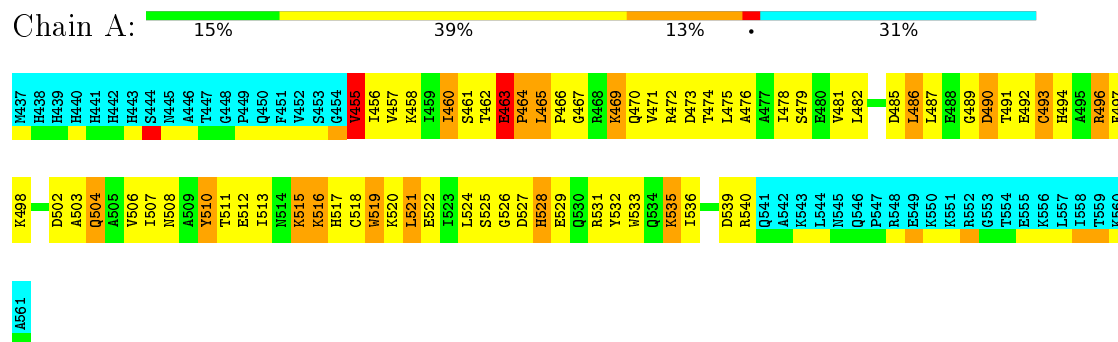
### 4.2.18 Score per residue for model 18

- Molecule 1: La-related protein 7



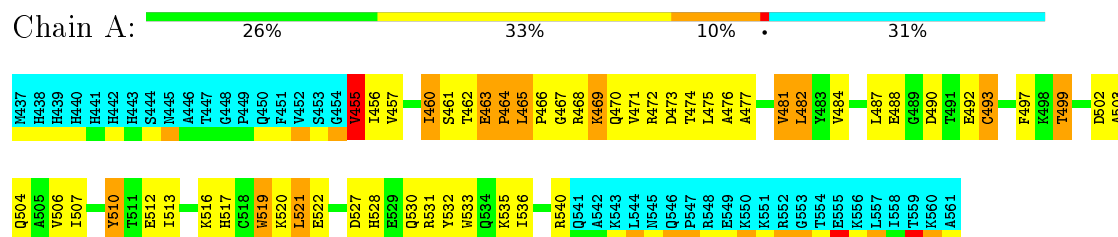
### 4.2.19 Score per residue for model 19

- Molecule 1: La-related protein 7



### 4.2.20 Score per residue for model 20

- Molecule 1: La-related protein 7



## 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: *structures with the lowest energy*.

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

Software name	Classification	Version
TALOS	geometry optimization	
X-PLOR NIH	refinement	

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

Chemical shift file(s)	5knw_cs.cif
Number of chemical shift lists	1
Total number of shifts	1511
Number of shifts mapped to atoms	1511
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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	700	711	708	70±9
All	All	14000	14220	14160	1398

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 50.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:TYR:CD1	1:A:521:LEU:HD13	0.97	1.94	2	4
1:A:520:LYS:O	1:A:521:LEU:HD13	0.95	1.60	8	7
1:A:486:LEU:HD22	1:A:487:LEU:N	0.93	1.78	15	3
1:A:510:TYR:CG	1:A:521:LEU:HD12	0.92	2.00	6	3
1:A:486:LEU:HD12	1:A:487:LEU:N	0.92	1.79	13	3
1:A:510:TYR:CD1	1:A:521:LEU:HD22	0.90	2.00	13	6
1:A:475:LEU:CD1	1:A:481:VAL:HG21	0.90	1.97	18	15
1:A:467:GLY:O	1:A:471:VAL:HG23	0.88	1.68	20	11
1:A:507:ILE:HD12	1:A:508:ASN:N	0.87	1.85	12	9
1:A:510:TYR:CD1	1:A:521:LEU:HD12	0.86	2.05	6	3
1:A:456:ILE:HD11	1:A:533:TRP:CE2	0.86	2.06	20	10
1:A:507:ILE:HG22	1:A:521:LEU:CB	0.85	2.01	15	5
1:A:461:SER:OG	1:A:465:LEU:HD12	0.84	1.72	17	10
1:A:507:ILE:HA	1:A:521:LEU:HD23	0.84	1.47	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:484:VAL:HG13	1:A:495:ALA:HB2	0.83	1.49	3	3
1:A:520:LYS:C	1:A:521:LEU:HD13	0.83	1.94	15	4
1:A:461:SER:HB3	1:A:465:LEU:HD12	0.82	1.52	9	8
1:A:460:ILE:HG22	1:A:520:LYS:HB2	0.81	1.52	14	20
1:A:507:ILE:HG22	1:A:521:LEU:HB3	0.81	1.51	8	10
1:A:486:LEU:HD12	1:A:493:CYS:HB3	0.79	1.55	3	4
1:A:481:VAL:HG12	1:A:497:PHE:CE1	0.78	2.13	8	9
1:A:510:TYR:CG	1:A:521:LEU:HD22	0.77	2.14	13	4
1:A:457:VAL:HG21	1:A:497:PHE:CE1	0.77	2.14	20	4
1:A:532:TYR:CE1	1:A:536:ILE:HD11	0.77	2.15	13	19
1:A:465:LEU:HD21	1:A:471:VAL:HG21	0.76	1.57	8	5
1:A:478:ILE:HD13	1:A:506:VAL:HG23	0.76	1.56	10	2
1:A:486:LEU:HD12	1:A:493:CYS:HB2	0.75	1.58	11	4
1:A:521:LEU:HD22	1:A:521:LEU:N	0.75	1.96	3	3
1:A:510:TYR:CE1	1:A:521:LEU:HD13	0.74	2.16	7	5
1:A:474:THR:O	1:A:478:ILE:HD12	0.74	1.82	16	6
1:A:521:LEU:N	1:A:521:LEU:HD22	0.74	1.98	8	4
1:A:457:VAL:HG21	1:A:497:PHE:CE2	0.74	2.18	15	10
1:A:510:TYR:CE2	1:A:513:ILE:HD11	0.74	2.17	19	1
1:A:481:VAL:HG12	1:A:497:PHE:CE2	0.74	2.18	14	5
1:A:533:TRP:CE3	1:A:536:ILE:HD12	0.73	2.18	5	18
1:A:455:VAL:HG11	1:A:500:PRO:HA	0.73	1.59	3	5
1:A:502:ASP:O	1:A:506:VAL:HG23	0.73	1.83	16	3
1:A:513:ILE:HG22	1:A:517:HIS:O	0.73	1.83	15	6
1:A:457:VAL:HG23	1:A:523:ILE:HD13	0.72	1.61	13	1
1:A:534:GLN:O	1:A:538:VAL:HG23	0.72	1.83	11	7
1:A:487:LEU:HD22	1:A:492:GLU:CG	0.71	2.15	7	1
1:A:465:LEU:HD13	1:A:491:THR:HA	0.71	1.61	19	1
1:A:507:ILE:HG22	1:A:521:LEU:HB2	0.71	1.62	15	1
1:A:456:ILE:HD11	1:A:533:TRP:CZ2	0.71	2.20	5	8
1:A:471:VAL:HG11	1:A:493:CYS:SG	0.71	2.26	13	5
1:A:532:TYR:HE1	1:A:536:ILE:HD11	0.69	1.46	8	20
1:A:468:ARG:HA	1:A:486:LEU:HD13	0.69	1.63	4	2
1:A:486:LEU:O	1:A:486:LEU:HD13	0.69	1.87	2	2
1:A:484:VAL:HG23	1:A:495:ALA:HB2	0.69	1.64	18	1
1:A:465:LEU:HD13	1:A:491:THR:CA	0.68	2.18	19	3
1:A:486:LEU:HD23	1:A:493:CYS:HB2	0.68	1.64	15	2
1:A:465:LEU:HD21	1:A:493:CYS:SG	0.67	2.29	20	1
1:A:507:ILE:HG22	1:A:521:LEU:CG	0.67	2.19	14	4
1:A:478:ILE:HG22	1:A:506:VAL:HG22	0.67	1.67	2	1
1:A:481:VAL:HG12	1:A:497:PHE:CD2	0.66	2.26	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:482:LEU:HD12	1:A:498:LYS:CG	0.66	2.19	2	1
1:A:507:ILE:HA	1:A:521:LEU:HD21	0.66	1.66	14	2
1:A:471:VAL:HG13	1:A:519:TRP:CH2	0.66	2.25	19	5
1:A:486:LEU:HD12	1:A:493:CYS:SG	0.65	2.32	12	2
1:A:520:LYS:C	1:A:521:LEU:HD22	0.65	2.12	18	5
1:A:478:ILE:HD13	1:A:510:TYR:CE2	0.65	2.27	2	5
1:A:507:ILE:HG22	1:A:521:LEU:HD11	0.65	1.69	7	1
1:A:482:LEU:HD12	1:A:482:LEU:C	0.65	2.12	20	1
1:A:478:ILE:HD13	1:A:510:TYR:HE2	0.65	1.49	2	7
1:A:510:TYR:CD1	1:A:521:LEU:CD1	0.65	2.80	10	5
1:A:484:VAL:HG13	1:A:484:VAL:O	0.64	1.92	6	4
1:A:507:ILE:HG22	1:A:521:LEU:HD21	0.64	1.69	2	3
1:A:486:LEU:HD22	1:A:489:GLY:CA	0.64	2.22	19	1
1:A:461:SER:CB	1:A:465:LEU:HD12	0.64	2.23	3	18
1:A:455:VAL:HG21	1:A:499:THR:C	0.64	2.13	4	10
1:A:460:ILE:HD13	1:A:461:SER:N	0.63	2.08	15	12
1:A:481:VAL:CG1	1:A:497:PHE:CE1	0.63	2.81	17	3
1:A:460:ILE:HD13	1:A:461:SER:O	0.63	1.92	16	14
1:A:536:ILE:HG23	1:A:540:ARG:NH1	0.63	2.09	18	1
1:A:457:VAL:HG23	1:A:523:ILE:CD1	0.63	2.23	13	1
1:A:457:VAL:CG2	1:A:497:PHE:CE1	0.62	2.82	20	3
1:A:486:LEU:HD22	1:A:489:GLY:HA2	0.62	1.71	19	1
1:A:507:ILE:HG22	1:A:521:LEU:HG	0.62	1.70	14	3
1:A:457:VAL:CG2	1:A:497:PHE:CE2	0.62	2.81	15	9
1:A:468:ARG:HD3	1:A:486:LEU:HD22	0.62	1.72	9	1
1:A:484:VAL:O	1:A:484:VAL:HG13	0.61	1.96	18	2
1:A:472:ARG:HB3	1:A:484:VAL:HG11	0.61	1.73	20	3
1:A:486:LEU:HD12	1:A:486:LEU:C	0.61	2.15	13	1
1:A:457:VAL:HG21	1:A:497:PHE:CZ	0.61	2.31	15	2
1:A:507:ILE:CB	1:A:521:LEU:HD21	0.61	2.26	2	2
1:A:465:LEU:CD2	1:A:471:VAL:HG21	0.60	2.26	5	6
1:A:521:LEU:O	1:A:521:LEU:HD23	0.60	1.95	7	3
1:A:481:VAL:CG1	1:A:497:PHE:CE2	0.60	2.84	14	2
1:A:486:LEU:HD13	1:A:493:CYS:HB3	0.60	1.70	10	2
1:A:479:SER:HB3	1:A:506:VAL:HG22	0.60	1.72	12	2
1:A:471:VAL:HG22	1:A:519:TRP:CZ2	0.59	2.32	15	9
1:A:532:TYR:CE2	1:A:535:LYS:CE	0.59	2.85	16	3
1:A:510:TYR:CD2	1:A:513:ILE:HD11	0.59	2.32	19	1
1:A:468:ARG:HB3	1:A:486:LEU:HD23	0.59	1.74	18	2
1:A:475:LEU:HD12	1:A:481:VAL:HG21	0.59	1.72	11	5
1:A:507:ILE:HG22	1:A:521:LEU:CD2	0.59	2.27	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:486:LEU:C	1:A:486:LEU:HD13	0.59	2.17	2	1
1:A:457:VAL:CG1	1:A:521:LEU:CD2	0.59	2.81	6	3
1:A:533:TRP:O	1:A:537:LEU:HD12	0.59	1.98	4	1
1:A:483:TYR:CD2	1:A:496:ARG:NH2	0.59	2.71	14	1
1:A:473:ASP:O	1:A:477:ALA:HB2	0.58	1.98	6	6
1:A:457:VAL:HG13	1:A:457:VAL:O	0.58	1.99	5	2
1:A:463:GLU:N	1:A:464:PRO:CD	0.58	2.66	20	19
1:A:496:ARG:HH11	1:A:536:ILE:HD13	0.58	1.59	2	1
1:A:462:THR:HG23	1:A:520:LYS:NZ	0.58	2.13	20	1
1:A:455:VAL:HG21	1:A:499:THR:O	0.58	1.98	13	5
1:A:516:LYS:CG	1:A:517:HIS:NE2	0.58	2.67	2	7
1:A:478:ILE:CG2	1:A:506:VAL:HG23	0.58	2.29	7	2
1:A:532:TYR:CD2	1:A:535:LYS:CE	0.58	2.87	18	2
1:A:507:ILE:CG2	1:A:521:LEU:HD21	0.58	2.29	2	2
1:A:478:ILE:HG21	1:A:506:VAL:HA	0.58	1.76	6	6
1:A:465:LEU:HD13	1:A:491:THR:O	0.57	1.98	2	8
1:A:478:ILE:HG21	1:A:506:VAL:HG23	0.57	1.76	13	2
1:A:475:LEU:HD12	1:A:476:ALA:N	0.57	2.14	20	9
1:A:472:ARG:HB2	1:A:484:VAL:HG21	0.57	1.76	13	2
1:A:532:TYR:CE2	1:A:535:LYS:HE2	0.57	2.35	5	5
1:A:472:ARG:HA	1:A:484:VAL:HG21	0.57	1.76	7	3
1:A:466:PRO:CG	1:A:470:GLN:CB	0.57	2.82	18	14
1:A:486:LEU:HD12	1:A:493:CYS:CB	0.57	2.30	1	5
1:A:482:LEU:HD12	1:A:498:LYS:HG3	0.57	1.75	2	1
1:A:456:ILE:HD11	1:A:533:TRP:NE1	0.57	2.15	17	1
1:A:478:ILE:CG2	1:A:506:VAL:HG22	0.56	2.30	8	1
1:A:465:LEU:HD23	1:A:471:VAL:HG21	0.56	1.76	20	1
1:A:516:LYS:HG3	1:A:517:HIS:CE1	0.56	2.35	9	5
1:A:532:TYR:CD2	1:A:535:LYS:HE2	0.56	2.35	18	4
1:A:475:LEU:HD13	1:A:481:VAL:HG11	0.56	1.78	11	8
1:A:487:LEU:N	1:A:487:LEU:CD2	0.56	2.68	11	1
1:A:462:THR:O	1:A:463:GLU:CB	0.56	2.53	11	20
1:A:467:GLY:O	1:A:470:GLN:N	0.56	2.38	9	1
1:A:486:LEU:C	1:A:486:LEU:HD12	0.56	2.20	18	2
1:A:497:PHE:HE1	1:A:506:VAL:HG21	0.56	1.61	16	1
1:A:472:ARG:O	1:A:476:ALA:HB3	0.56	2.01	6	4
1:A:486:LEU:HD23	1:A:493:CYS:HB3	0.56	1.76	2	2
1:A:487:LEU:HD13	1:A:492:GLU:HG3	0.56	1.76	9	2
1:A:510:TYR:CE1	1:A:521:LEU:CD2	0.55	2.88	20	1
1:A:457:VAL:CG1	1:A:521:LEU:HD21	0.55	2.31	19	3
1:A:471:VAL:HG22	1:A:519:TRP:CH2	0.55	2.36	11	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:516:LYS:CD	1:A:517:HIS:CE1	0.55	2.89	6	2
1:A:503:ALA:O	1:A:506:VAL:HG12	0.55	2.02	17	11
1:A:516:LYS:HD3	1:A:517:HIS:CE1	0.55	2.37	19	2
1:A:486:LEU:HD12	1:A:487:LEU:H	0.55	1.60	10	1
1:A:483:TYR:CE1	1:A:485:ASP:OD2	0.55	2.59	16	1
1:A:474:THR:O	1:A:477:ALA:N	0.55	2.40	3	11
1:A:475:LEU:HD11	1:A:481:VAL:HG21	0.55	1.77	18	4
1:A:507:ILE:HG22	1:A:521:LEU:CD1	0.55	2.32	7	1
1:A:455:VAL:HG21	1:A:497:PHE:O	0.54	2.01	14	3
1:A:456:ILE:HD12	1:A:532:TYR:CE1	0.54	2.37	15	1
1:A:507:ILE:HG21	1:A:523:ILE:HD11	0.54	1.78	18	1
1:A:510:TYR:CE1	1:A:521:LEU:HD22	0.54	2.36	11	1
1:A:483:TYR:CE1	1:A:484:VAL:O	0.54	2.61	6	1
1:A:468:ARG:HB3	1:A:486:LEU:HD22	0.54	1.78	4	1
1:A:481:VAL:HG12	1:A:497:PHE:CD1	0.54	2.37	18	4
1:A:510:TYR:CD1	1:A:521:LEU:HG	0.54	2.38	20	4
1:A:521:LEU:CD2	1:A:521:LEU:N	0.54	2.71	18	4
1:A:458:LYS:HB2	1:A:524:LEU:HD21	0.53	1.80	10	3
1:A:503:ALA:O	1:A:506:VAL:CG1	0.53	2.56	17	7
1:A:478:ILE:HG13	1:A:510:TYR:CE2	0.53	2.39	19	1
1:A:521:LEU:N	1:A:521:LEU:CD2	0.53	2.70	8	2
1:A:472:ARG:O	1:A:476:ALA:CB	0.53	2.56	6	8
1:A:455:VAL:CB	1:A:497:PHE:O	0.53	2.56	18	5
1:A:457:VAL:O	1:A:457:VAL:CG1	0.53	2.56	5	1
1:A:507:ILE:HG12	1:A:523:ILE:HD11	0.53	1.81	14	2
1:A:486:LEU:HD22	1:A:486:LEU:C	0.53	2.22	15	2
1:A:460:ILE:CG2	1:A:520:LYS:HB2	0.52	2.34	13	19
1:A:496:ARG:HD2	1:A:533:TRP:CH2	0.52	2.40	10	5
1:A:510:TYR:CD1	1:A:521:LEU:CD2	0.52	2.92	20	1
1:A:471:VAL:O	1:A:475:LEU:CD2	0.52	2.57	8	2
1:A:487:LEU:O	1:A:490:ASP:N	0.52	2.43	13	15
1:A:466:PRO:HG2	1:A:470:GLN:CB	0.52	2.34	11	13
1:A:484:VAL:CG1	1:A:484:VAL:O	0.52	2.58	18	2
1:A:463:GLU:N	1:A:464:PRO:HD2	0.52	2.20	11	19
1:A:534:GLN:O	1:A:538:VAL:CG2	0.52	2.58	2	3
1:A:516:LYS:HG2	1:A:517:HIS:CE1	0.52	2.39	4	1
1:A:480:GLU:CG	1:A:480:GLU:O	0.52	2.57	12	1
1:A:496:ARG:CZ	1:A:536:ILE:HD13	0.52	2.35	19	1
1:A:516:LYS:C	1:A:517:HIS:CG	0.52	2.83	13	6
1:A:461:SER:HB2	1:A:519:TRP:CD1	0.51	2.40	1	4
1:A:484:VAL:HG13	1:A:495:ALA:CB	0.51	2.30	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:504:GLN:OE1	1:A:508:ASN:ND2	0.51	2.43	3	1
1:A:517:HIS:O	1:A:519:TRP:N	0.51	2.43	13	2
1:A:466:PRO:CG	1:A:470:GLN:HB3	0.51	2.35	7	11
1:A:460:ILE:CD1	1:A:461:SER:O	0.51	2.57	9	5
1:A:457:VAL:CG1	1:A:521:LEU:CD1	0.51	2.87	17	1
1:A:510:TYR:CD1	1:A:521:LEU:HD23	0.51	2.40	20	1
1:A:462:THR:O	1:A:463:GLU:CG	0.51	2.58	13	12
1:A:529:GLU:OE1	1:A:533:TRP:CD1	0.51	2.63	13	1
1:A:461:SER:OG	1:A:462:THR:N	0.51	2.43	14	3
1:A:513:ILE:HG21	1:A:519:TRP:HB2	0.51	1.82	4	5
1:A:521:LEU:CG	1:A:521:LEU:O	0.51	2.58	14	1
1:A:507:ILE:HG22	1:A:521:LEU:HD12	0.51	1.81	17	2
1:A:483:TYR:C	1:A:483:TYR:CD1	0.51	2.84	7	6
1:A:467:GLY:O	1:A:471:VAL:CG2	0.51	2.58	16	5
1:A:485:ASP:O	1:A:493:CYS:CB	0.51	2.58	19	1
1:A:510:TYR:CG	1:A:513:ILE:HG13	0.51	2.40	19	2
1:A:461:SER:OG	1:A:465:LEU:CD1	0.50	2.57	8	5
1:A:524:LEU:CD1	1:A:528:HIS:ND1	0.50	2.74	15	1
1:A:507:ILE:CA	1:A:521:LEU:HD23	0.50	2.31	1	2
1:A:486:LEU:HD22	1:A:487:LEU:H	0.50	1.60	15	2
1:A:510:TYR:O	1:A:513:ILE:CG1	0.50	2.59	19	1
1:A:485:ASP:CB	1:A:494:HIS:O	0.50	2.59	4	1
1:A:521:LEU:CD2	1:A:521:LEU:O	0.50	2.60	7	1
1:A:518:CYS:O	1:A:520:LYS:NZ	0.50	2.44	8	1
1:A:513:ILE:HG21	1:A:519:TRP:CB	0.50	2.36	7	4
1:A:524:LEU:CD2	1:A:524:LEU:N	0.50	2.75	2	1
1:A:475:LEU:CD1	1:A:481:VAL:CG2	0.50	2.85	14	1
1:A:507:ILE:CA	1:A:521:LEU:HD21	0.50	2.37	14	2
1:A:516:LYS:HG3	1:A:517:HIS:NE2	0.50	2.21	8	6
1:A:521:LEU:O	1:A:521:LEU:CD2	0.50	2.59	14	1
1:A:532:TYR:CG	1:A:535:LYS:HE3	0.50	2.41	18	1
1:A:482:LEU:HD12	1:A:498:LYS:HB3	0.50	1.82	10	1
1:A:508:ASN:O	1:A:511:THR:HG22	0.49	2.07	14	5
1:A:482:LEU:HD13	1:A:498:LYS:HG3	0.49	1.84	18	1
1:A:486:LEU:C	1:A:486:LEU:HD22	0.49	2.27	2	1
1:A:456:ILE:HG22	1:A:524:LEU:HD23	0.49	1.84	7	1
1:A:516:LYS:HG2	1:A:517:HIS:NE2	0.49	2.22	5	6
1:A:455:VAL:CG2	1:A:497:PHE:O	0.49	2.60	14	3
1:A:516:LYS:O	1:A:517:HIS:CG	0.49	2.66	12	1
1:A:472:ARG:HG3	1:A:473:ASP:N	0.49	2.23	9	8
1:A:483:TYR:C	1:A:483:TYR:CD2	0.49	2.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:457:VAL:CG1	1:A:457:VAL:O	0.49	2.61	13	1
1:A:485:ASP:OD2	1:A:485:ASP:N	0.49	2.46	13	1
1:A:464:PRO:O	1:A:466:PRO:N	0.49	2.46	12	5
1:A:524:LEU:HD13	1:A:528:HIS:ND1	0.49	2.23	15	1
1:A:504:GLN:O	1:A:508:ASN:ND2	0.49	2.45	8	12
1:A:478:ILE:HG21	1:A:506:VAL:HG13	0.49	1.83	2	1
1:A:478:ILE:HB	1:A:506:VAL:HG23	0.49	1.83	19	2
1:A:475:LEU:HD11	1:A:484:VAL:CG2	0.49	2.38	7	1
1:A:494:HIS:CD2	1:A:532:TYR:CE2	0.49	3.01	8	2
1:A:466:PRO:HB2	1:A:470:GLN:CB	0.49	2.37	16	4
1:A:512:GLU:O	1:A:515:LYS:CG	0.48	2.61	10	3
1:A:510:TYR:CD1	1:A:521:LEU:HB3	0.48	2.43	14	2
1:A:516:LYS:HB3	1:A:517:HIS:CD2	0.48	2.44	6	9
1:A:465:LEU:CD1	1:A:491:THR:O	0.48	2.61	2	3
1:A:516:LYS:CG	1:A:517:HIS:CE1	0.48	2.97	9	1
1:A:473:ASP:O	1:A:477:ALA:CB	0.48	2.61	14	3
1:A:513:ILE:HG21	1:A:519:TRP:HB3	0.48	1.84	7	2
1:A:514:ASN:ND2	1:A:518:CYS:SG	0.48	2.86	8	1
1:A:513:ILE:HD13	1:A:519:TRP:CE3	0.48	2.43	17	1
1:A:486:LEU:HD13	1:A:486:LEU:C	0.48	2.28	15	2
1:A:532:TYR:CD1	1:A:535:LYS:HE3	0.48	2.44	18	1
1:A:466:PRO:HB2	1:A:470:GLN:CG	0.48	2.39	4	1
1:A:494:HIS:HB2	1:A:532:TYR:CZ	0.48	2.44	13	2
1:A:460:ILE:HD12	1:A:491:THR:O	0.47	2.09	1	1
1:A:483:TYR:CD1	1:A:483:TYR:C	0.47	2.88	8	3
1:A:466:PRO:CB	1:A:470:GLN:CB	0.47	2.92	16	1
1:A:504:GLN:O	1:A:507:ILE:HG13	0.47	2.09	7	20
1:A:456:ILE:HG21	1:A:532:TYR:CG	0.47	2.44	14	1
1:A:459:ILE:HD13	1:A:521:LEU:HD21	0.47	1.86	17	1
1:A:482:LEU:O	1:A:483:TYR:CB	0.47	2.61	4	1
1:A:455:VAL:HB	1:A:497:PHE:O	0.47	2.10	18	5
1:A:510:TYR:CE1	1:A:519:TRP:CE3	0.47	3.02	18	2
1:A:510:TYR:CD1	1:A:521:LEU:CG	0.47	2.98	10	2
1:A:479:SER:HB3	1:A:506:VAL:CG2	0.47	2.39	2	1
1:A:526:GLY:O	1:A:529:GLU:N	0.47	2.48	5	5
1:A:486:LEU:CD2	1:A:493:CYS:HB3	0.47	2.39	8	1
1:A:489:GLY:O	1:A:490:ASP:O	0.47	2.32	10	2
1:A:508:ASN:O	1:A:511:THR:HG23	0.47	2.09	6	2
1:A:535:LYS:HD2	1:A:536:ILE:N	0.47	2.24	1	3
1:A:456:ILE:HG12	1:A:533:TRP:NE1	0.47	2.25	13	7
1:A:529:GLU:CG	1:A:530:GLN:N	0.47	2.78	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:456:ILE:O	1:A:524:LEU:HD23	0.47	2.10	7	1
1:A:483:TYR:CD2	1:A:483:TYR:C	0.46	2.88	5	1
1:A:486:LEU:O	1:A:488:GLU:N	0.46	2.48	7	1
1:A:531:ARG:C	1:A:531:ARG:CD	0.46	2.82	6	2
1:A:516:LYS:HA	1:A:516:LYS:CE	0.46	2.41	18	4
1:A:484:VAL:HG22	1:A:495:ALA:CB	0.46	2.40	15	1
1:A:464:PRO:O	1:A:465:LEU:C	0.46	2.54	12	12
1:A:475:LEU:N	1:A:510:TYR:OH	0.46	2.48	3	2
1:A:459:ILE:HG21	1:A:519:TRP:CZ2	0.46	2.45	3	2
1:A:482:LEU:O	1:A:483:TYR:HB2	0.46	2.11	4	2
1:A:468:ARG:CA	1:A:486:LEU:HD13	0.46	2.40	9	1
1:A:487:LEU:O	1:A:490:ASP:CB	0.46	2.63	17	2
1:A:486:LEU:HD13	1:A:486:LEU:O	0.46	2.11	16	1
1:A:521:LEU:O	1:A:521:LEU:CG	0.46	2.63	7	1
1:A:478:ILE:HG13	1:A:510:TYR:CD2	0.46	2.45	19	1
1:A:479:SER:CB	1:A:506:VAL:CG2	0.46	2.94	2	1
1:A:481:VAL:HG12	1:A:497:PHE:CZ	0.46	2.45	5	1
1:A:467:GLY:O	1:A:468:ARG:C	0.46	2.53	9	1
1:A:471:VAL:O	1:A:474:THR:OG1	0.46	2.30	17	11
1:A:499:THR:OG1	1:A:502:ASP:OD2	0.46	2.33	8	2
1:A:530:GLN:OE1	1:A:534:GLN:CG	0.46	2.64	16	2
1:A:464:PRO:O	1:A:465:LEU:O	0.46	2.34	16	1
1:A:472:ARG:HA	1:A:475:LEU:HD21	0.46	1.87	2	1
1:A:455:VAL:HG23	1:A:497:PHE:O	0.46	2.10	3	2
1:A:484:VAL:O	1:A:484:VAL:CG1	0.46	2.64	4	1
1:A:486:LEU:HA	1:A:493:CYS:CB	0.46	2.41	7	2
1:A:482:LEU:HD23	1:A:496:ARG:HB2	0.46	1.87	4	1
1:A:487:LEU:O	1:A:488:GLU:C	0.45	2.54	8	12
1:A:524:LEU:HD23	1:A:524:LEU:N	0.45	2.25	2	1
1:A:482:LEU:HD12	1:A:482:LEU:O	0.45	2.10	20	1
1:A:487:LEU:HD22	1:A:492:GLU:HG3	0.45	1.88	7	1
1:A:487:LEU:HB3	1:A:490:ASP:CB	0.45	2.41	14	5
1:A:492:GLU:O	1:A:492:GLU:CG	0.45	2.63	10	1
1:A:486:LEU:CD1	1:A:493:CYS:HB2	0.45	2.40	4	4
1:A:507:ILE:HA	1:A:521:LEU:HD13	0.45	1.87	19	3
1:A:521:LEU:HG	1:A:521:LEU:O	0.45	2.12	14	1
1:A:501:GLU:HG3	1:A:502:ASP:N	0.45	2.26	1	1
1:A:471:VAL:HA	1:A:474:THR:OG1	0.45	2.12	5	3
1:A:478:ILE:CB	1:A:506:VAL:HG23	0.45	2.42	3	1
1:A:455:VAL:HG12	1:A:500:PRO:N	0.45	2.27	5	1
1:A:456:ILE:CD1	1:A:496:ARG:HB3	0.45	2.42	12	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:468:ARG:HG3	1:A:469:LYS:N	0.45	2.26	15	1
1:A:497:PHE:N	1:A:497:PHE:CD1	0.45	2.84	14	2
1:A:516:LYS:CG	1:A:517:HIS:CD2	0.45	3.00	8	1
1:A:475:LEU:HD13	1:A:481:VAL:HG21	0.45	1.86	14	1
1:A:466:PRO:HB2	1:A:470:GLN:HB2	0.45	1.89	16	1
1:A:513:ILE:HD13	1:A:519:TRP:HE3	0.45	1.72	17	1
1:A:459:ILE:CG2	1:A:519:TRP:CE2	0.45	2.99	3	1
1:A:456:ILE:HG22	1:A:456:ILE:O	0.45	2.12	16	1
1:A:483:TYR:CD1	1:A:485:ASP:OD2	0.45	2.70	16	1
1:A:510:TYR:CG	1:A:521:LEU:HD13	0.45	2.43	2	1
1:A:530:GLN:HG3	1:A:531:ARG:N	0.45	2.27	18	6
1:A:456:ILE:O	1:A:524:LEU:CD2	0.45	2.65	7	1
1:A:494:HIS:HB2	1:A:532:TYR:OH	0.45	2.11	8	1
1:A:507:ILE:HG21	1:A:523:ILE:CD1	0.44	2.42	2	1
1:A:455:VAL:HG12	1:A:499:THR:C	0.44	2.32	5	2
1:A:485:ASP:HB2	1:A:496:ARG:NH1	0.44	2.27	14	1
1:A:465:LEU:CD2	1:A:471:VAL:CG2	0.44	2.95	8	2
1:A:518:CYS:SG	1:A:520:LYS:CE	0.44	3.06	6	2
1:A:535:LYS:HG2	1:A:536:ILE:N	0.44	2.27	18	3
1:A:469:LYS:HG3	1:A:470:GLN:N	0.44	2.28	8	1
1:A:535:LYS:O	1:A:539:ASP:HB2	0.44	2.12	19	3
1:A:485:ASP:OD1	1:A:494:HIS:O	0.44	2.35	16	1
1:A:470:GLN:O	1:A:474:THR:OG1	0.44	2.33	1	2
1:A:483:TYR:CD1	1:A:484:VAL:N	0.44	2.85	3	3
1:A:486:LEU:CG	1:A:493:CYS:HB3	0.44	2.43	8	1
1:A:480:GLU:HG3	1:A:480:GLU:O	0.44	2.12	12	1
1:A:460:ILE:O	1:A:520:LYS:HG2	0.44	2.12	10	11
1:A:518:CYS:O	1:A:518:CYS:SG	0.44	2.76	3	1
1:A:526:GLY:O	1:A:528:HIS:N	0.44	2.51	5	3
1:A:472:ARG:CB	1:A:484:VAL:HG11	0.44	2.42	1	3
1:A:464:PRO:O	1:A:466:PRO:CD	0.44	2.66	2	3
1:A:485:ASP:HB3	1:A:494:HIS:O	0.44	2.12	4	1
1:A:466:PRO:HG2	1:A:470:GLN:HB3	0.44	1.89	10	3
1:A:516:LYS:CE	1:A:516:LYS:HA	0.44	2.43	13	2
1:A:484:VAL:HG22	1:A:495:ALA:HB1	0.44	1.89	15	1
1:A:535:LYS:O	1:A:539:ASP:CB	0.44	2.66	15	2
1:A:530:GLN:OE1	1:A:534:GLN:HG2	0.44	2.12	16	1
1:A:497:PHE:N	1:A:497:PHE:CD2	0.43	2.86	8	2
1:A:503:ALA:O	1:A:507:ILE:HG12	0.43	2.13	8	1
1:A:487:LEU:CD1	1:A:492:GLU:O	0.43	2.66	12	1
1:A:463:GLU:O	1:A:465:LEU:N	0.43	2.51	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:510:TYR:CE1	1:A:521:LEU:HD23	0.43	2.47	20	1
1:A:471:VAL:HG13	1:A:519:TRP:HH2	0.43	1.73	16	1
1:A:536:ILE:CG2	1:A:540:ARG:NH1	0.43	2.81	18	1
1:A:457:VAL:HG13	1:A:521:LEU:CD1	0.43	2.43	20	1
1:A:532:TYR:CZ	1:A:535:LYS:HE3	0.43	2.47	17	4
1:A:522:GLU:OE2	1:A:523:ILE:O	0.43	2.37	3	1
1:A:532:TYR:CE2	1:A:535:LYS:NZ	0.43	2.84	6	1
1:A:487:LEU:HD22	1:A:492:GLU:HG2	0.43	1.87	7	1
1:A:461:SER:HB3	1:A:519:TRP:NE1	0.43	2.28	7	3
1:A:510:TYR:O	1:A:513:ILE:HG12	0.43	2.14	7	3
1:A:471:VAL:HG12	1:A:475:LEU:CD2	0.43	2.43	8	1
1:A:530:GLN:O	1:A:534:GLN:HG3	0.43	2.13	9	1
1:A:458:LYS:HG3	1:A:494:HIS:CE1	0.43	2.49	11	1
1:A:461:SER:HB2	1:A:519:TRP:NE1	0.43	2.29	10	4
1:A:466:PRO:HG2	1:A:470:GLN:HB2	0.43	1.91	7	4
1:A:456:ILE:HG13	1:A:532:TYR:CD1	0.43	2.49	18	3
1:A:462:THR:O	1:A:463:GLU:HB2	0.43	2.14	18	5
1:A:469:LYS:O	1:A:472:ARG:HG2	0.43	2.14	19	5
1:A:466:PRO:O	1:A:470:GLN:OE1	0.43	2.36	9	1
1:A:516:LYS:O	1:A:517:HIS:ND1	0.43	2.52	12	1
1:A:512:GLU:HG3	1:A:513:ILE:N	0.43	2.29	15	1
1:A:512:GLU:O	1:A:515:LYS:HG2	0.42	2.14	15	2
1:A:458:LYS:HG3	1:A:494:HIS:NE2	0.42	2.29	11	4
1:A:468:ARG:N	1:A:486:LEU:HD13	0.42	2.29	9	1
1:A:507:ILE:HD12	1:A:507:ILE:C	0.42	2.34	12	1
1:A:512:GLU:O	1:A:515:LYS:N	0.42	2.44	19	2
1:A:492:GLU:N	1:A:492:GLU:OE2	0.42	2.52	19	1
1:A:468:ARG:HG2	1:A:469:LYS:N	0.42	2.29	20	1
1:A:460:ILE:HG23	1:A:520:LYS:HG3	0.42	1.91	6	4
1:A:466:PRO:HB3	1:A:470:GLN:HB3	0.42	1.92	9	1
1:A:471:VAL:HG22	1:A:519:TRP:HZ2	0.42	1.69	15	1
1:A:514:ASN:ND2	1:A:514:ASN:O	0.42	2.52	2	1
1:A:487:LEU:HD13	1:A:492:GLU:O	0.42	2.14	7	1
1:A:476:ALA:O	1:A:479:SER:O	0.42	2.38	10	1
1:A:485:ASP:OD2	1:A:496:ARG:CG	0.42	2.68	13	1
1:A:479:SER:O	1:A:480:GLU:C	0.42	2.57	14	1
1:A:486:LEU:CD1	1:A:493:CYS:HB3	0.42	2.42	1	1
1:A:525:SER:CA	1:A:529:GLU:HB3	0.42	2.45	12	1
1:A:486:LEU:CG	1:A:493:CYS:HB2	0.42	2.45	4	2
1:A:507:ILE:HG13	1:A:508:ASN:N	0.42	2.29	7	1
1:A:468:ARG:O	1:A:472:ARG:HB3	0.42	2.15	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:484:VAL:CG2	1:A:493:CYS:SG	0.42	3.07	16	1
1:A:535:LYS:CD	1:A:536:ILE:N	0.42	2.83	1	1
1:A:503:ALA:O	1:A:507:ILE:CG1	0.42	2.68	8	1
1:A:472:ARG:CG	1:A:473:ASP:N	0.41	2.83	6	3
1:A:532:TYR:C	1:A:532:TYR:CD1	0.41	2.93	5	1
1:A:512:GLU:O	1:A:513:ILE:C	0.41	2.59	18	3
1:A:457:VAL:O	1:A:494:HIS:HA	0.41	2.16	10	3
1:A:456:ILE:CG2	1:A:494:HIS:HB3	0.41	2.45	5	1
1:A:469:LYS:O	1:A:473:ASP:OD2	0.41	2.38	7	1
1:A:532:TYR:CD2	1:A:535:LYS:HE3	0.41	2.49	18	1
1:A:464:PRO:O	1:A:466:PRO:HD3	0.41	2.15	5	4
1:A:486:LEU:CB	1:A:493:CYS:HB3	0.41	2.45	9	3
1:A:483:TYR:CE2	1:A:484:VAL:O	0.41	2.72	4	1
1:A:507:ILE:HG21	1:A:523:ILE:HG13	0.41	1.93	12	1
1:A:510:TYR:CD1	1:A:521:LEU:HD11	0.41	2.51	15	1
1:A:483:TYR:CD2	1:A:496:ARG:CZ	0.41	3.03	14	2
1:A:475:LEU:CD1	1:A:481:VAL:HG11	0.41	2.46	8	2
1:A:503:ALA:HB1	1:A:523:ILE:HD12	0.41	1.92	13	1
1:A:468:ARG:O	1:A:472:ARG:CB	0.41	2.69	14	1
1:A:524:LEU:CD1	1:A:528:HIS:CE1	0.41	3.04	15	1
1:A:460:ILE:CD1	1:A:492:GLU:HG2	0.41	2.46	1	1
1:A:532:TYR:CE2	1:A:535:LYS:HE3	0.41	2.50	2	2
1:A:510:TYR:CD2	1:A:513:ILE:HG13	0.41	2.51	20	1
1:A:531:ARG:CD	1:A:531:ARG:C	0.41	2.88	3	2
1:A:486:LEU:HG	1:A:493:CYS:CB	0.41	2.46	8	1
1:A:458:LYS:HB2	1:A:494:HIS:CD2	0.41	2.50	14	1
1:A:482:LEU:HD12	1:A:498:LYS:HG2	0.41	1.92	2	1
1:A:526:GLY:O	1:A:527:ASP:C	0.41	2.58	5	1
1:A:526:GLY:C	1:A:528:HIS:N	0.41	2.74	5	1
1:A:501:GLU:CD	1:A:502:ASP:N	0.41	2.74	5	1
1:A:468:ARG:CB	1:A:486:LEU:HD13	0.41	2.45	8	1
1:A:466:PRO:HB3	1:A:470:GLN:CB	0.41	2.46	9	1
1:A:468:ARG:CB	1:A:486:LEU:HD23	0.41	2.45	13	1
1:A:460:ILE:HG22	1:A:520:LYS:CB	0.41	2.39	15	2
1:A:487:LEU:CB	1:A:490:ASP:HB3	0.41	2.46	15	1
1:A:532:TYR:CD1	1:A:532:TYR:C	0.41	2.94	18	1
1:A:530:GLN:O	1:A:534:GLN:CG	0.41	2.69	18	1
1:A:469:LYS:CG	1:A:470:GLN:N	0.41	2.83	19	1
1:A:462:THR:CG2	1:A:520:LYS:NZ	0.41	2.83	20	1
1:A:475:LEU:HD12	1:A:481:VAL:HG11	0.41	1.93	8	1
1:A:497:PHE:CD1	1:A:497:PHE:N	0.41	2.89	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:457:VAL:HG13	1:A:521:LEU:CD2	0.40	2.47	10	1
1:A:476:ALA:HA	1:A:479:SER:O	0.40	2.17	15	2
1:A:524:LEU:CD1	1:A:528:HIS:CG	0.40	3.04	15	1
1:A:466:PRO:HB2	1:A:470:GLN:HG3	0.40	1.93	3	1
1:A:458:LYS:CB	1:A:524:LEU:HD21	0.40	2.46	6	1
1:A:487:LEU:N	1:A:487:LEU:HD12	0.40	2.31	7	1
1:A:510:TYR:CE1	1:A:521:LEU:CD1	0.40	2.99	7	1
1:A:524:LEU:HD12	1:A:528:HIS:CG	0.40	2.51	7	1
1:A:497:PHE:CD2	1:A:497:PHE:N	0.40	2.88	9	2
1:A:473:ASP:OD1	1:A:473:ASP:C	0.40	2.60	15	1
1:A:462:THR:O	1:A:463:GLU:HG3	0.40	2.16	10	1
1:A:510:TYR:CD1	1:A:521:LEU:HB2	0.40	2.52	11	1
1:A:475:LEU:HD12	1:A:481:VAL:CG2	0.40	2.46	18	1
1:A:515:LYS:HG3	1:A:516:LYS:N	0.40	2.31	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	86/125 (69%)	74±2 (86±2%)	8±2 (10±2%)	3±1 (4±1%)	6	33
All	All	1720/2500 (69%)	1484 (86%)	168 (10%)	68 (4%)	6	33

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	463	GLU	20
1	A	455	VAL	15
1	A	474	THR	9
1	A	487	LEU	7
1	A	527	ASP	3
1	A	490	ASP	3
1	A	518	CYS	3
1	A	483	TYR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	465	LEU	2
1	A	464	PRO	2
1	A	468	ARG	1
1	A	488	GLU	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	77/110 (70%)	54±3 (70±4%)	23±3 (30±4%)	2	16
All	All	1540/2200 (70%)	1071 (70%)	469 (30%)	2	16

All 56 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	465	LEU	20
1	A	519	TRP	20
1	A	510	TYR	20
1	A	516	LYS	18
1	A	535	LYS	17
1	A	531	ARG	16
1	A	460	ILE	16
1	A	521	LEU	16
1	A	486	LEU	15
1	A	499	THR	15
1	A	455	VAL	14
1	A	528	HIS	14
1	A	498	LYS	13
1	A	474	THR	13
1	A	520	LYS	12
1	A	463	GLU	11
1	A	482	LEU	11
1	A	530	GLN	10
1	A	479	SER	9
1	A	496	ARG	9
1	A	469	LYS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	515	LYS	9
1	A	540	ARG	9
1	A	522	GLU	9
1	A	502	ASP	9
1	A	493	CYS	8
1	A	504	GLN	8
1	A	487	LEU	8
1	A	537	LEU	8
1	A	492	GLU	7
1	A	488	GLU	7
1	A	525	SER	7
1	A	527	ASP	6
1	A	480	GLU	6
1	A	512	GLU	6
1	A	473	ASP	6
1	A	468	ARG	6
1	A	507	ILE	5
1	A	518	CYS	5
1	A	524	LEU	5
1	A	475	LEU	4
1	A	491	THR	4
1	A	501	GLU	4
1	A	485	ASP	3
1	A	490	ASP	3
1	A	462	THR	3
1	A	472	ARG	3
1	A	534	GLN	3
1	A	511	THR	2
1	A	481	VAL	2
1	A	539	ASP	1
1	A	470	GLN	1
1	A	458	LYS	1
1	A	461	SER	1
1	A	459	ILE	1
1	A	517	HIS	1

### 6.3.3 RNA ⓘ

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 84% for the entire structure.

### 7.1 Chemical shift list 1

File name: 5knw\_cs.cif

Chemical shift list name: *cs-full\_noA.txt*

#### 7.1.1 Bookkeeping [i](#)

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

Total number of shifts	1511
Number of shifts mapped to atoms	1511
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 [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	119	$-0.55 \pm 0.08$	Should be applied
$^{13}\text{C}_\beta$	113	$-0.18 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	106	$0.09 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	113	$-0.29 \pm 0.29$	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 90%, i.e. 998 atoms were assigned a chemical shift out of a possible 1107. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	416/424 (98%)	169/169 (100%)	164/172 (95%)	83/83 (100%)
Sidechain	514/602 (85%)	316/350 (90%)	194/224 (87%)	4/28 (14%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	68/81 (84%)	35/41 (85%)	32/32 (100%)	1/8 (12%)
Overall	998/1107 (90%)	520/560 (93%)	390/428 (91%)	88/119 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 84%, i.e. 1360 atoms were assigned a chemical shift out of a possible 1618. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	570/615 (93%)	232/245 (95%)	225/250 (90%)	113/120 (94%)
Sidechain	711/865 (82%)	441/508 (87%)	263/313 (84%)	7/44 (16%)
Aromatic	79/138 (57%)	42/70 (60%)	36/48 (75%)	1/20 (5%)
Overall	1360/1618 (84%)	715/823 (87%)	524/611 (86%)	121/184 (66%)

#### 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:

