



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:44 PM BST

PDB ID : 1RH8  
Title : Three-dimensional structure of the calcium-free Piccolo C2A-domain  
Authors : Garcia, J.; Gerber, S.H.; Sugita, S.; Sudhof, T.C.; Rizo, J.  
Deposited on : 2003-11-14

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-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

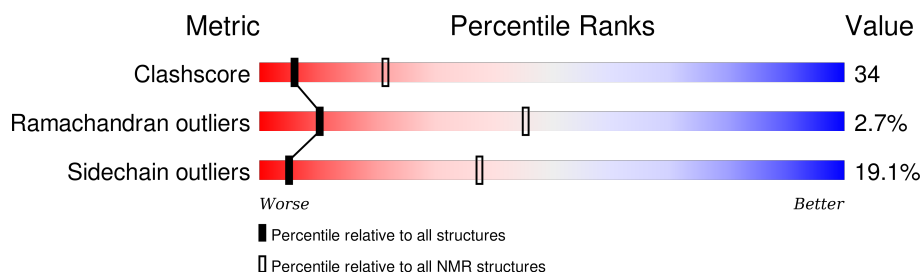
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	142	<div> <div></div> <div>35%</div> <div>44%</div> <div>8%</div> <div>14%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 5 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:4637-A:4666, A:4673-A:4683, A:4687-A:4739, A:4745-A:4772 (122)	0.29	5

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 1 single-model cluster was found.

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

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

There is only 1 type of molecule in this entry. The entry contains 2317 atoms, of which 1155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Piccolo protein.

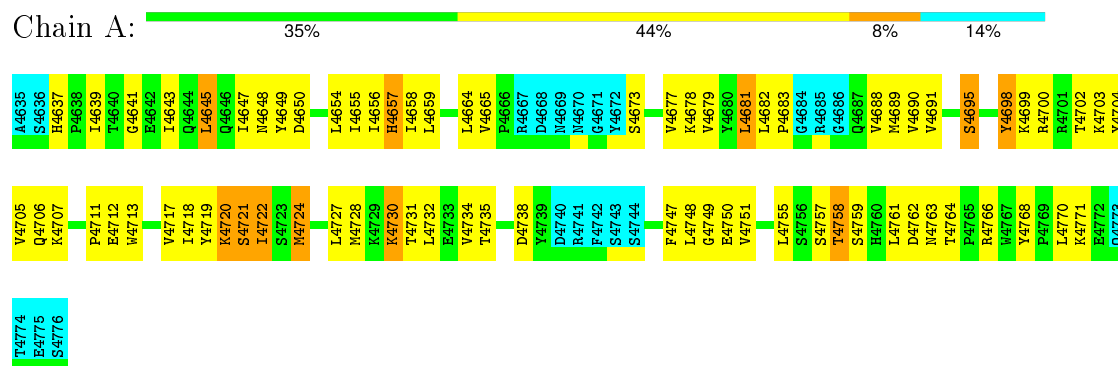
Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2317	738	1155	199	222	3	

## 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: Piccolo protein

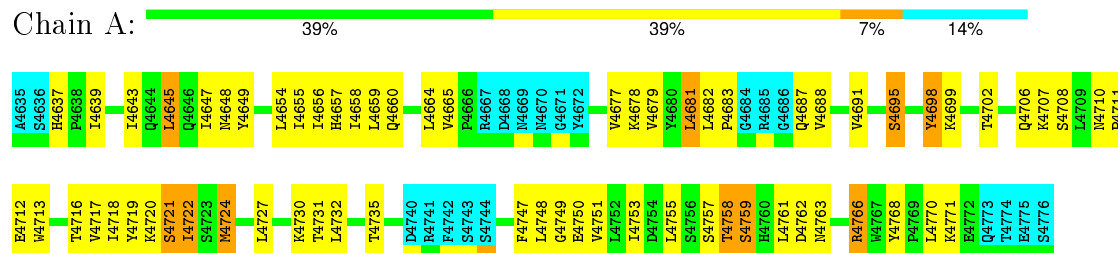


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

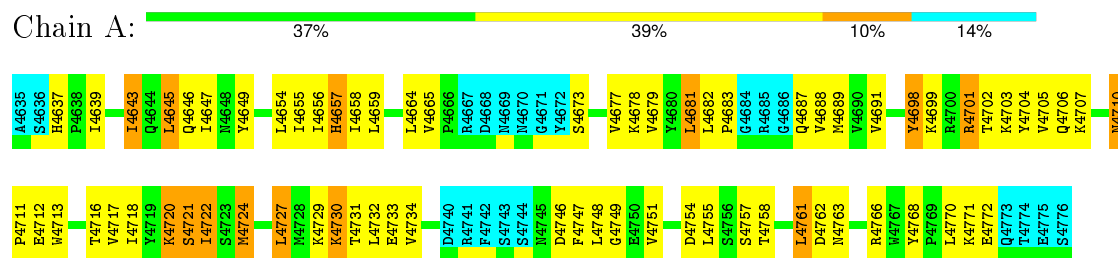
#### 4.2.1 Score per residue for model 1

- Molecule 1: Piccolo protein



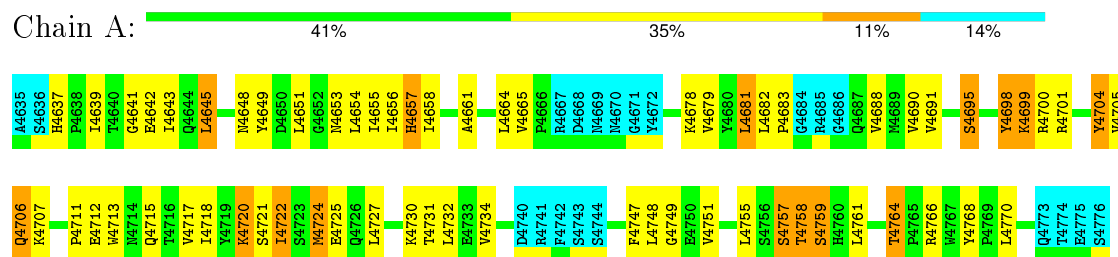
## 4.2.2 Score per residue for model 2

- Molecule 1: Piccolo protein



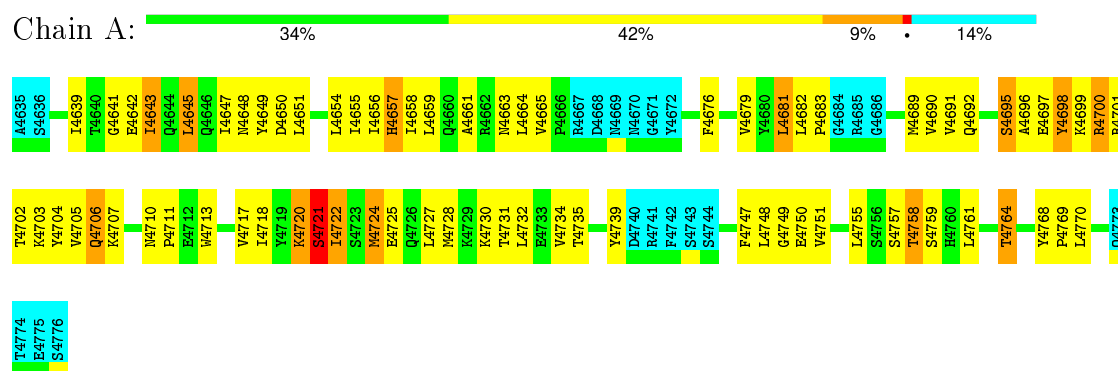
## 4.2.3 Score per residue for model 3

- Molecule 1: Piccolo protein



## 4.2.4 Score per residue for model 4

- Molecule 1: Piccolo protein

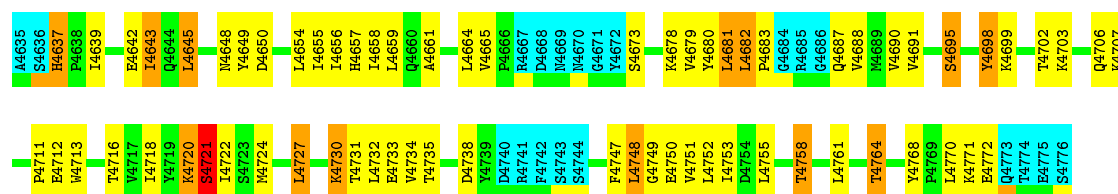


## 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Piccolo protein

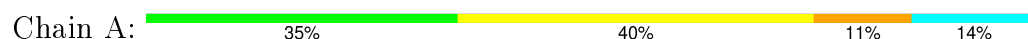






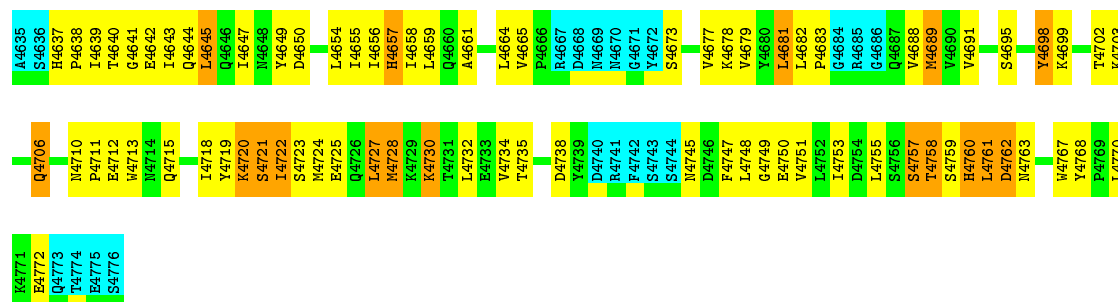
#### 4.2.9 Score per residue for model 9

- Molecule 1: Piccolo protein



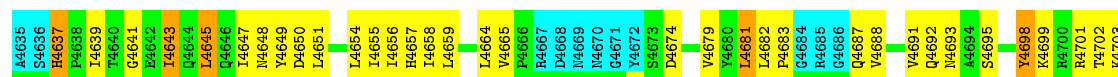
#### 4.2.10 Score per residue for model 10

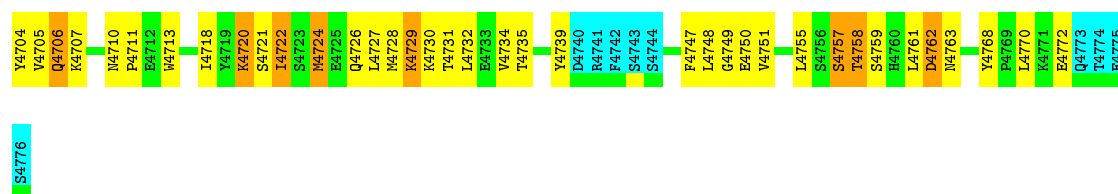
- Molecule 1: Piccolo protein



#### 4.2.11 Score per residue for model 11

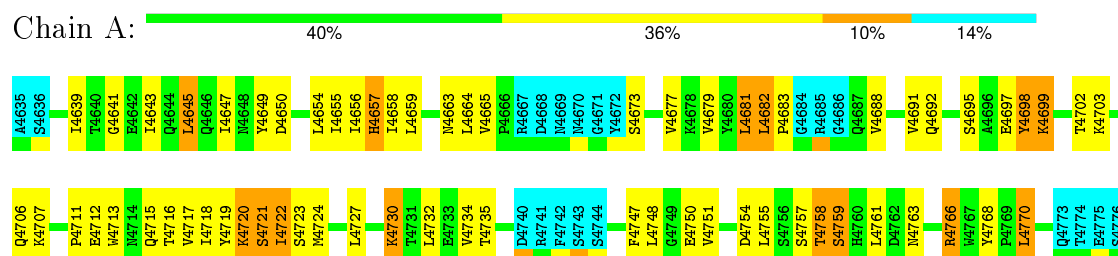
- Molecule 1: Piccolo protein





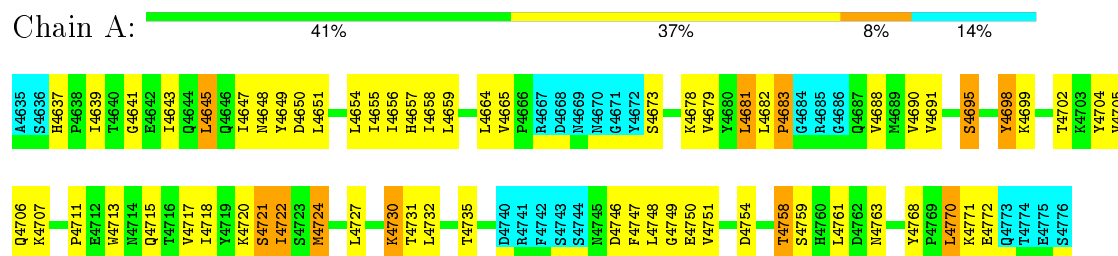
#### 4.2.12 Score per residue for model 12

- Molecule 1: Piccolo protein



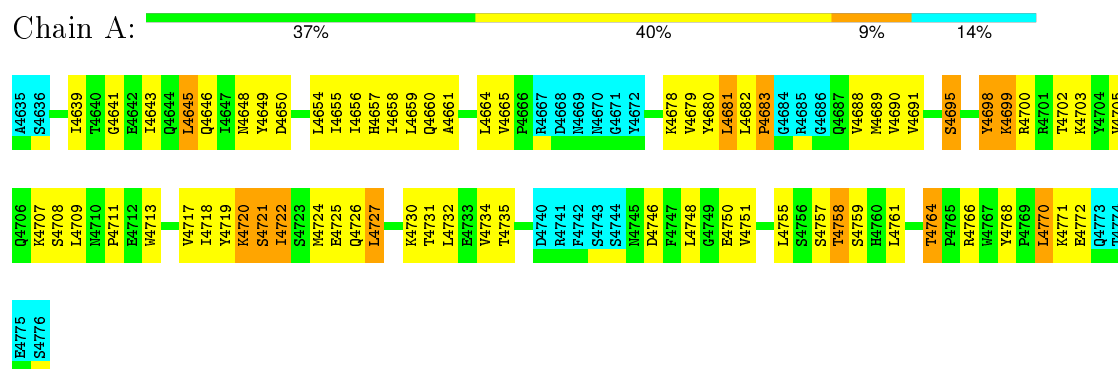
#### 4.2.13 Score per residue for model 13

- Molecule 1: Piccolo protein



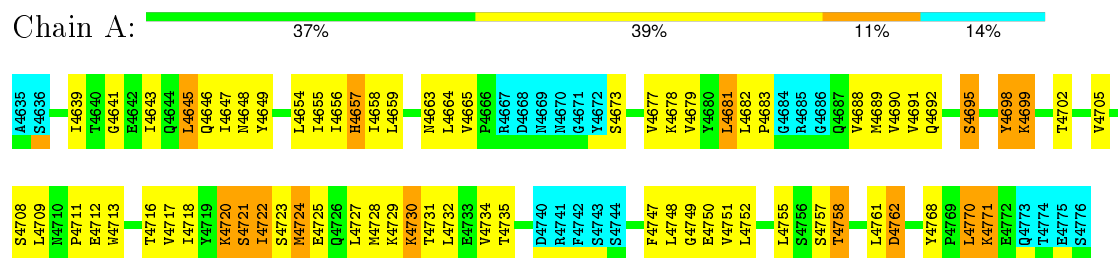
#### 4.2.14 Score per residue for model 14

- Molecule 1: Piccolo protein



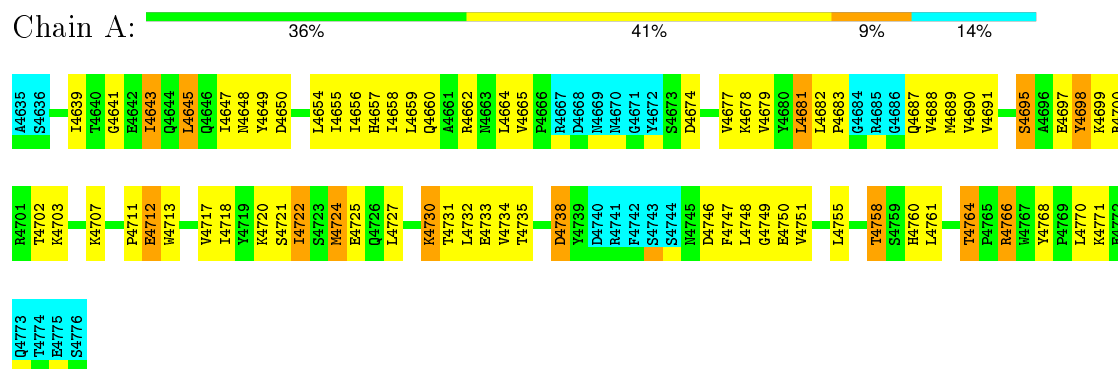
### 4.2.15 Score per residue for model 15

- Molecule 1: Piccolo protein



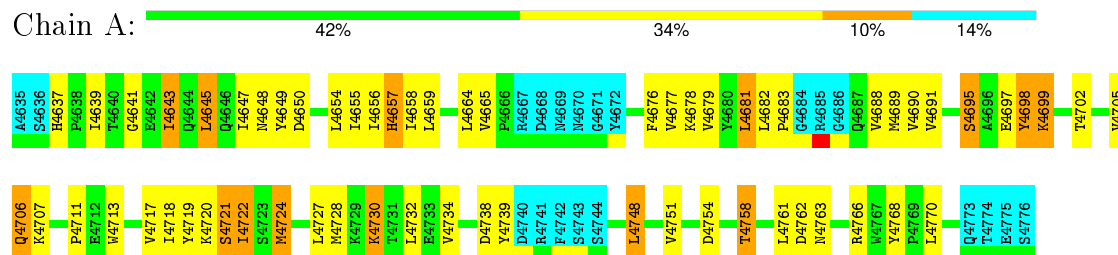
### 4.2.16 Score per residue for model 16

- Molecule 1: Piccolo protein



### 4.2.17 Score per residue for model 17

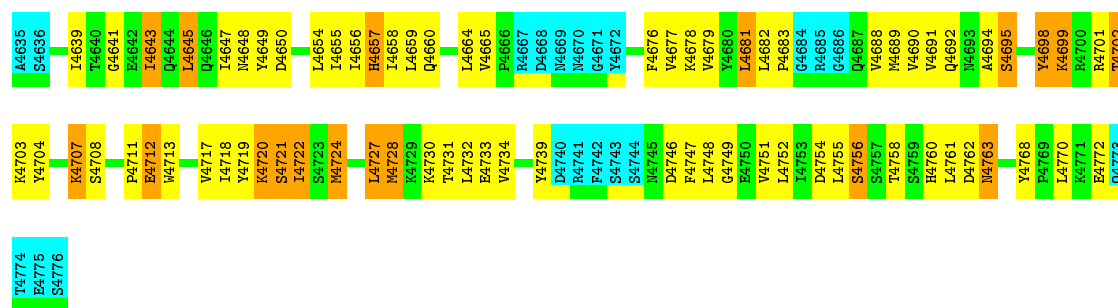
- Molecule 1: Piccolo protein



### 4.2.18 Score per residue for model 18

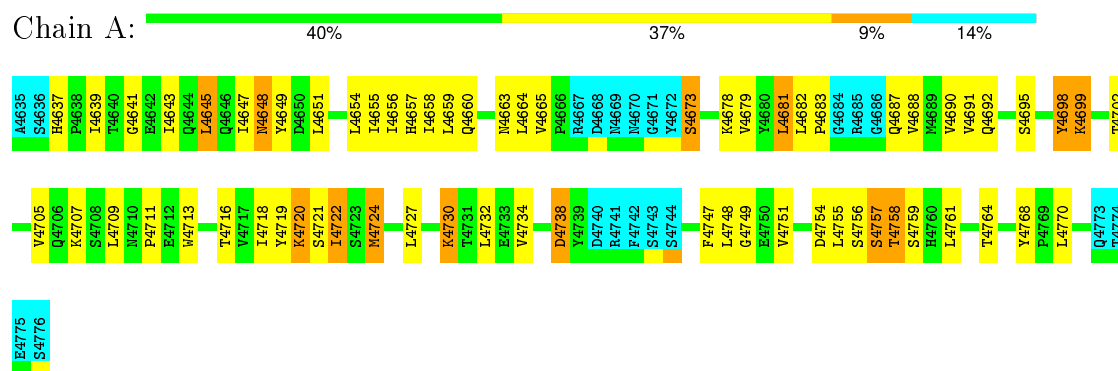
- Molecule 1: Piccolo protein





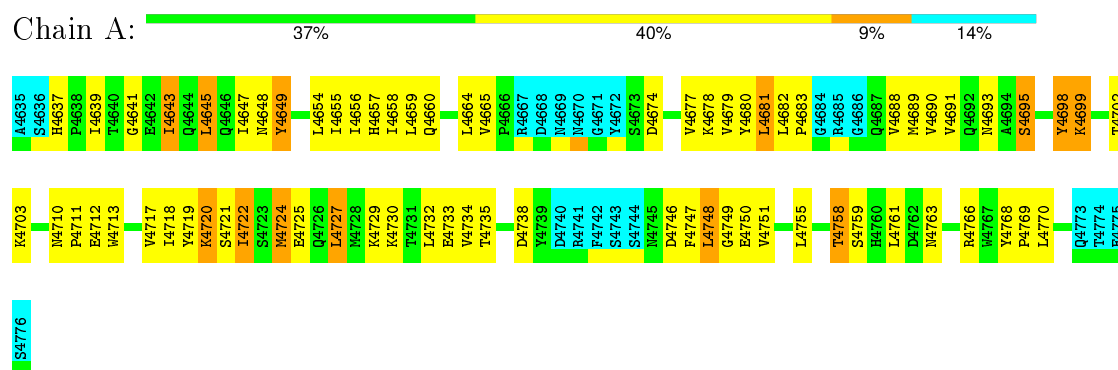
#### 4.2.19 Score per residue for model 19

- Molecule 1: Piccolo protein



#### 4.2.20 Score per residue for model 20

- Molecule 1: Piccolo protein



## 5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *torsion angle dynamics*.

Of the 1000 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
CNS	structure solution	0.9
CNS	refinement	0.9

No chemical shift data was provided. 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	1007	1021	1018	69±7
All	All	20140	20420	20360	1379

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 34.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4654:LEU:HD13	1:A:4727:LEU:HD11	1.03	1.26	9	19
1:A:4753:ILE:HG21	1:A:4760:HIS:CE1	0.91	1.99	10	1
1:A:4751:VAL:HG23	1:A:4770:LEU:HD23	0.88	1.45	8	17
1:A:4658:ILE:HD13	1:A:4691:VAL:HG22	0.87	1.46	4	14
1:A:4654:LEU:HD13	1:A:4727:LEU:CD1	0.84	2.01	9	19
1:A:4654:LEU:HD23	1:A:4656:ILE:HD11	0.83	1.49	15	7
1:A:4751:VAL:CG2	1:A:4770:LEU:HD23	0.82	2.05	13	19
1:A:4654:LEU:CD2	1:A:4656:ILE:HD11	0.82	2.05	15	7
1:A:4647:ILE:HD13	1:A:4656:ILE:HG23	0.80	1.53	10	16
1:A:4658:ILE:HD13	1:A:4691:VAL:CG2	0.79	2.07	15	14
1:A:4647:ILE:CD1	1:A:4656:ILE:HG23	0.79	2.08	10	14
1:A:4654:LEU:HD22	1:A:4730:LYS:NZ	0.79	1.92	5	2
1:A:4755:LEU:HA	1:A:4758:THR:HG23	0.78	1.54	10	1
1:A:4639:ILE:HG23	1:A:4748:LEU:O	0.76	1.80	11	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4751:VAL:HG11	1:A:4768:TYR:HB3	0.75	1.58	10	20
1:A:4727:LEU:HD12	1:A:4755:LEU:HD13	0.75	1.59	12	2
1:A:4654:LEU:CD1	1:A:4727:LEU:HD11	0.74	2.12	18	2
1:A:4722:ILE:HD11	1:A:4730:LYS:HE3	0.74	1.58	13	14
1:A:4658:ILE:HG22	1:A:4713:TRP:CE3	0.74	2.17	12	19
1:A:4758:THR:HG23	1:A:4761:LEU:CD1	0.74	2.12	2	4
1:A:4704:TYR:CD2	1:A:4705:VAL:HG22	0.74	2.18	13	2
1:A:4641:GLY:O	1:A:4770:LEU:HD12	0.73	1.84	5	14
1:A:4664:LEU:HD12	1:A:4711:PRO:CD	0.73	2.14	5	17
1:A:4655:ILE:HG23	1:A:4718:ILE:HD13	0.72	1.61	13	1
1:A:4641:GLY:C	1:A:4770:LEU:HD12	0.72	2.06	20	16
1:A:4689:MET:HG2	1:A:4717:VAL:HG11	0.71	1.61	4	9
1:A:4645:LEU:HD12	1:A:4768:TYR:CD1	0.71	2.21	2	12
1:A:4647:ILE:HG22	1:A:4761:LEU:HD23	0.71	1.63	9	3
1:A:4758:THR:HG23	1:A:4761:LEU:HD11	0.71	1.61	2	2
1:A:4722:ILE:HD11	1:A:4730:LYS:CE	0.70	2.16	11	17
1:A:4681:LEU:HD11	1:A:4755:LEU:HD12	0.70	1.62	12	7
1:A:4645:LEU:CD1	1:A:4734:VAL:HG21	0.68	2.18	16	5
1:A:4655:ILE:HG23	1:A:4718:ILE:CD1	0.68	2.18	13	1
1:A:4735:THR:HG22	1:A:4750:GLU:HG3	0.68	1.65	15	12
1:A:4643:ILE:HG12	1:A:4645:LEU:HD21	0.68	1.65	18	7
1:A:4702:THR:HG21	1:A:4712:GLU:OE2	0.68	1.89	8	5
1:A:4751:VAL:HG11	1:A:4768:TYR:CB	0.68	2.18	17	18
1:A:4681:LEU:HD21	1:A:4730:LYS:HE2	0.67	1.66	8	1
1:A:4643:ILE:HG22	1:A:4751:VAL:HG21	0.67	1.66	16	5
1:A:4718:ILE:HD12	1:A:4718:ILE:N	0.67	2.05	17	3
1:A:4718:ILE:N	1:A:4718:ILE:HD12	0.67	2.05	14	2
1:A:4679:VAL:CG1	1:A:4732:LEU:HD11	0.66	2.20	10	20
1:A:4681:LEU:HD11	1:A:4755:LEU:CD1	0.66	2.21	12	13
1:A:4752:LEU:HD12	1:A:4771:LYS:NZ	0.66	2.05	15	1
1:A:4682:LEU:HD11	1:A:4752:LEU:HD21	0.66	1.68	8	2
1:A:4699:LYS:HA	1:A:4702:THR:HG22	0.65	1.68	20	14
1:A:4678:LYS:HD3	1:A:4688:VAL:HG21	0.65	1.69	17	11
1:A:4724:MET:HE2	1:A:4727:LEU:HD23	0.64	1.69	4	3
1:A:4717:VAL:C	1:A:4718:ILE:HD12	0.64	2.13	9	5
1:A:4722:ILE:CG2	1:A:4727:LEU:HD13	0.64	2.23	13	1
1:A:4681:LEU:HB3	1:A:4683:PRO:HD3	0.64	1.70	8	1
1:A:4751:VAL:HG22	1:A:4770:LEU:HA	0.64	1.70	7	12
1:A:4656:ILE:HG21	1:A:4732:LEU:HD21	0.64	1.68	6	12
1:A:4645:LEU:HD21	1:A:4734:VAL:HG11	0.63	1.71	17	7
1:A:4643:ILE:HB	1:A:4770:LEU:HD21	0.63	1.70	12	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4665:VAL:HG12	1:A:4748:LEU:HD21	0.63	1.68	6	6
1:A:4738:ASP:HB2	1:A:4748:LEU:HD12	0.63	1.70	17	6
1:A:4679:VAL:HG22	1:A:4734:VAL:HA	0.63	1.71	15	11
1:A:4705:VAL:O	1:A:4709:LEU:HD12	0.62	1.94	15	3
1:A:4724:MET:HA	1:A:4727:LEU:HD23	0.62	1.71	8	1
1:A:4758:THR:HG23	1:A:4761:LEU:HG	0.61	1.72	20	16
1:A:4654:LEU:HD13	1:A:4727:LEU:HD13	0.61	1.71	8	1
1:A:4757:SER:O	1:A:4759:SER:N	0.61	2.33	10	10
1:A:4681:LEU:HD11	1:A:4755:LEU:HD11	0.61	1.71	19	3
1:A:4696:ALA:O	1:A:4700:ARG:N	0.61	2.33	4	3
1:A:4698:TYR:O	1:A:4702:THR:HG23	0.61	1.95	11	3
1:A:4758:THR:CG2	1:A:4761:LEU:HD11	0.61	2.26	2	2
1:A:4691:VAL:HG13	1:A:4715:GLN:HB2	0.61	1.73	5	7
1:A:4717:VAL:O	1:A:4718:ILE:HD13	0.60	1.96	13	1
1:A:4664:LEU:HD12	1:A:4711:PRO:HD3	0.60	1.74	17	18
1:A:4682:LEU:HB2	1:A:4683:PRO:HD3	0.60	1.72	17	19
1:A:4656:ILE:HD12	1:A:4656:ILE:N	0.59	2.11	5	10
1:A:4657:HIS:CD2	1:A:4716:THR:HG23	0.59	2.32	12	1
1:A:4643:ILE:HG23	1:A:4645:LEU:HD11	0.59	1.74	20	8
1:A:4727:LEU:HA	1:A:4730:LYS:CG	0.59	2.27	5	2
1:A:4758:THR:HB	1:A:4761:LEU:HG	0.59	1.75	10	2
1:A:4656:ILE:N	1:A:4656:ILE:HD12	0.59	2.13	20	9
1:A:4637:HIS:HB2	1:A:4665:VAL:HG21	0.58	1.75	11	12
1:A:4645:LEU:HD12	1:A:4768:TYR:CE1	0.58	2.33	18	6
1:A:4731:THR:HG23	1:A:4753:ILE:C	0.58	2.19	1	3
1:A:4704:TYR:CE2	1:A:4705:VAL:HG22	0.58	2.34	13	3
1:A:4682:LEU:CB	1:A:4683:PRO:CD	0.58	2.82	12	3
1:A:4689:MET:CG	1:A:4717:VAL:HG11	0.57	2.28	7	8
1:A:4678:LYS:HG2	1:A:4690:VAL:HG22	0.57	1.75	17	2
1:A:4724:MET:HA	1:A:4727:LEU:HB3	0.57	1.77	15	9
1:A:4655:ILE:HG23	1:A:4718:ILE:HG13	0.57	1.76	20	4
1:A:4665:VAL:HG12	1:A:4748:LEU:CD2	0.56	2.31	9	6
1:A:4647:ILE:CG2	1:A:4761:LEU:HD23	0.56	2.30	9	2
1:A:4681:LEU:HD12	1:A:4731:THR:N	0.56	2.16	2	14
1:A:4678:LYS:CD	1:A:4688:VAL:HG21	0.56	2.31	13	7
1:A:4655:ILE:HG23	1:A:4718:ILE:HG12	0.56	1.78	16	7
1:A:4645:LEU:HD11	1:A:4734:VAL:HG21	0.56	1.78	12	4
1:A:4643:ILE:CG2	1:A:4751:VAL:HG21	0.56	2.31	16	5
1:A:4682:LEU:HD11	1:A:4752:LEU:CD2	0.56	2.30	8	2
1:A:4764:THR:HG22	1:A:4764:THR:O	0.56	2.01	8	4
1:A:4645:LEU:HD23	1:A:4658:ILE:HG13	0.55	1.77	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4655:ILE:HG13	1:A:4718:ILE:HG23	0.55	1.79	12	19
1:A:4664:LEU:HD22	1:A:4748:LEU:HD22	0.55	1.77	20	2
1:A:4751:VAL:HG13	1:A:4769:PRO:O	0.55	2.02	9	3
1:A:4727:LEU:CD1	1:A:4755:LEU:HD13	0.55	2.31	12	5
1:A:4752:LEU:HD12	1:A:4771:LYS:HZ1	0.55	1.60	15	1
1:A:4682:LEU:CB	1:A:4683:PRO:HD3	0.54	2.33	12	5
1:A:4682:LEU:HD21	1:A:4733:GLU:HB2	0.54	1.79	2	2
1:A:4696:ALA:O	1:A:4700:ARG:HG3	0.54	2.03	6	2
1:A:4704:TYR:HD2	1:A:4705:VAL:HG23	0.54	1.62	4	1
1:A:4696:ALA:O	1:A:4700:ARG:CG	0.54	2.56	7	3
1:A:4720:LYS:O	1:A:4721:SER:CB	0.53	2.57	10	20
1:A:4654:LEU:HD11	1:A:4755:LEU:HD22	0.53	1.80	8	1
1:A:4665:VAL:HG13	1:A:4665:VAL:O	0.53	2.04	2	8
1:A:4704:TYR:CE2	1:A:4705:VAL:HG13	0.53	2.38	2	1
1:A:4764:THR:O	1:A:4764:THR:HG22	0.53	2.04	16	2
1:A:4657:HIS:CD2	1:A:4657:HIS:N	0.52	2.77	18	12
1:A:4665:VAL:O	1:A:4665:VAL:HG13	0.52	2.05	9	11
1:A:4681:LEU:HD12	1:A:4730:LYS:HB3	0.52	1.80	4	14
1:A:4655:ILE:CG1	1:A:4718:ILE:HD12	0.52	2.35	13	1
1:A:4661:ALA:HB3	1:A:4711:PRO:HD2	0.52	1.81	14	1
1:A:4681:LEU:HD21	1:A:4730:LYS:NZ	0.51	2.21	5	1
1:A:4640:THR:O	1:A:4664:LEU:HD23	0.51	2.05	5	3
1:A:4761:LEU:O	1:A:4763:ASN:N	0.51	2.43	10	6
1:A:4699:LYS:HE2	1:A:4712:GLU:CB	0.51	2.35	15	1
1:A:4758:THR:CB	1:A:4761:LEU:HG	0.51	2.36	18	1
1:A:4645:LEU:HD13	1:A:4734:VAL:HG21	0.51	1.83	16	1
1:A:4659:LEU:O	1:A:4713:TRP:N	0.51	2.43	11	18
1:A:4758:THR:HG23	1:A:4761:LEU:CG	0.51	2.36	13	2
1:A:4724:MET:CE	1:A:4727:LEU:HD21	0.51	2.35	8	1
1:A:4688:VAL:O	1:A:4688:VAL:HG13	0.50	2.06	12	5
1:A:4680:TYR:HB3	1:A:4688:VAL:HA	0.50	1.83	8	3
1:A:4758:THR:HG23	1:A:4758:THR:O	0.50	2.06	9	1
1:A:4679:VAL:HG11	1:A:4732:LEU:HD11	0.50	1.83	8	15
1:A:4698:TYR:CZ	1:A:4699:LYS:HD3	0.50	2.41	13	20
1:A:4645:LEU:HD23	1:A:4658:ILE:HA	0.50	1.83	14	4
1:A:4654:LEU:HD23	1:A:4719:TYR:HD2	0.50	1.66	1	3
1:A:4701:ARG:O	1:A:4704:TYR:CE2	0.50	2.64	9	1
1:A:4688:VAL:HG13	1:A:4688:VAL:O	0.50	2.07	1	9
1:A:4758:THR:O	1:A:4758:THR:HG23	0.50	2.07	2	1
1:A:4698:TYR:CZ	1:A:4699:LYS:CD	0.50	2.95	14	13
1:A:4655:ILE:HG23	1:A:4717:VAL:O	0.50	2.07	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4637:HIS:CE1	1:A:4665:VAL:HG11	0.49	2.42	3	2
1:A:4681:LEU:CD1	1:A:4731:THR:C	0.49	2.81	5	2
1:A:4694:ALA:HB2	1:A:4713:TRP:O	0.49	2.07	18	1
1:A:4643:ILE:HD11	1:A:4713:TRP:CZ3	0.49	2.42	4	2
1:A:4731:THR:HG23	1:A:4754:ASP:HA	0.49	1.83	6	3
1:A:4681:LEU:HD21	1:A:4730:LYS:CE	0.49	2.37	8	1
1:A:4722:ILE:HD11	1:A:4730:LYS:HE2	0.49	1.85	2	3
1:A:4701:ARG:O	1:A:4704:TYR:CZ	0.49	2.66	3	2
1:A:4705:VAL:HG23	1:A:4706:GLN:N	0.49	2.23	2	6
1:A:4657:HIS:N	1:A:4657:HIS:CD2	0.49	2.81	4	8
1:A:4722:ILE:HG22	1:A:4722:ILE:O	0.49	2.08	18	9
1:A:4698:TYR:O	1:A:4702:THR:HG22	0.49	2.08	4	4
1:A:4681:LEU:C	1:A:4682:LEU:HD23	0.48	2.27	8	1
1:A:4643:ILE:HG12	1:A:4645:LEU:HD11	0.48	1.85	1	1
1:A:4698:TYR:CE2	1:A:4699:LYS:HD3	0.48	2.44	11	5
1:A:4665:VAL:HG12	1:A:4748:LEU:HD22	0.48	1.84	1	4
1:A:4718:ILE:CD1	1:A:4718:ILE:N	0.48	2.76	14	2
1:A:4727:LEU:HA	1:A:4730:LYS:HG3	0.48	1.85	8	2
1:A:4722:ILE:O	1:A:4722:ILE:HG22	0.48	2.08	12	9
1:A:4649:TYR:HB3	1:A:4761:LEU:HD22	0.48	1.86	20	1
1:A:4642:GLU:O	1:A:4661:ALA:HB1	0.48	2.08	8	7
1:A:4697:GLU:HA	1:A:4700:ARG:CG	0.48	2.37	7	3
1:A:4749:GLY:HA3	1:A:4770:LEU:HD22	0.48	1.86	2	2
1:A:4677:VAL:HB	1:A:4691:VAL:HG21	0.47	1.86	7	4
1:A:4704:TYR:HD2	1:A:4705:VAL:HG13	0.47	1.70	7	3
1:A:4722:ILE:HD11	1:A:4730:LYS:NZ	0.47	2.24	12	1
1:A:4682:LEU:N	1:A:4682:LEU:HD23	0.47	2.25	8	1
1:A:4728:MET:HE1	1:A:4755:LEU:O	0.47	2.09	6	1
1:A:4681:LEU:HD21	1:A:4730:LYS:HZ3	0.47	1.70	5	1
1:A:4657:HIS:CE1	1:A:4716:THR:HG23	0.47	2.44	6	5
1:A:4704:TYR:CE2	1:A:4705:VAL:CG1	0.47	2.98	2	1
1:A:4657:HIS:CE1	1:A:4716:THR:CG2	0.47	2.98	2	6
1:A:4648:ASN:HA	1:A:4761:LEU:O	0.46	2.10	1	13
1:A:4717:VAL:HG12	1:A:4718:ILE:N	0.46	2.26	5	6
1:A:4681:LEU:HD12	1:A:4730:LYS:CB	0.46	2.41	4	3
1:A:4706:GLN:O	1:A:4710:ASN:N	0.46	2.49	11	6
1:A:4681:LEU:HD23	1:A:4719:TYR:CD2	0.46	2.46	6	2
1:A:4718:ILE:N	1:A:4718:ILE:CD1	0.46	2.79	18	3
1:A:4702:THR:HB	1:A:4706:GLN:HB2	0.46	1.88	11	1
1:A:4660:GLN:HA	1:A:4713:TRP:CZ3	0.46	2.46	7	5
1:A:4699:LYS:HB3	1:A:4699:LYS:HZ3	0.46	1.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4724:MET:HE1	1:A:4727:LEU:HD21	0.46	1.87	8	1
1:A:4647:ILE:HG13	1:A:4760:HIS:ND1	0.46	2.25	10	1
1:A:4639:ILE:HG21	1:A:4747:PHE:CE2	0.46	2.45	12	4
1:A:4656:ILE:HD13	1:A:4719:TYR:CE2	0.46	2.45	14	3
1:A:4658:ILE:HG13	1:A:4691:VAL:CG2	0.46	2.41	1	6
1:A:4689:MET:CE	1:A:4719:TYR:CE1	0.45	2.99	10	1
1:A:4645:LEU:HD23	1:A:4658:ILE:CG1	0.45	2.41	5	2
1:A:4755:LEU:HA	1:A:4758:THR:CG2	0.45	2.41	18	1
1:A:4681:LEU:HD13	1:A:4731:THR:O	0.45	2.11	15	5
1:A:4722:ILE:HG23	1:A:4727:LEU:HB2	0.45	1.88	10	3
1:A:4718:ILE:HG22	1:A:4719:TYR:N	0.45	2.27	18	5
1:A:4643:ILE:CD1	1:A:4713:TRP:CZ3	0.45	2.99	4	1
1:A:4643:ILE:CG2	1:A:4645:LEU:HD11	0.45	2.41	13	3
1:A:4681:LEU:CD1	1:A:4730:LYS:HB3	0.45	2.41	20	11
1:A:4727:LEU:HD12	1:A:4730:LYS:CE	0.45	2.41	5	1
1:A:4702:THR:O	1:A:4702:THR:HG23	0.45	2.12	7	2
1:A:4724:MET:HE1	1:A:4761:LEU:HD13	0.45	1.87	13	2
1:A:4658:ILE:HG21	1:A:4677:VAL:HG21	0.45	1.89	17	3
1:A:4683:PRO:CD	1:A:4730:LYS:HA	0.45	2.42	11	1
1:A:4701:ARG:O	1:A:4704:TYR:CE1	0.45	2.69	3	3
1:A:4768:TYR:N	1:A:4768:TYR:CD1	0.45	2.84	13	2
1:A:4755:LEU:HD23	1:A:4758:THR:HG21	0.44	1.88	8	1
1:A:4698:TYR:CE2	1:A:4699:LYS:CD	0.44	3.00	7	2
1:A:4728:MET:CE	1:A:4755:LEU:O	0.44	2.66	10	2
1:A:4758:THR:OG1	1:A:4761:LEU:HG	0.44	2.12	18	1
1:A:4655:ILE:C	1:A:4656:ILE:HD12	0.44	2.32	3	3
1:A:4730:LYS:CD	1:A:4755:LEU:HD13	0.44	2.42	5	2
1:A:4724:MET:CE	1:A:4727:LEU:CD2	0.44	2.96	6	11
1:A:4760:HIS:N	1:A:4760:HIS:CD2	0.44	2.84	18	1
1:A:4691:VAL:HG13	1:A:4715:GLN:CG	0.44	2.43	9	1
1:A:4755:LEU:O	1:A:4758:THR:HG22	0.44	2.13	2	2
1:A:4690:VAL:HG12	1:A:4691:VAL:N	0.44	2.28	18	12
1:A:4682:LEU:HB2	1:A:4683:PRO:CD	0.44	2.42	12	2
1:A:4689:MET:HG3	1:A:4717:VAL:HG11	0.44	1.89	9	1
1:A:4724:MET:HE2	1:A:4727:LEU:CD2	0.44	2.42	18	1
1:A:4676:PHE:CE1	1:A:4739:TYR:CD2	0.44	3.05	17	3
1:A:4656:ILE:CD1	1:A:4656:ILE:N	0.44	2.81	5	2
1:A:4728:MET:HE1	1:A:4756:SER:O	0.44	2.13	18	1
1:A:4658:ILE:HD13	1:A:4691:VAL:HG21	0.44	1.86	14	2
1:A:4698:TYR:CE2	1:A:4699:LYS:HG2	0.44	2.48	4	2
1:A:4687:GLN:O	1:A:4687:GLN:CG	0.44	2.66	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4747:PHE:CZ	1:A:4749:GLY:C	0.43	2.92	15	14
1:A:4681:LEU:HG	1:A:4730:LYS:HB2	0.43	1.88	5	2
1:A:4761:LEU:C	1:A:4763:ASN:N	0.43	2.72	2	3
1:A:4658:ILE:CG2	1:A:4713:TRP:CE3	0.43	3.00	19	7
1:A:4724:MET:HA	1:A:4727:LEU:CB	0.43	2.43	13	1
1:A:4747:PHE:CZ	1:A:4749:GLY:CA	0.43	3.02	13	2
1:A:4730:LYS:CD	1:A:4755:LEU:CD1	0.43	2.97	5	1
1:A:4677:VAL:HG12	1:A:4678:LYS:N	0.43	2.29	9	5
1:A:4681:LEU:CD2	1:A:4730:LYS:HE2	0.43	2.42	8	1
1:A:4697:GLU:HA	1:A:4700:ARG:HG2	0.43	1.89	7	2
1:A:4755:LEU:O	1:A:4758:THR:HG23	0.42	2.14	18	1
1:A:4658:ILE:HG13	1:A:4691:VAL:HG22	0.42	1.89	18	1
1:A:4644:GLN:C	1:A:4645:LEU:HG	0.42	2.35	9	1
1:A:4738:ASP:OD2	1:A:4748:LEU:HD11	0.42	2.14	16	2
1:A:4681:LEU:C	1:A:4683:PRO:HD3	0.42	2.34	8	1
1:A:4655:ILE:HG22	1:A:4657:HIS:NE2	0.42	2.29	6	1
1:A:4678:LYS:HA	1:A:4689:MET:O	0.42	2.14	9	1
1:A:4654:LEU:HD22	1:A:4730:LYS:HZ2	0.42	1.72	5	1
1:A:4679:VAL:CG1	1:A:4732:LEU:CD1	0.42	2.97	5	10
1:A:4733:GLU:OE2	1:A:4752:LEU:HD21	0.42	2.14	9	1
1:A:4698:TYR:CD1	1:A:4698:TYR:C	0.42	2.92	5	1
1:A:4682:LEU:N	1:A:4683:PRO:CD	0.42	2.82	8	6
1:A:4681:LEU:CD1	1:A:4730:LYS:CB	0.42	2.97	4	6
1:A:4691:VAL:HG13	1:A:4715:GLN:CB	0.42	2.44	5	1
1:A:4677:VAL:HB	1:A:4691:VAL:CG2	0.42	2.45	18	1
1:A:4648:ASN:O	1:A:4655:ILE:HB	0.42	2.14	19	6
1:A:4664:LEU:HD12	1:A:4711:PRO:CG	0.42	2.44	4	2
1:A:4699:LYS:O	1:A:4703:LYS:N	0.42	2.53	10	1
1:A:4702:THR:HG23	1:A:4702:THR:O	0.42	2.13	12	2
1:A:4647:ILE:HD12	1:A:4732:LEU:HD22	0.42	1.91	1	1
1:A:4764:THR:CG2	1:A:4764:THR:O	0.42	2.67	8	2
1:A:4726:GLN:O	1:A:4729:LYS:CG	0.42	2.67	11	1
1:A:4638:PRO:O	1:A:4665:VAL:HB	0.42	2.15	10	1
1:A:4677:VAL:CG1	1:A:4678:LYS:N	0.42	2.82	17	6
1:A:4698:TYR:C	1:A:4698:TYR:CD1	0.42	2.93	18	1
1:A:4724:MET:HE1	1:A:4761:LEU:CD1	0.41	2.45	20	1
1:A:4704:TYR:CD2	1:A:4705:VAL:HG23	0.41	2.47	4	1
1:A:4695:SER:O	1:A:4698:TYR:CD2	0.41	2.73	5	1
1:A:4766:ARG:O	1:A:4768:TYR:CE1	0.41	2.74	20	6
1:A:4689:MET:HE2	1:A:4719:TYR:CE1	0.41	2.50	10	1
1:A:4760:HIS:CE1	1:A:4766:ARG:CD	0.41	3.03	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4658:ILE:HG21	1:A:4691:VAL:HG21	0.41	1.92	18	1
1:A:4699:LYS:HE2	1:A:4712:GLU:HB2	0.41	1.91	15	1
1:A:4637:HIS:NE2	1:A:4665:VAL:HG11	0.41	2.31	20	1
1:A:4724:MET:HE3	1:A:4727:LEU:CD2	0.41	2.45	13	1
1:A:4654:LEU:HG	1:A:4656:ILE:HD11	0.41	1.93	9	2
1:A:4679:VAL:O	1:A:4719:TYR:OH	0.41	2.38	5	1
1:A:4722:ILE:HD13	1:A:4730:LYS:HE2	0.41	1.92	5	1
1:A:4731:THR:HG23	1:A:4754:ASP:N	0.41	2.31	5	1
1:A:4683:PRO:CG	1:A:4730:LYS:HA	0.41	2.46	1	2
1:A:4699:LYS:O	1:A:4702:THR:N	0.41	2.53	10	2
1:A:4760:HIS:CE1	1:A:4768:TYR:CE2	0.41	3.09	18	1
1:A:4722:ILE:HG21	1:A:4727:LEU:HD13	0.41	1.91	13	1
1:A:4704:TYR:O	1:A:4707:LYS:HG2	0.41	2.16	18	1
1:A:4681:LEU:HA	1:A:4681:LEU:HD13	0.40	1.80	16	1
1:A:4722:ILE:CG2	1:A:4722:ILE:O	0.40	2.69	12	1
1:A:4655:ILE:CG2	1:A:4716:THR:CG2	0.40	3.00	12	1
1:A:4766:ARG:HG3	1:A:4768:TYR:CZ	0.40	2.51	2	1
1:A:4644:GLN:NE2	1:A:4767:TRP:NE1	0.40	2.70	7	1
1:A:4647:ILE:HG22	1:A:4761:LEU:CD2	0.40	2.40	9	1
1:A:4644:GLN:OE1	1:A:4767:TRP:CZ2	0.40	2.74	10	1
1:A:4680:TYR:CZ	1:A:4733:GLU:OE1	0.40	2.74	20	1
1:A:4656:ILE:N	1:A:4656:ILE:CD1	0.40	2.84	16	1
1:A:4681:LEU:HD13	1:A:4681:LEU:HA	0.40	1.80	11	1
1:A:4701:ARG:O	1:A:4704:TYR:CD1	0.40	2.74	11	1
1:A:4644:GLN:O	1:A:4659:LEU:HB2	0.40	2.16	10	1
1:A:4639:ILE:HG21	1:A:4747:PHE:HE2	0.40	1.77	13	1
1:A:4660:GLN:HA	1:A:4713:TRP:CE3	0.40	2.52	19	1
1:A:4653:ASN:ND2	1:A:4720:LYS:CG	0.40	2.85	3	1
1:A:4665:VAL:HG12	1:A:4748:LEU:HD23	0.40	1.92	8	1
1:A:4646:GLN:O	1:A:4657:HIS:CD2	0.40	2.75	14	1
1:A:4724:MET:O	1:A:4728:MET:CG	0.40	2.70	4	1
1:A:4679:VAL:HG12	1:A:4719:TYR:OH	0.40	2.16	10	1
1:A:4682:LEU:N	1:A:4683:PRO:HD3	0.40	2.32	8	1
1:A:4692:GLN:O	1:A:4715:GLN:NE2	0.40	2.55	12	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	122/142 (86%)	106±2 (87±2%)	13±2 (10±2%)	3±1 (3±1%)	10	45
All	All	2440/2840 (86%)	2123 (87%)	250 (10%)	67 (3%)	10	45

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	4758	THR	18
1	A	4695	SER	15
1	A	4721	SER	12
1	A	4763	ASN	7
1	A	4762	ASP	7
1	A	4761	LEU	3
1	A	4683	PRO	3
1	A	4682	LEU	1
1	A	4745	ASN	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	116/132 (88%)	94±3 (81±2%)	22±3 (19±2%)	5	37
All	All	2320/2640 (88%)	1877 (81%)	443 (19%)	5	37

All 62 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	4698	TYR	20
1	A	4649	TYR	20
1	A	4645	LEU	20
1	A	4722	ILE	20
1	A	4681	LEU	20
1	A	4724	MET	17
1	A	4707	LYS	16

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Mol	Chain	Res	Type	Models (Total)
1	A	4720	LYS	14
1	A	4695	SER	14
1	A	4730	LYS	12
1	A	4771	LYS	11
1	A	4650	ASP	11
1	A	4706	GLN	11
1	A	4657	HIS	10
1	A	4643	ILE	10
1	A	4703	LYS	10
1	A	4725	GLU	9
1	A	4699	LYS	9
1	A	4757	SER	8
1	A	4727	LEU	8
1	A	4673	SER	8
1	A	4728	MET	8
1	A	4746	ASP	8
1	A	4700	ARG	8
1	A	4759	SER	7
1	A	4692	GLN	7
1	A	4748	LEU	7
1	A	4772	GLU	7
1	A	4764	THR	7
1	A	4762	ASP	6
1	A	4651	LEU	6
1	A	4712	GLU	6
1	A	4754	ASP	5
1	A	4766	ARG	5
1	A	4663	ASN	5
1	A	4729	LYS	5
1	A	4687	GLN	5
1	A	4770	LEU	5
1	A	4701	ARG	5
1	A	4697	GLU	4
1	A	4723	SER	4
1	A	4721	SER	4
1	A	4674	ASP	4
1	A	4708	SER	4
1	A	4693	ASN	4
1	A	4648	ASN	3
1	A	4738	ASP	3
1	A	4756	SER	2
1	A	4710	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	4704	TYR	2
1	A	4662	ARG	2
1	A	4637	HIS	2
1	A	4733	GLU	2
1	A	4689	MET	2
1	A	4646	GLN	2
1	A	4682	LEU	1
1	A	4760	HIS	1
1	A	4660	GLN	1
1	A	4739	TYR	1
1	A	4763	ASN	1
1	A	4726	GLN	1
1	A	4702	THR	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

No chemical shift data were provided