



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:08 AM BST

PDB ID : 2N03  
Title : Solution NMR Structure plectin repeat domain 6 (4403-4606) of Plectin from Homo sapiens, Northeast Structural Genomics Consortium (NESG) Target HR6354E  
Authors : Pulavarti, S.; Eletsky, A.; Huang, Y.; Janjua, H.; Xiao, R.; Acton, T.; Everett, J.; Montelione, G.; Szyperski, T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2015-03-04

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

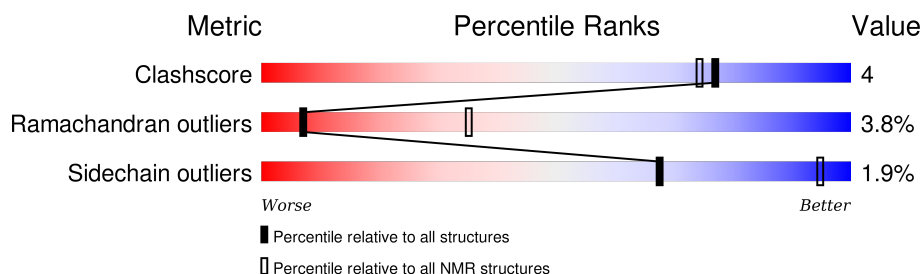
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 49%.

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	215	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:4416-A:4497, A:4504-A:4573, A:4580-A:4606 (179)	0.95	17

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

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

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

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3327 atoms, of which 1662 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Plectin.

Mol	Chain	Residues	Atoms						Trace
1	A	215	Total	C	H	N	O	S	0
			3327	1038	1662	297	321	9	

There are 11 discrepancies between the modelled and reference sequences:

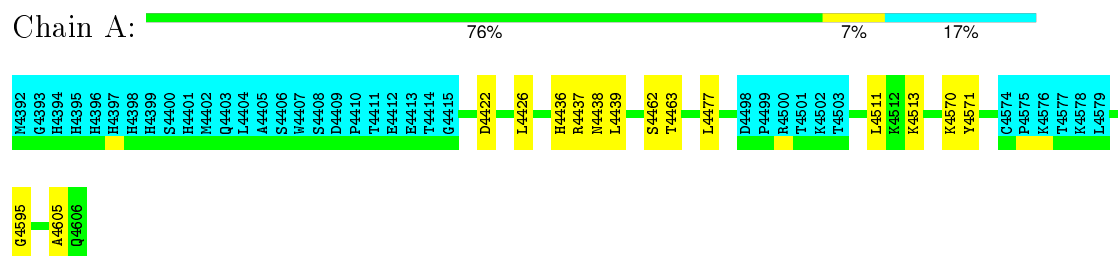
Chain	Residue	Modelled	Actual	Comment	Reference
A	4392	MET	-	EXPRESSION TAG	UNP Q15149
A	4393	GLY	-	EXPRESSION TAG	UNP Q15149
A	4394	HIS	-	EXPRESSION TAG	UNP Q15149
A	4395	HIS	-	EXPRESSION TAG	UNP Q15149
A	4396	HIS	-	EXPRESSION TAG	UNP Q15149
A	4397	HIS	-	EXPRESSION TAG	UNP Q15149
A	4398	HIS	-	EXPRESSION TAG	UNP Q15149
A	4399	HIS	-	EXPRESSION TAG	UNP Q15149
A	4400	SER	-	EXPRESSION TAG	UNP Q15149
A	4401	HIS	-	EXPRESSION TAG	UNP Q15149
A	4402	MET	-	EXPRESSION TAG	UNP Q15149

## 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: Plectin

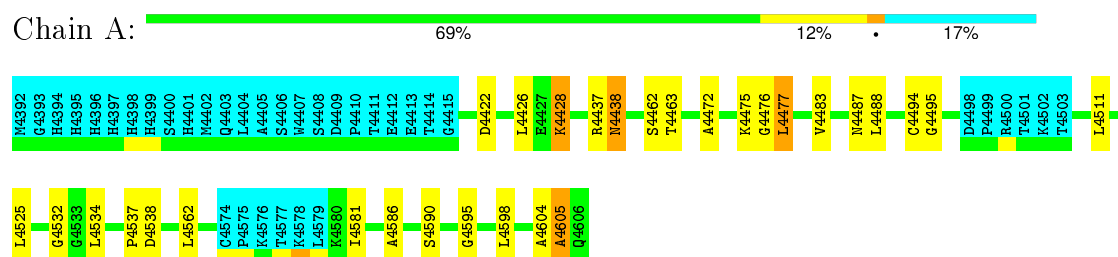


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

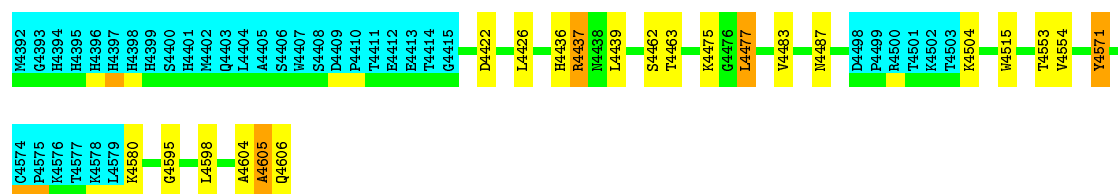
- Molecule 1: Plectin



#### 4.2.2 Score per residue for model 2

- Molecule 1: Plectin

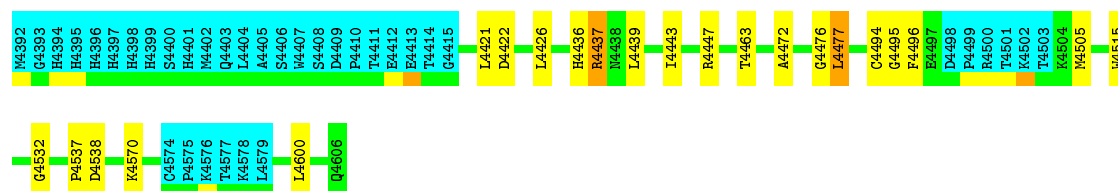




### 4.2.3 Score per residue for model 3

- Molecule 1: Plectin

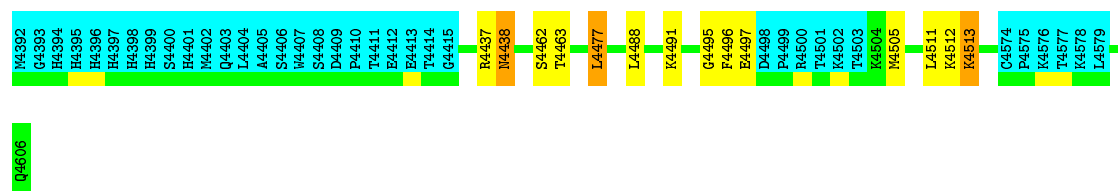
Chain A: 73% 9% 17%



### 4.2.4 Score per residue for model 4

- Molecule 1: Plectin

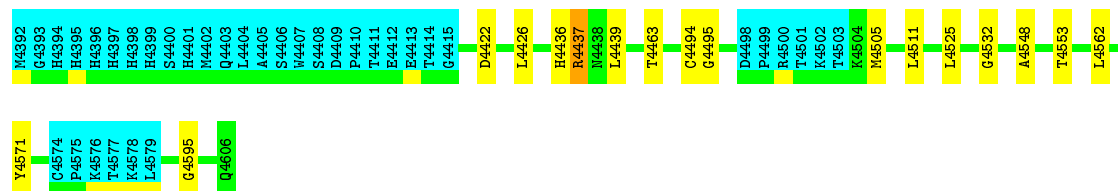
Chain A: 77% 5% 17%



### 4.2.5 Score per residue for model 5

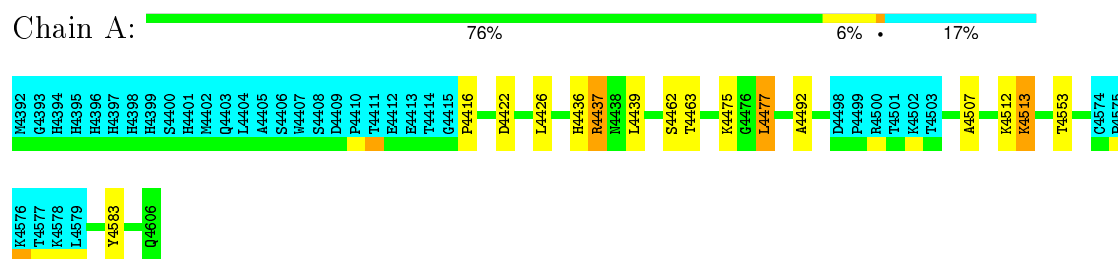
- Molecule 1: Plectin

Chain A: 75% 7% 17%



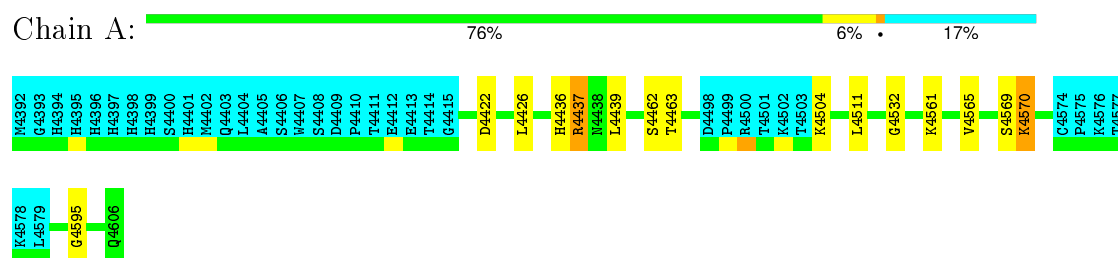
## 4.2.6 Score per residue for model 6

- Molecule 1: Plectin



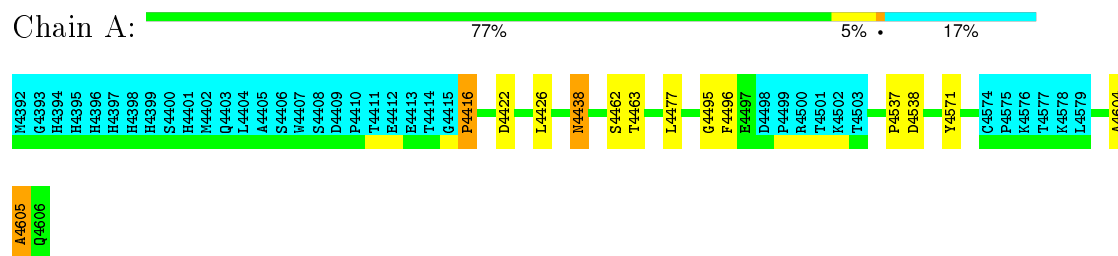
## 4.2.7 Score per residue for model 7

- Molecule 1: Plectin



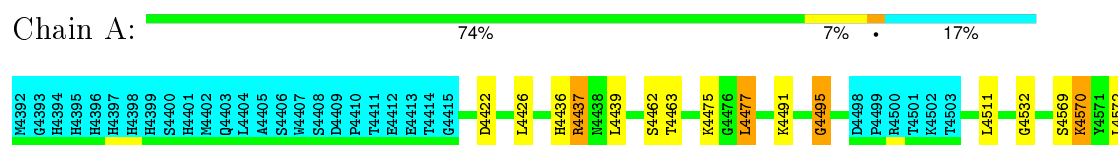
## 4.2.8 Score per residue for model 8

- Molecule 1: Plectin



## 4.2.9 Score per residue for model 9

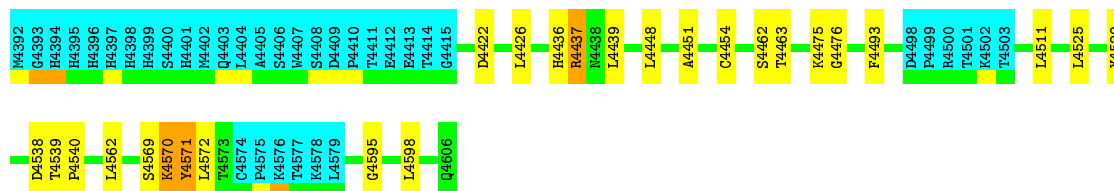
- Molecule 1: Plectin





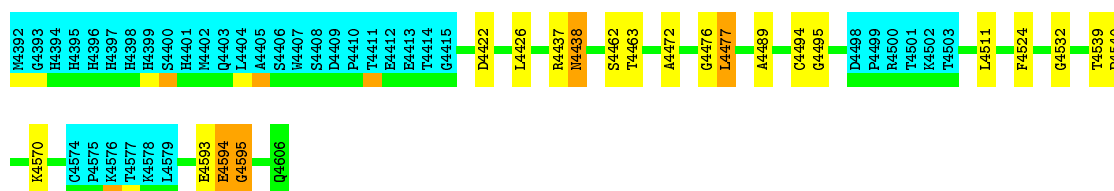
#### 4.2.10 Score per residue for model 10

- Molecule 1: Plectin



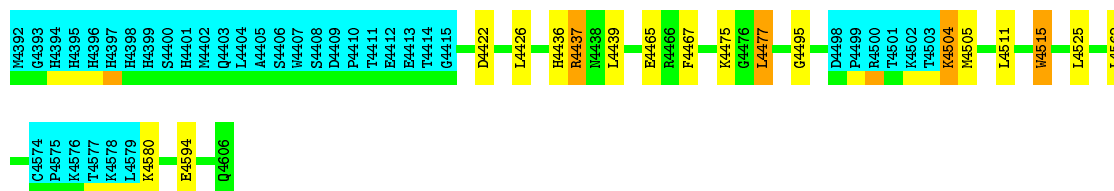
#### 4.2.11 Score per residue for model 11

- Molecule 1: Plectin



#### 4.2.12 Score per residue for model 12

- Molecule 1: Plectin

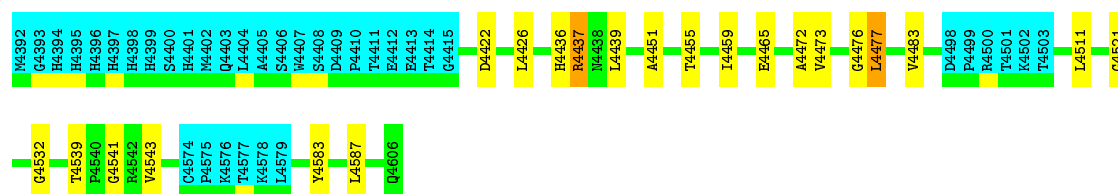


#### 4.2.13 Score per residue for model 13

- Molecule 1: Plectin

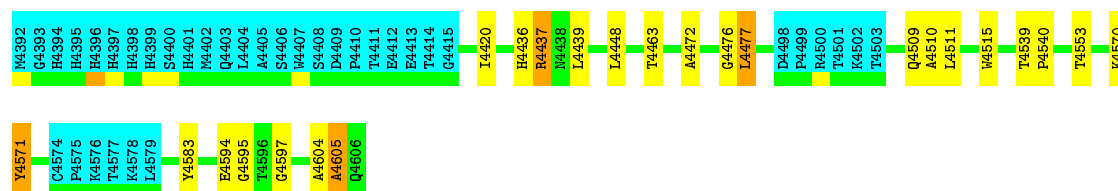






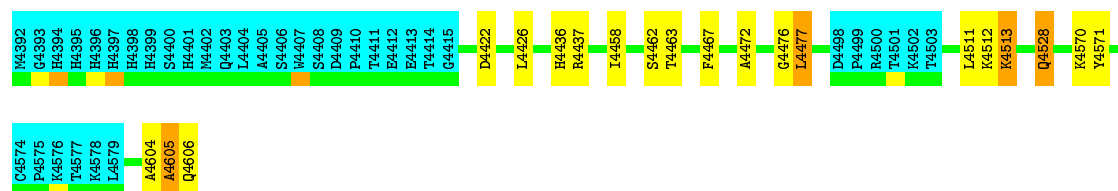
#### 4.2.14 Score per residue for model 14

- Molecule 1: Plectin



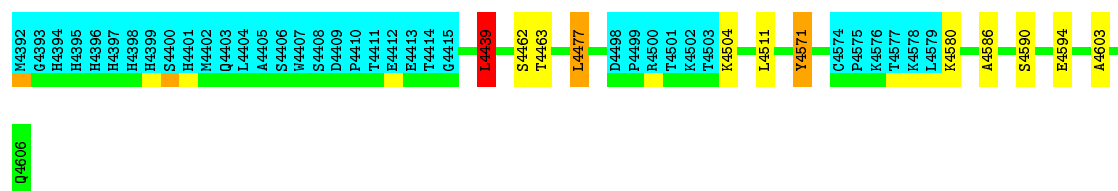
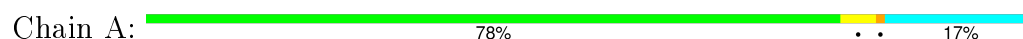
#### 4.2.15 Score per residue for model 15

- Molecule 1: Plectin



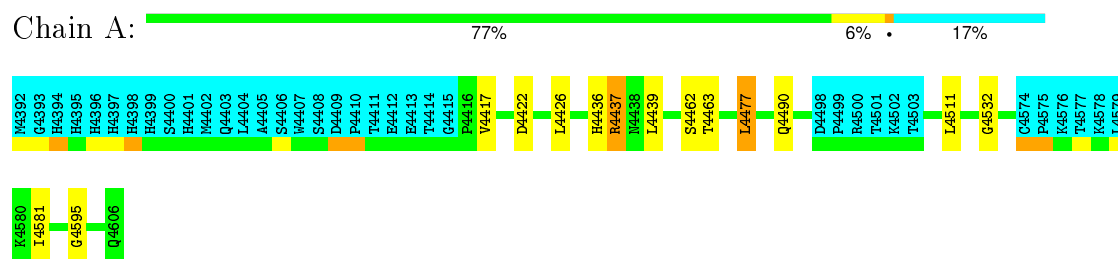
#### 4.2.16 Score per residue for model 16

- Molecule 1: Plectin



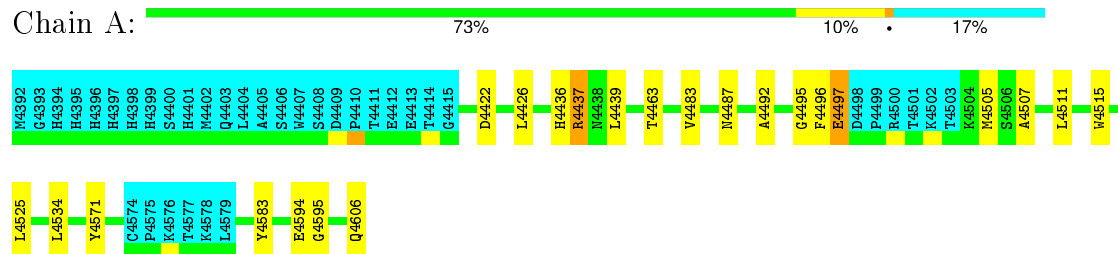
### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Plectin



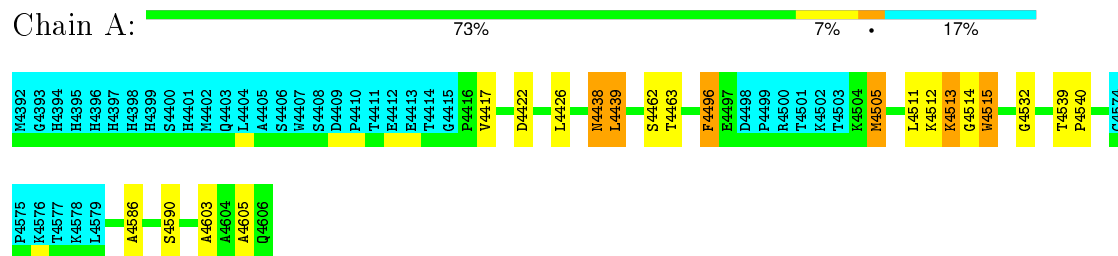
### 4.2.18 Score per residue for model 18

- Molecule 1: Plectin



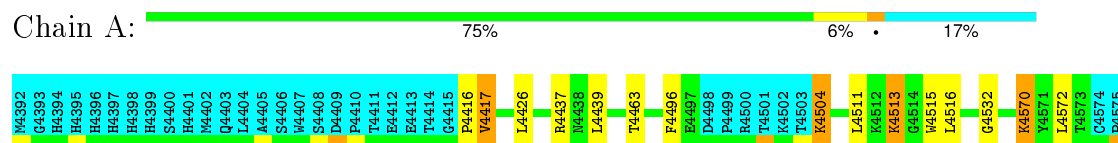
### 4.2.19 Score per residue for model 19

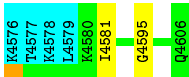
- Molecule 1: Plectin



### 4.2.20 Score per residue for model 20

- Molecule 1: Plectin





## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	
rosetta	refinement	
CYANA	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)	2n03_cs.str
Number of chemical shift lists	1
Total number of shifts	1340
Number of shifts mapped to atoms	1340
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	49%

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

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.01	0±0/1393 (0.0±0.0%)	0.54±0.00	0±0/1879 (0.0±0.0%)
All	All	0.68	1/27860 (0.0%)	0.54	0/37580 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
All	All	0	1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	4416	PRO	N-CD	5.43	1.55	1.47	8	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	4476	GLY	Peptide	1

### 6.2 Too-close contacts [i](#)

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	1375	1394	1394	10±4
All	All	27500	27880	27880	205

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4477:LEU:CD2	1:A:4477:LEU:N	0.79	2.46	9	2
1:A:4477:LEU:N	1:A:4477:LEU:HD23	0.76	1.95	12	2
1:A:4421:LEU:HB3	1:A:4600:LEU:HD11	0.76	1.57	3	1
1:A:4571:TYR:O	1:A:4571:TYR:CG	0.72	2.43	14	1
1:A:4477:LEU:H	1:A:4477:LEU:CD2	0.71	1.98	9	1
1:A:4512:LYS:O	1:A:4513:LYS:CB	0.69	2.41	4	4
1:A:4421:LEU:CB	1:A:4600:LEU:HD11	0.68	2.18	3	1
1:A:4569:SER:O	1:A:4570:LYS:CB	0.67	2.41	9	3
1:A:4477:LEU:N	1:A:4477:LEU:HD22	0.67	2.03	9	1
1:A:4570:LYS:HG2	1:A:4570:LYS:O	0.67	1.90	7	1
1:A:4581:ILE:HD12	1:A:4581:ILE:O	0.67	1.90	20	1
1:A:4477:LEU:HD23	1:A:4477:LEU:H	0.66	1.48	12	1
1:A:4570:LYS:O	1:A:4571:TYR:CB	0.63	2.46	14	1
1:A:4571:TYR:O	1:A:4571:TYR:CD2	0.63	2.52	14	2
1:A:4528:GLN:HA	1:A:4528:GLN:HE21	0.62	1.54	15	1
1:A:4473:VAL:HG21	1:A:4483:VAL:CG2	0.60	2.26	13	1
1:A:4606:GLN:HG2	1:A:4606:GLN:OXT	0.60	1.97	18	2
1:A:4561:LYS:O	1:A:4565:VAL:HG13	0.59	1.98	7	1
1:A:4439:LEU:HD22	1:A:4605:ALA:HB2	0.58	1.75	19	1
1:A:4473:VAL:HG21	1:A:4483:VAL:HG22	0.58	1.75	13	1
1:A:4439:LEU:O	1:A:4439:LEU:HD13	0.57	1.99	16	1
1:A:4422:ASP:O	1:A:4426:LEU:N	0.57	2.37	10	16
1:A:4428:LYS:HD2	1:A:4428:LYS:O	0.57	1.99	1	1
1:A:4496:PHE:CD1	1:A:4496:PHE:O	0.56	2.58	19	1
1:A:4477:LEU:CD2	1:A:4477:LEU:C	0.56	2.73	3	3
1:A:4438:ASN:O	1:A:4438:ASN:ND2	0.56	2.39	4	1
1:A:4436:HIS:O	1:A:4437:ARG:CB	0.56	2.54	7	9
1:A:4477:LEU:N	1:A:4477:LEU:HD13	0.55	2.16	11	6
1:A:4477:LEU:HD13	1:A:4477:LEU:N	0.55	2.16	17	4
1:A:4569:SER:O	1:A:4570:LYS:HB2	0.55	2.02	9	3
1:A:4477:LEU:C	1:A:4477:LEU:CD2	0.55	2.76	2	6
1:A:4436:HIS:O	1:A:4437:ARG:HB3	0.54	2.02	7	12
1:A:4570:LYS:HD2	1:A:4570:LYS:N	0.54	2.17	11	3
1:A:4505:MET:SD	1:A:4515:TRP:CE3	0.53	3.01	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4477:LEU:O	1:A:4477:LEU:HD23	0.53	2.02	15	3
1:A:4438:ASN:ND2	1:A:4438:ASN:O	0.53	2.41	1	1
1:A:4437:ARG:O	1:A:4438:ASN:HB2	0.53	2.04	4	3
1:A:4477:LEU:C	1:A:4477:LEU:HD22	0.53	2.24	2	1
1:A:4512:LYS:O	1:A:4513:LYS:HB3	0.52	2.04	15	3
1:A:4439:LEU:HD11	1:A:4603:ALA:HB3	0.52	1.82	16	2
1:A:4472:ALA:O	1:A:4476:GLY:N	0.51	2.43	14	6
1:A:4513:LYS:HG2	1:A:4513:LYS:O	0.51	2.05	20	1
1:A:4515:TRP:C	1:A:4515:TRP:CD1	0.51	2.83	12	2
1:A:4604:ALA:O	1:A:4605:ALA:HB2	0.51	2.05	15	1
1:A:4492:ALA:O	1:A:4507:ALA:HB2	0.51	2.06	6	1
1:A:4570:LYS:O	1:A:4571:TYR:HB2	0.51	2.05	14	1
1:A:4537:PRO:O	1:A:4538:ASP:HB2	0.51	2.06	8	2
1:A:4416:PRO:O	1:A:4417:VAL:HB	0.51	2.05	20	1
1:A:4477:LEU:O	1:A:4477:LEU:CD2	0.51	2.59	15	1
1:A:4571:TYR:CD2	1:A:4571:TYR:O	0.50	2.65	16	1
1:A:4428:LYS:O	1:A:4428:LYS:CD	0.50	2.59	1	1
1:A:4428:LYS:CG	1:A:4428:LYS:O	0.50	2.59	1	1
1:A:4483:VAL:O	1:A:4487:ASN:HB2	0.50	2.06	2	3
1:A:4586:ALA:O	1:A:4590:SER:N	0.50	2.44	19	4
1:A:4570:LYS:O	1:A:4571:TYR:CG	0.50	2.64	10	1
1:A:4489:ALA:HB2	1:A:4524:PHE:CE1	0.50	2.41	11	1
1:A:4528:GLN:HA	1:A:4528:GLN:NE2	0.50	2.20	15	1
1:A:4477:LEU:HD22	1:A:4477:LEU:C	0.50	2.26	3	1
1:A:4604:ALA:O	1:A:4605:ALA:HB3	0.49	2.07	2	4
1:A:4570:LYS:HD2	1:A:4570:LYS:H	0.49	1.67	15	1
1:A:4420:ILE:HD11	1:A:4448:LEU:CD1	0.49	2.38	14	1
1:A:4525:LEU:HD22	1:A:4534:LEU:HD22	0.48	1.83	18	2
1:A:4572:LEU:HD12	1:A:4586:ALA:HB2	0.48	1.84	9	1
1:A:4475:LYS:HG2	1:A:4475:LYS:O	0.47	2.09	12	4
1:A:4525:LEU:HB3	1:A:4562:LEU:HD11	0.47	1.87	5	4
1:A:4436:HIS:O	1:A:4437:ARG:HB2	0.47	2.10	15	1
1:A:4477:LEU:H	1:A:4477:LEU:HD23	0.47	1.68	9	1
1:A:4553:THR:HG23	1:A:4554:VAL:HG13	0.47	1.85	2	1
1:A:4451:ALA:O	1:A:4454:CYS:SG	0.46	2.69	10	1
1:A:4600:LEU:C	1:A:4600:LEU:HD13	0.46	2.31	3	1
1:A:4510:ALA:HB2	1:A:4515:TRP:CZ2	0.46	2.46	14	1
1:A:4537:PRO:O	1:A:4538:ASP:HB3	0.46	2.11	1	1
1:A:4512:LYS:O	1:A:4513:LYS:HB2	0.46	2.10	19	1
1:A:4493:PHE:N	1:A:4493:PHE:CD1	0.45	2.80	10	1
1:A:4529:TYR:HB2	1:A:4562:LEU:HD12	0.45	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4593:GLU:O	1:A:4594:GLU:HB2	0.45	2.11	11	1
1:A:4495:GLY:O	1:A:4496:PHE:HB2	0.45	2.12	3	2
1:A:4605:ALA:O	1:A:4606:GLN:C	0.44	2.55	15	1
1:A:4451:ALA:O	1:A:4455:THR:HG23	0.44	2.13	13	1
1:A:4491:LYS:O	1:A:4495:GLY:N	0.44	2.51	9	1
1:A:4539:THR:HB	1:A:4540:PRO:HD2	0.44	1.89	19	4
1:A:4437:ARG:O	1:A:4438:ASN:CB	0.43	2.66	4	1
1:A:4438:ASN:O	1:A:4438:ASN:CG	0.43	2.56	4	1
1:A:4492:ALA:HB1	1:A:4507:ALA:HB2	0.43	1.89	18	1
1:A:4448:LEU:O	1:A:4451:ALA:HB3	0.43	2.13	10	1
1:A:4539:THR:HG21	1:A:4543:VAL:HG23	0.43	1.90	13	1
1:A:4537:PRO:O	1:A:4538:ASP:CB	0.43	2.67	1	1
1:A:4505:MET:HE2	1:A:4515:TRP:CE3	0.43	2.49	19	1
1:A:4570:LYS:O	1:A:4570:LYS:CG	0.43	2.61	7	1
1:A:4570:LYS:HD3	1:A:4570:LYS:H	0.42	1.73	20	1
1:A:4548:ALA:HB1	1:A:4553:THR:OG1	0.42	2.14	5	1
1:A:4511:LEU:HD21	1:A:4521:GLY:HA3	0.42	1.90	13	1
1:A:4495:GLY:O	1:A:4496:PHE:CB	0.42	2.68	3	1
1:A:4495:GLY:O	1:A:4496:PHE:HB3	0.42	2.15	8	1
1:A:4459:ILE:HA	1:A:4465:GLU:O	0.42	2.15	13	1
1:A:4572:LEU:CD1	1:A:4586:ALA:HB2	0.42	2.44	9	1
1:A:4583:TYR:O	1:A:4587:LEU:HG	0.41	2.14	13	1
1:A:4477:LEU:H	1:A:4477:LEU:HD22	0.41	1.61	9	1
1:A:4488:LEU:HD12	1:A:4491:LYS:HE3	0.41	1.92	4	1
1:A:4472:ALA:O	1:A:4476:GLY:CA	0.41	2.69	14	3
1:A:4496:PHE:CZ	1:A:4516:LEU:HD22	0.41	2.50	20	1
1:A:4475:LYS:O	1:A:4475:LYS:HG2	0.41	2.16	1	2
1:A:4496:PHE:O	1:A:4497:GLU:C	0.41	2.60	18	1
1:A:4509:GLN:HG3	1:A:4553:THR:OG1	0.41	2.16	14	1
1:A:4495:GLY:O	1:A:4497:GLU:N	0.40	2.54	4	1
1:A:4458:ILE:N	1:A:4467:PHE:O	0.40	2.54	15	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	178/215 (83%)	161±2 (90±1%)	11±3 (6±2%)	7±2 (4±1%)	7	35
All	All	3560/4300 (83%)	3212 (90%)	214 (6%)	134 (4%)	7	35

All 23 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	4463	THR	18
1	A	4439	LEU	14
1	A	4437	ARG	13
1	A	4462	SER	13
1	A	4595	GLY	10
1	A	4532	GLY	10
1	A	4571	TYR	8
1	A	4495	GLY	6
1	A	4594	GLU	5
1	A	4605	ALA	5
1	A	4504	LYS	5
1	A	4513	LYS	5
1	A	4438	ASN	5
1	A	4494	CYS	4
1	A	4417	VAL	3
1	A	4570	LYS	3
1	A	4416	PRO	1
1	A	4541	GLY	1
1	A	4598	LEU	1
1	A	4538	ASP	1
1	A	4515	TRP	1
1	A	4497	GLU	1
1	A	4514	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	144/177 (81%)	141±1 (98±1%)	3±1 (2±1%)	67	95
All	All	2880/3540 (81%)	2825 (98%)	55 (2%)	67	95

All 17 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	4511	LEU	15
1	A	4477	LEU	13
1	A	4505	MET	4
1	A	4583	TYR	4
1	A	4515	TRP	3
1	A	4598	LEU	3
1	A	4439	LEU	2
1	A	4438	ASN	2
1	A	4572	LEU	1
1	A	4570	LYS	1
1	A	4488	LEU	1
1	A	4581	ILE	1
1	A	4428	LYS	1
1	A	4528	GLN	1
1	A	4426	LEU	1
1	A	4496	PHE	1
1	A	4553	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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 49% for the well-defined parts and 46% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2n03\_cs.str

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	1340
Number of shifts mapped to atoms	1340
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
$^{13}\text{C}_\alpha$	203	$0.33 \pm 0.10$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	187	$1.07 \pm 0.13$	Should be applied
$^{13}\text{C}'$	188	$-0.16 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	195	$1.10 \pm 0.24$	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 49%, i.e. 1047 atoms were assigned a chemical shift out of a possible 2153. 30 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	737/883 (83%)	224/352 (64%)	340/358 (95%)	173/173 (100%)
Sidechain	310/1167 (27%)	70/677 (10%)	240/433 (55%)	0/57 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/103 (0%)	0/54 (0%)	0/47 (0%)	0/2 (0%)
Overall	1047/2153 (49%)	294/1083 (27%)	580/838 (69%)	173/232 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 46%, i.e. 1189 atoms were assigned a chemical shift out of a possible 2596. 32 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	844/1057 (80%)	258/421 (61%)	391/430 (91%)	195/206 (95%)
Sidechain	345/1375 (25%)	76/803 (9%)	269/508 (53%)	0/64 (0%)
Aromatic	0/164 (0%)	0/88 (0%)	0/66 (0%)	0/10 (0%)
Overall	1189/2596 (46%)	334/1312 (25%)	660/1004 (66%)	195/280 (70%)

#### 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:

