



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:09 AM BST

PDB ID : 2N2H
Title : Solution structure of Sds3 in complex with Sin3A
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Deposited on : 2015-05-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

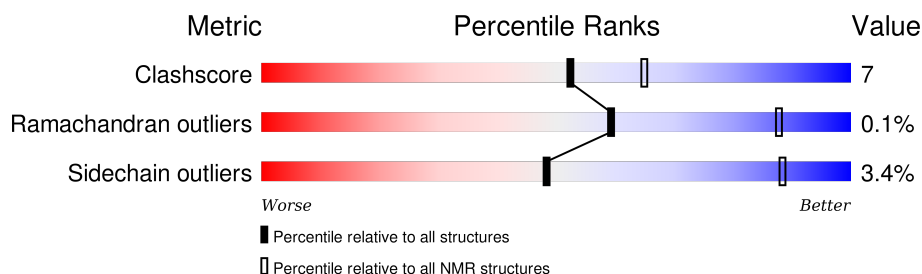
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 86%.

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 ≥ 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	27	
2	B	125	

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:207-A:224, B:616-B:658, B:662-B:716 (116)	0.43	1

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

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

The models can be grouped into 5 clusters and 6 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2537 atoms, of which 1285 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Sin3 histone deacetylase corepressor complex component SDS3.

Mol	Chain	Residues	Atoms						Trace
1	A	27	Total	C	H	N	O	S	0
			442	134	224	37	46	1	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	SER	-	EXPRESSION TAG	UNP Q8BR65
A	203	ASN	-	EXPRESSION TAG	UNP Q8BR65
A	204	ALA	-	EXPRESSION TAG	UNP Q8BR65

- Molecule 2 is a protein called Paired amphipathic helix protein Sin3a.

Mol	Chain	Residues	Atoms						Trace
2	B	125	Total	C	H	N	O	S	0
			2095	649	1061	190	193	2	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	SER	-	EXPRESSION TAG	UNP Q60520
B	606	ASN	-	EXPRESSION TAG	UNP Q60520
B	607	ALA	-	EXPRESSION TAG	UNP Q60520

4 Residue-property plots

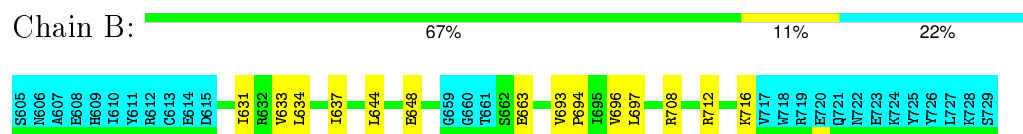
4.1 Average score per residue in the NMR ensemble

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: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



4.2 Scores per residue for each member of the ensemble

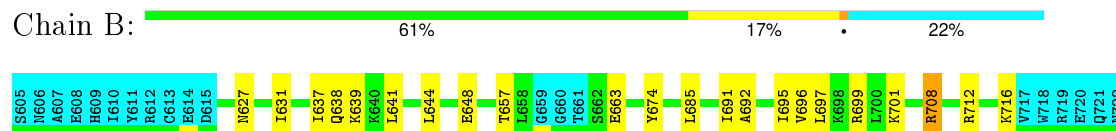
Colouring as in section 4.1 above.

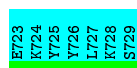
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



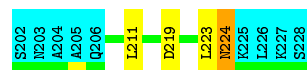
- Molecule 2: Paired amphipathic helix protein Sin3a





4.2.2 Score per residue for model 2

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



4.2.3 Score per residue for model 3

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



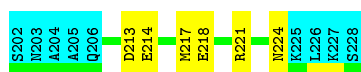
- Molecule 2: Paired amphipathic helix protein Sin3a



4.2.4 Score per residue for model 4

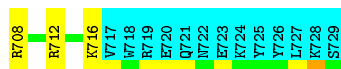
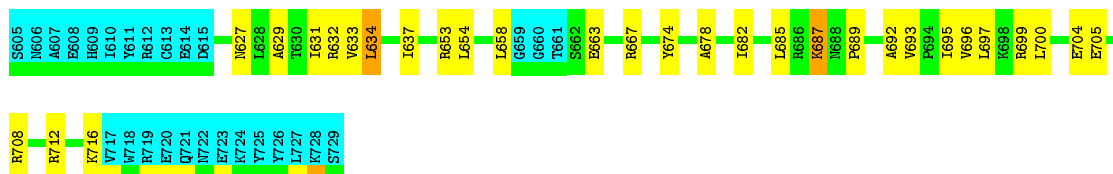
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3





- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 54% 22% 22%



4.2.5 Score per residue for model 5

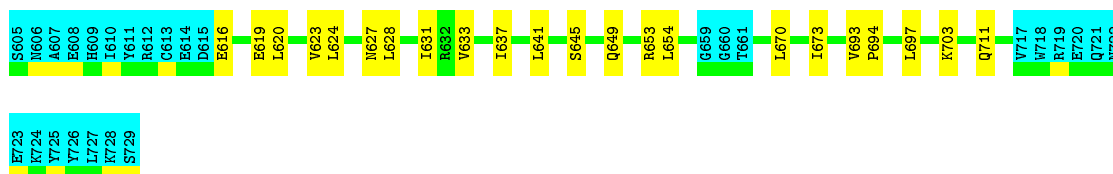
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 63% 33%



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 61% 18% 22%



4.2.6 Score per residue for model 6

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 52% 15% 33%



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 64% 14% 22%



S729

4.2.7 Score per residue for model 7

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 

S202 N203 A204 A205 Q206 L207 N208 Y209 D219 T222 L223 K224 K225 L226 K227 S228

- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 

S605 M606 A607 E608 H609 I610 V611 H612 G613 E614 D615 T626 I627 L628 A629 I631 T630 K632 V633 L634 E635 K639 V640 L641 L644 E648 G659 G660 T661 I665 L670 Q671 R672 L673 V674 A675 L685 V693 P694 I695 V696 L700 E704 R712 R716 V717 R718 E720 Q721 N722 K723 Y725 L726 K728 S729

4.2.8 Score per residue for model 8

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 

S202 N203 A204 A205 Q206 R221 K225 L226 K227 S228

- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 

S605 M606 A607 E608 H609 I610 V611 H612 G613 E614 D615 V633 I637 L641 L644 E648 G659 G660 T661 A678 I682 I691 A692 V693 P694 I695 R699 E709 R712 K716 V717 R718 E720 Q721 N722 K723 Y725 L726 K728 S729

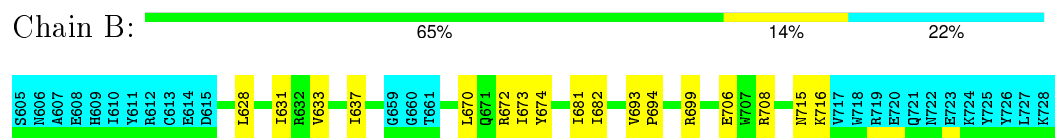
4.2.9 Score per residue for model 9

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 

S202 N203 A204 A205 Q206 L207 N208 L211 I216 D219 L220 R221 T222 L223 N224 K225 L226 K227 S228

- Molecule 2: Paired amphipathic helix protein Sin3a

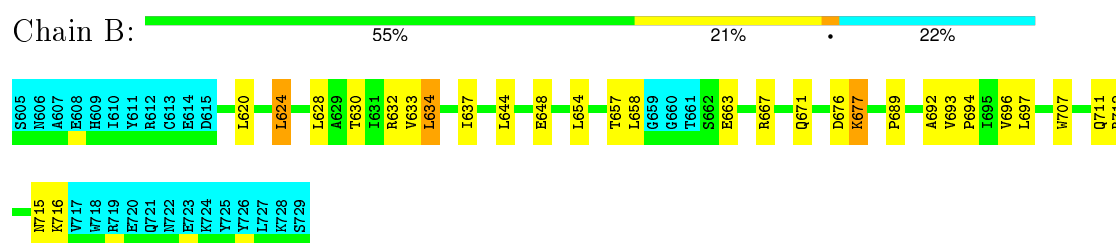


4.2.10 Score per residue for model 10

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

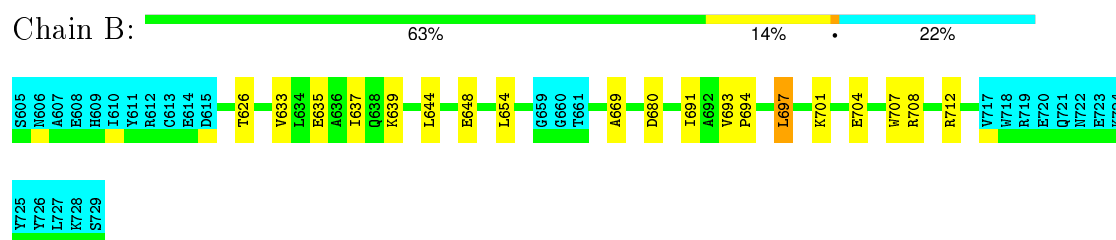


4.2.11 Score per residue for model 11

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



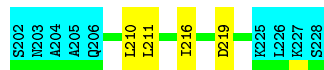
- Molecule 2: Paired amphipathic helix protein Sin3a



4.2.12 Score per residue for model 12

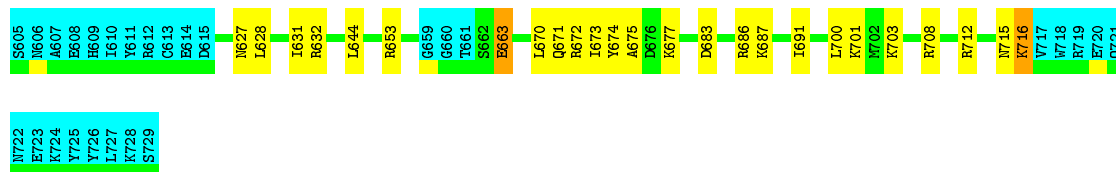
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



4.2.13 Score per residue for model 13

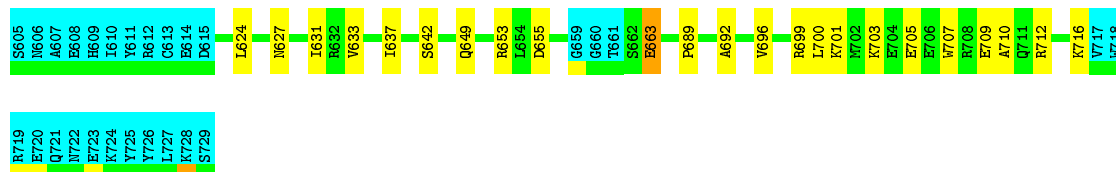
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 




- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



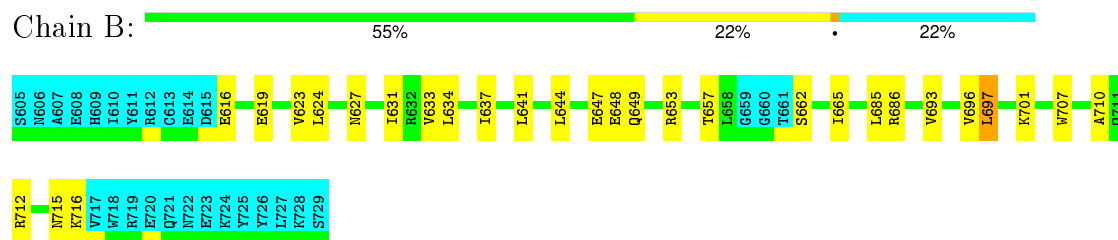
4.2.14 Score per residue for model 14

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

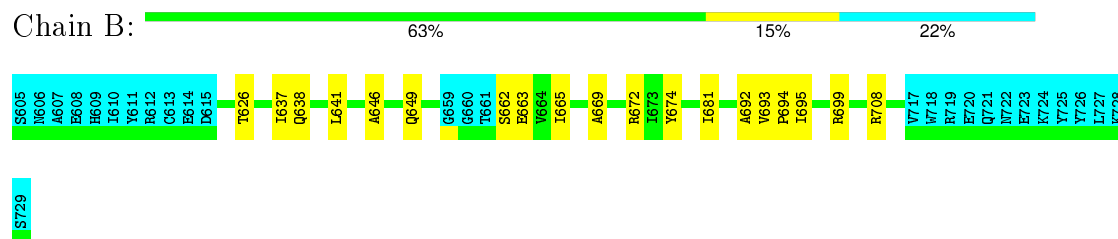


4.2.15 Score per residue for model 15

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a

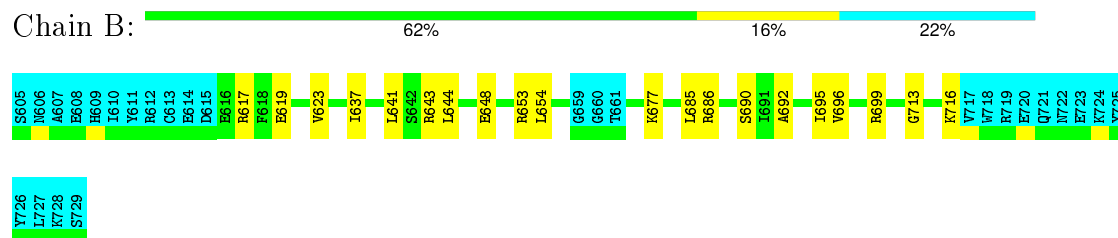


4.2.16 Score per residue for model 16

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



4.2.17 Score per residue for model 17

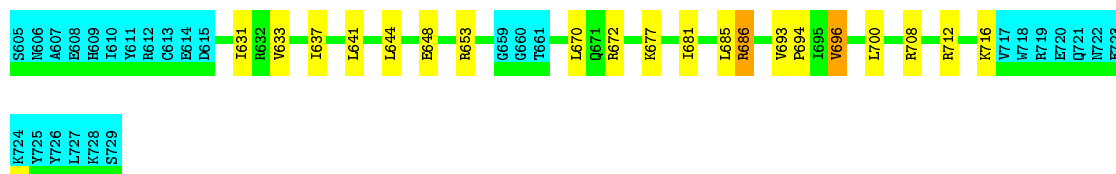
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

Chain B: 



4.2.18 Score per residue for model 18

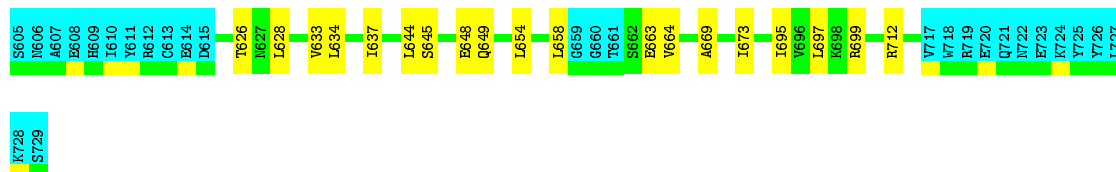
- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

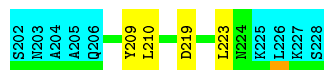
Chain B: 



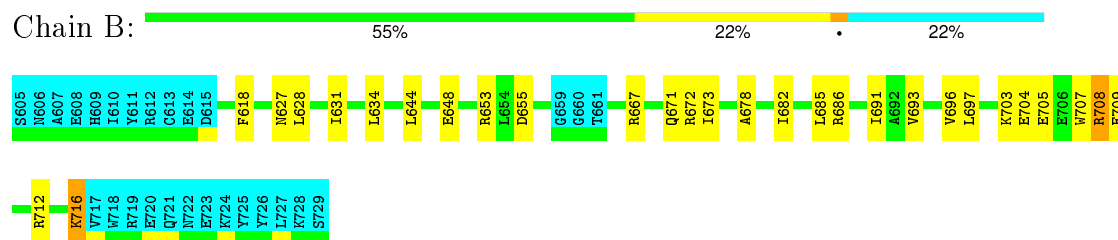
4.2.19 Score per residue for model 19

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3

Chain A: 



- Molecule 2: Paired amphipathic helix protein Sin3a

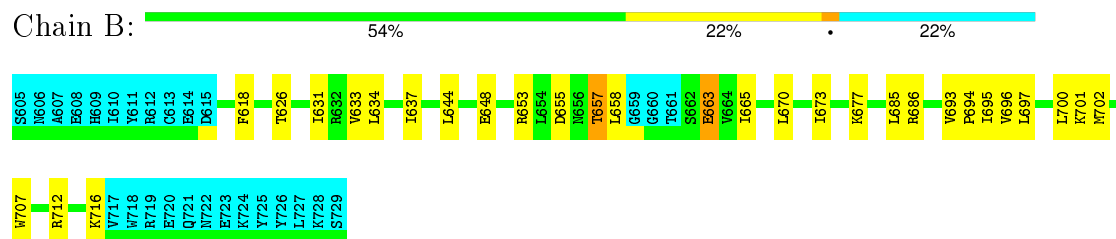


4.2.20 Score per residue for model 20

- Molecule 1: Sin3 histone deacetylase corepressor complex component SDS3



- Molecule 2: Paired amphipathic helix protein Sin3a



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
ARIA	structure solution	
CNS	refinement	

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

Chemical shift file(s)	2n2h_cs.str
Number of chemical shift lists	2
Total number of shifts	1790
Number of shifts mapped to atoms	1790
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	152	151	151	2±1
2	B	803	850	849	12±4
All	All	19100	20020	20000	269

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:634:LEU:HB3	2:B:697:LEU:HD13	0.81	1.50	20	5
2:B:634:LEU:HB3	2:B:697:LEU:HG	0.68	1.64	6	3
1:A:216:ILE:HG21	2:B:677:LYS:HB3	0.67	1.65	12	1
2:B:685:LEU:HD21	2:B:696:VAL:HG21	0.65	1.67	19	5
2:B:670:LEU:HD23	2:B:682:ILE:HG12	0.64	1.69	9	1
2:B:712:ARG:HA	2:B:716:LYS:HB3	0.61	1.72	4	4
2:B:644:LEU:HB3	2:B:648:GLU:HB2	0.61	1.73	10	11
2:B:667:ARG:HG3	2:B:682:ILE:HG12	0.59	1.72	19	1
2:B:635:GLU:O	2:B:639:LYS:HG2	0.59	1.97	11	1
2:B:704:GLU:O	2:B:708:ARG:HG2	0.58	1.98	4	2
2:B:683:ASP:OD2	2:B:687:LYS:HE2	0.58	1.98	12	1
2:B:633:VAL:O	2:B:637:ILE:HG12	0.57	1.99	6	11
1:A:209:TYR:HB3	2:B:672:ARG:HD2	0.56	1.76	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:654:LEU:HD23	2:B:658:LEU:HD21	0.56	1.78	2	1
2:B:619:GLU:O	2:B:623:VAL:HG23	0.56	2.00	5	2
2:B:641:LEU:O	2:B:644:LEU:HG	0.55	2.01	2	3
2:B:673:ILE:HG21	2:B:703:LYS:HG3	0.55	1.76	19	1
2:B:667:ARG:O	2:B:671:GLN:HG3	0.55	2.01	19	2
1:A:219:ASP:O	1:A:223:LEU:HG	0.54	2.01	19	9
1:A:217:MET:SD	2:B:677:LYS:HE2	0.54	2.41	16	1
1:A:216:ILE:O	1:A:220:LEU:HB2	0.54	2.02	9	1
2:B:674:TYR:CD1	2:B:681:ILE:HG13	0.54	2.37	9	2
1:A:211:LEU:HG	2:B:673:ILE:HB	0.54	1.79	9	1
2:B:671:GLN:O	2:B:675:ALA:HA	0.54	2.03	7	2
1:A:211:LEU:HD21	2:B:703:LYS:HD2	0.53	1.80	12	1
2:B:673:ILE:HG21	2:B:703:LYS:HG2	0.53	1.79	2	1
2:B:653:ARG:HD2	2:B:686:ARG:O	0.53	2.04	2	4
2:B:693:VAL:HB	2:B:694:PRO:HD3	0.53	1.80	20	7
2:B:643:ARG:HA	2:B:690:SER:OG	0.53	2.03	16	1
2:B:634:LEU:CB	2:B:697:LEU:HD13	0.53	2.33	2	1
1:A:220:LEU:HD11	2:B:677:LYS:HG2	0.53	1.80	20	1
2:B:631:ILE:CD1	2:B:700:LEU:HB3	0.52	2.35	13	2
2:B:712:ARG:HA	2:B:716:LYS:CB	0.52	2.33	6	4
2:B:654:LEU:HA	2:B:657:THR:OG1	0.52	2.03	3	1
2:B:693:VAL:O	2:B:697:LEU:HB2	0.52	2.05	11	4
2:B:674:TYR:OH	2:B:699:ARG:HG3	0.52	2.05	9	2
2:B:708:ARG:O	2:B:712:ARG:HB2	0.52	2.03	11	1
2:B:629:ALA:O	2:B:633:VAL:HG23	0.51	2.05	4	2
2:B:634:LEU:HD13	2:B:693:VAL:HG13	0.51	1.81	4	1
2:B:627:ASN:O	2:B:631:ILE:HG12	0.51	2.06	13	8
1:A:209:TYR:HD2	2:B:707:TRP:HE1	0.51	1.49	11	1
2:B:631:ILE:HD13	2:B:700:LEU:HB3	0.51	1.83	4	2
2:B:695:ILE:O	2:B:699:ARG:HG2	0.51	2.06	18	5
2:B:637:ILE:O	2:B:641:LEU:HG	0.51	2.06	16	7
2:B:708:ARG:O	2:B:712:ARG:HG2	0.50	2.05	1	1
2:B:654:LEU:HD12	2:B:658:LEU:HD13	0.50	1.81	18	1
2:B:671:GLN:HG2	2:B:678:ALA:HB1	0.50	1.81	19	1
2:B:654:LEU:CD1	2:B:689:PRO:HB3	0.50	2.36	10	2
2:B:685:LEU:HD21	2:B:696:VAL:HG11	0.50	1.83	17	4
2:B:658:LEU:HB2	2:B:663:GLU:HG3	0.50	1.82	10	1
2:B:672:ARG:NE	2:B:672:ARG:HA	0.50	2.22	9	1
2:B:692:ALA:O	2:B:696:VAL:HG22	0.50	2.07	4	4
2:B:662:SER:HB2	2:B:665:ILE:HB	0.50	1.82	15	1
2:B:663:GLU:OE2	2:B:667:ARG:HB2	0.50	2.07	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:693:VAL:HG12	2:B:694:PRO:HD3	0.50	1.83	7	1
2:B:712:ARG:O	2:B:716:LYS:HB3	0.50	2.06	17	2
2:B:629:ALA:HA	2:B:632:ARG:HH21	0.50	1.67	4	1
2:B:626:THR:HG22	2:B:669:ALA:HB2	0.49	1.84	15	3
2:B:697:LEU:O	2:B:701:LYS:HG2	0.49	2.07	1	3
2:B:653:ARG:HG3	2:B:689:PRO:HD3	0.49	1.84	4	1
2:B:704:GLU:O	2:B:708:ARG:HB2	0.49	2.07	19	1
2:B:663:GLU:O	2:B:667:ARG:HD3	0.49	2.06	3	1
2:B:626:THR:HG23	2:B:665:ILE:HB	0.49	1.83	7	3
2:B:712:ARG:HA	2:B:716:LYS:CG	0.49	2.37	8	1
1:A:211:LEU:HB2	2:B:673:ILE:HB	0.49	1.81	3	2
2:B:649:GLN:O	2:B:653:ARG:HB2	0.48	2.07	5	1
2:B:673:ILE:HG13	2:B:674:TYR:CD2	0.48	2.42	12	1
2:B:711:GLN:HG3	2:B:715:ASN:HB3	0.48	1.86	2	1
2:B:712:ARG:HA	2:B:716:LYS:HB2	0.48	1.84	19	3
2:B:637:ILE:HG21	2:B:654:LEU:HD21	0.48	1.84	5	4
1:A:208:ASN:HB2	2:B:706:GLU:OE2	0.48	2.09	9	1
2:B:636:ALA:O	2:B:640:LYS:HG2	0.48	2.07	3	1
1:A:223:LEU:CD2	2:B:692:ALA:HA	0.47	2.38	1	3
2:B:689:PRO:O	2:B:693:VAL:HB	0.47	2.09	6	1
1:A:217:MET:O	1:A:221:ARG:HG3	0.47	2.09	13	1
1:A:216:ILE:HG21	2:B:677:LYS:HB2	0.47	1.85	16	1
1:A:223:LEU:HD23	2:B:695:ILE:HD12	0.47	1.85	16	2
2:B:628:LEU:O	2:B:632:ARG:HG2	0.47	2.09	12	1
1:A:217:MET:O	1:A:221:ARG:HG2	0.47	2.10	15	3
1:A:221:ARG:HE	1:A:221:ARG:HA	0.46	1.71	8	1
2:B:712:ARG:HG3	2:B:716:LYS:HD3	0.46	1.86	13	1
2:B:673:ILE:HG22	2:B:703:LYS:HG3	0.46	1.86	5	1
2:B:635:GLU:O	2:B:639:LYS:HG3	0.46	2.10	7	1
2:B:624:LEU:CD2	2:B:707:TRP:HB3	0.46	2.41	13	2
1:A:209:TYR:HD1	2:B:707:TRP:HE1	0.45	1.55	19	2
2:B:667:ARG:HG3	2:B:682:ILE:HD13	0.45	1.88	6	1
2:B:620:LEU:HB3	2:B:711:GLN:OE1	0.45	2.12	10	1
2:B:634:LEU:CD1	2:B:693:VAL:HG13	0.45	2.42	4	1
2:B:653:ARG:HG3	2:B:686:ARG:O	0.45	2.12	17	1
1:A:210:LEU:HA	2:B:672:ARG:O	0.45	2.12	12	1
2:B:670:LEU:HD12	2:B:673:ILE:HD11	0.44	1.89	7	2
2:B:654:LEU:HD22	2:B:658:LEU:HD13	0.44	1.87	4	1
2:B:678:ALA:O	2:B:682:ILE:HG12	0.44	2.12	8	2
2:B:644:LEU:HD22	2:B:648:GLU:HB3	0.44	1.88	11	1
2:B:624:LEU:HG	2:B:711:GLN:HG2	0.44	1.88	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:662:SER:HB3	2:B:665:ILE:HD11	0.44	1.89	14	1
2:B:644:LEU:HB3	2:B:648:GLU:CB	0.44	2.43	20	1
2:B:677:LYS:O	2:B:681:ILE:HG12	0.44	2.13	17	1
2:B:631:ILE:HD11	2:B:700:LEU:HG	0.44	1.89	17	1
2:B:694:PRO:O	2:B:698:LYS:HG3	0.44	2.13	3	1
2:B:653:ARG:HD2	2:B:655:ASP:OD1	0.44	2.12	13	1
1:A:216:ILE:HG12	2:B:674:TYR:HD1	0.44	1.73	1	1
1:A:210:LEU:HD23	2:B:672:ARG:O	0.44	2.12	19	1
2:B:705:GLU:O	2:B:709:GLU:HG2	0.43	2.13	13	2
2:B:619:GLU:O	2:B:623:VAL:HG12	0.43	2.12	14	1
2:B:701:LYS:O	2:B:704:GLU:HB3	0.43	2.14	11	1
2:B:633:VAL:O	2:B:637:ILE:HG13	0.43	2.14	17	1
1:A:214:GLU:O	1:A:218:GLU:HB2	0.43	2.14	4	1
2:B:646:ALA:HA	2:B:649:GLN:HE21	0.43	1.74	15	1
2:B:702:MET:O	2:B:705:GLU:HB2	0.43	2.14	3	1
1:A:210:LEU:HD13	2:B:672:ARG:O	0.43	2.14	15	1
2:B:631:ILE:CD1	2:B:700:LEU:HG	0.43	2.43	2	4
1:A:221:ARG:HA	1:A:221:ARG:NE	0.43	2.28	6	1
1:A:211:LEU:HB2	2:B:673:ILE:O	0.43	2.13	18	1
2:B:649:GLN:OE1	2:B:689:PRO:HG2	0.42	2.14	2	1
2:B:654:LEU:HG	2:B:658:LEU:HD12	0.42	1.89	6	1
2:B:629:ALA:HA	2:B:632:ARG:NH2	0.42	2.29	4	1
2:B:634:LEU:HB3	2:B:697:LEU:HD23	0.42	1.91	4	1
2:B:645:SER:O	2:B:649:GLN:HG3	0.42	2.14	18	2
2:B:624:LEU:HG	2:B:711:GLN:OE1	0.42	2.14	5	1
2:B:654:LEU:N	2:B:654:LEU:HD12	0.42	2.29	2	1
2:B:653:ARG:HA	2:B:689:PRO:HG3	0.42	1.90	4	1
1:A:207:LEU:HD23	2:B:710:ALA:HB1	0.42	1.91	13	1
1:A:209:TYR:O	2:B:673:ILE:HG22	0.42	2.15	20	1
2:B:632:ARG:HA	2:B:632:ARG:NE	0.42	2.29	3	1
2:B:693:VAL:HA	2:B:696:VAL:HG22	0.42	1.91	19	1
2:B:707:TRP:O	2:B:711:GLN:HB2	0.42	2.15	10	1
2:B:673:ILE:CG2	2:B:703:LYS:HG3	0.42	2.45	5	1
2:B:649:GLN:HB3	2:B:689:PRO:HG2	0.41	1.90	13	1
2:B:653:ARG:HD3	2:B:686:ARG:O	0.41	2.16	20	2
2:B:630:THR:O	2:B:634:LEU:HB2	0.41	2.15	10	1
1:A:216:ILE:HG12	2:B:674:TYR:CD1	0.41	2.51	1	1
2:B:676:ASP:OD1	2:B:677:LYS:HG2	0.41	2.16	10	1
1:A:207:LEU:HB3	1:A:209:TYR:CE2	0.41	2.49	7	1
1:A:213:ASP:O	1:A:217:MET:HG3	0.41	2.15	15	1
2:B:647:GLU:CD	2:B:647:GLU:H	0.41	2.19	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:224:ASN:N	1:A:224:ASN:HD22	0.41	2.13	2	1
2:B:627:ASN:OD1	2:B:704:GLU:HA	0.41	2.16	7	1
2:B:634:LEU:HD12	2:B:697:LEU:HB2	0.41	1.91	4	1
2:B:709:GLU:O	2:B:712:ARG:HG2	0.41	2.15	8	1
2:B:693:VAL:N	2:B:694:PRO:HD2	0.41	2.31	15	2
2:B:657:THR:HB	2:B:658:LEU:HD12	0.41	1.93	20	1
2:B:711:GLN:NE2	2:B:715:ASN:HB2	0.41	2.31	10	1
2:B:620:LEU:O	2:B:624:LEU:HD23	0.41	2.16	5	1
2:B:641:LEU:HD22	2:B:649:GLN:OE1	0.40	2.17	14	1
2:B:628:LEU:O	2:B:632:ARG:HG3	0.40	2.17	10	1
2:B:645:SER:O	2:B:649:GLN:HG2	0.40	2.17	2	1
2:B:687:LYS:HZ3	2:B:687:LYS:HB2	0.40	1.76	4	1
2:B:663:GLU:HG3	2:B:664:VAL:N	0.40	2.32	18	1

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

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	18/27 (67%)	17±1 (96±4%)	1±1 (4±4%)	0±0 (0±0%)	100	100
2	B	98/125 (78%)	91±2 (93±2%)	7±2 (7±2%)	0±0 (0±0%)	56	85
All	All	2320/3040 (76%)	2171 (94%)	146 (6%)	3 (0%)	59	88

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	655	ASP	2
2	B	642	SER	1

6.3.2 Protein sidechains [i](#)

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	18/25 (72%)	17±1 (96±5%)	1±1 (4±5%)	43	85
2	B	86/110 (78%)	83±2 (97±2%)	3±2 (3±2%)	49	89
All	All	2080/2700 (77%)	2010 (97%)	70 (3%)	48	88

All 33 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)
2	B	708	ARG	6
1	A	224	ASN	5
2	B	657	THR	5
2	B	628	LEU	5
2	B	663	GLU	4
2	B	701	LYS	3
2	B	716	LYS	3
2	B	670	LEU	3
2	B	638	GLN	3
2	B	697	LEU	2
1	A	217	MET	2
2	B	677	LYS	2
2	B	699	ARG	2
2	B	634	LEU	2
2	B	715	ASN	2
2	B	702	MET	2
2	B	617	ARG	2
1	A	219	ASP	2
1	A	213	ASP	1
1	A	220	LEU	1
2	B	696	VAL	1
2	B	644	LEU	1
1	A	207	LEU	1
1	A	211	LEU	1
2	B	705	GLU	1
2	B	680	ASP	1
2	B	631	ILE	1
2	B	703	LYS	1
1	A	218	GLU	1
2	B	639	LYS	1
2	B	686	ARG	1
2	B	687	LYS	1

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Mol	Chain	Res	Type	Models (Total)
2	B	624	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 86% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: 2n2h_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	1518
Number of shifts mapped to atoms	1518
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
$^{13}\text{C}_\alpha$	125	-0.59 ± 0.19	Should be applied
$^{13}\text{C}_\beta$	121	0.02 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	122	-0.44 ± 0.10	None needed (< 0.5 ppm)
^{15}N	116	0.65 ± 0.22	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 74%, i.e. 1148 atoms were assigned a chemical shift out of a possible 1555. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	478/576 (83%)	191/230 (83%)	195/232 (84%)	92/114 (81%)
Sidechain	637/916 (70%)	398/533 (75%)	231/329 (70%)	8/54 (15%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	33/63 (52%)	20/33 (61%)	12/27 (44%)	1/3 (33%)
Overall	1148/1555 (74%)	609/796 (77%)	438/588 (74%)	101/171 (59%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1448 atoms were assigned a chemical shift out of a possible 2013. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	605/756 (80%)	242/302 (80%)	247/304 (81%)	116/150 (77%)
Sidechain	779/1150 (68%)	489/672 (73%)	279/409 (68%)	11/69 (16%)
Aromatic	64/107 (60%)	38/55 (69%)	24/46 (52%)	2/6 (33%)
Overall	1448/2013 (72%)	769/1029 (75%)	550/759 (72%)	129/225 (57%)

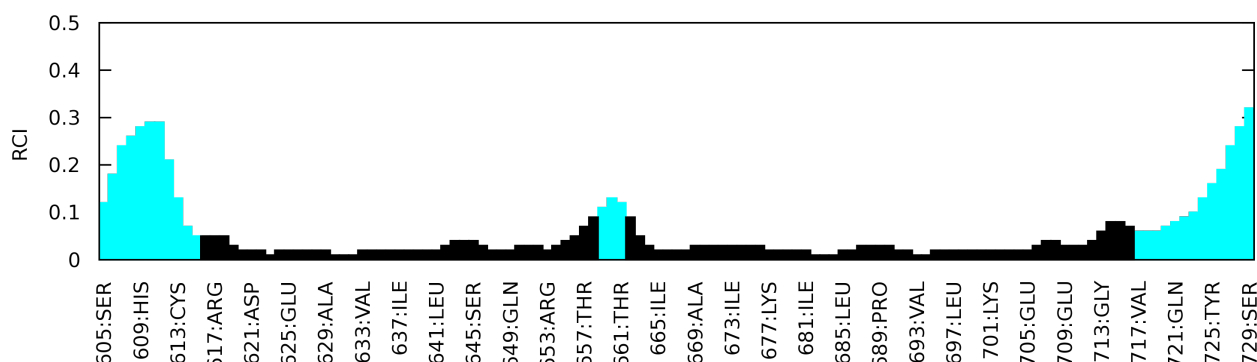
7.1.4 Statistically unusual chemical shifts [i](#)

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 B:



7.2 Chemical shift list 2

File name: 2n2h_cs.str

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	272
Number of shifts mapped to atoms	272
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

7.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	22	-0.65 ± 0.22	Should be applied
$^{13}\text{C}_\beta$	23	0.11 ± 0.24	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	23	-0.49 ± 0.40	None needed (< 0.5 ppm)

7.2.3 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 12%, i.e. 183 atoms were assigned a chemical shift out of a possible 1555. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	69/576 (12%)	35/230 (15%)	17/232 (7%)	17/114 (15%)
Sidechain	110/916 (12%)	69/533 (13%)	39/329 (12%)	2/54 (4%)
Aromatic	4/63 (6%)	4/33 (12%)	0/27 (0%)	0/3 (0%)
Overall	183/1555 (12%)	108/796 (14%)	56/588 (10%)	19/171 (11%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 250 atoms were assigned a chemical shift out of a possible 2013. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	93/756 (12%)	48/302 (16%)	22/304 (7%)	23/150 (15%)

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	Total	¹H	¹³C	¹⁵N
Sidechain	153/1150 (13%)	98/672 (15%)	53/409 (13%)	2/69 (3%)
Aromatic	4/107 (4%)	4/55 (7%)	0/46 (0%)	0/6 (0%)
Overall	250/2013 (12%)	150/1029 (15%)	75/759 (10%)	25/225 (11%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 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:

