



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:29 pm BST

PDB ID : 2M41
Title : Solution Structure of the AXH domain of Ataxin-1 in complex with ligand peptide from Capicua
Authors : de Chiara, C.; Kelly, G.; Pastore, A.
Deposited on : 2013-01-28

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

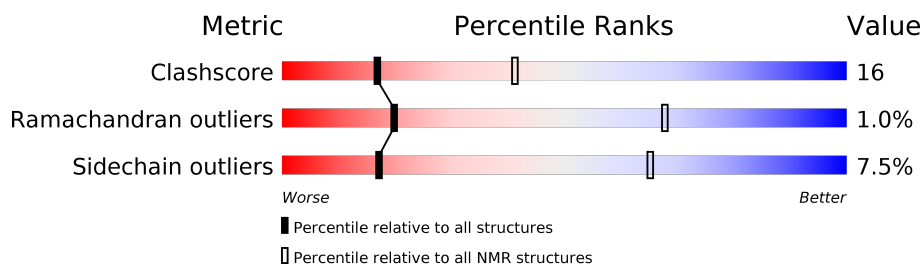
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 77%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 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	15	
2	B	126	

2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 14 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:35-A:43, B:571-B:605, B:609-B:689 (125)	0.27	14

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. No single-model clusters were found.

Cluster number	Models
1	1, 4, 7, 8, 11, 12, 15
2	3, 6, 10, 13, 14
3	2, 5, 9

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2138 atoms, of which 1065 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein capicua homolog.

Mol	Chain	Residues	Atoms					Trace
1	A	15	Total	C	H	N	O	0
			246	86	122	19	19	

- Molecule 2 is a protein called Ataxin-1.

Mol	Chain	Residues	Atoms						Trace
2	B	123	Total	C	H	N	O	S	0
			1892	605	943	152	187	5	

There are 3 discrepancies between the modelled and reference sequences:

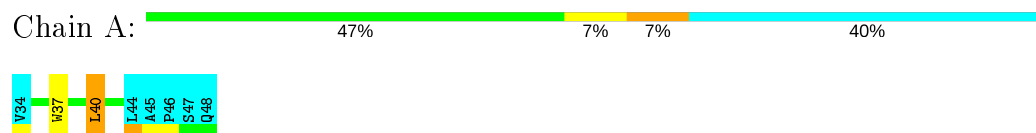
Chain	Residue	Modelled	Actual	Comment	Reference
B	564	GLY	-	EXPRESSION TAG	UNP P54253
B	565	ALA	-	EXPRESSION TAG	UNP P54253
B	566	MET	-	EXPRESSION TAG	UNP P54253

4 Residue-property plots

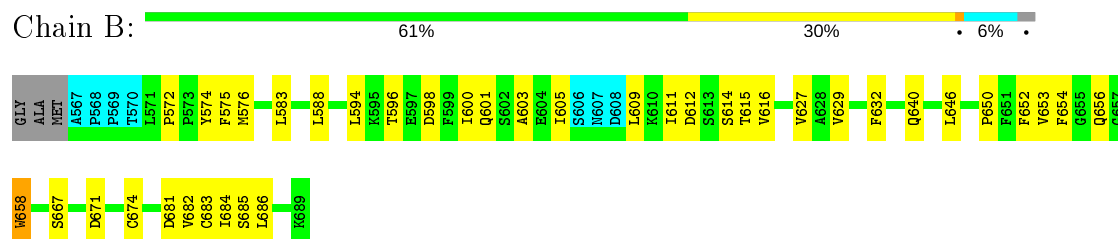
4.1 Average score per residue in the NMR ensemble

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: Protein capicua homolog



- Molecule 2: Ataxin-1

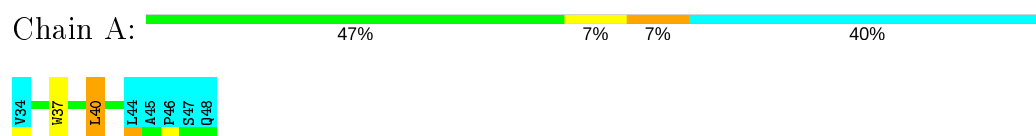


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Protein capicua homolog



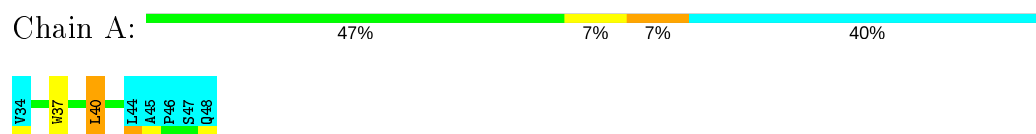
- Molecule 2: Ataxin-1



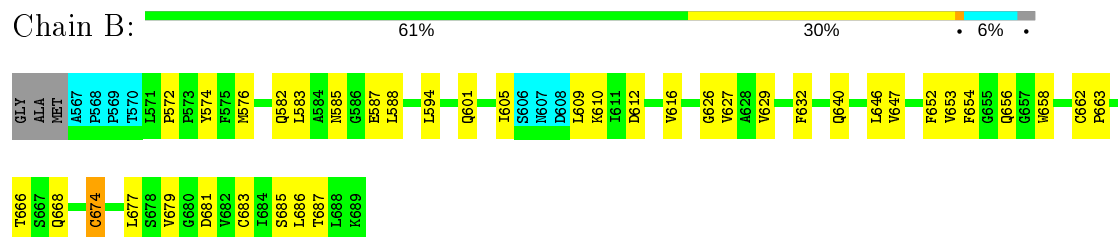


4.2.2 Score per residue for model 2

- Molecule 1: Protein capicua homolog

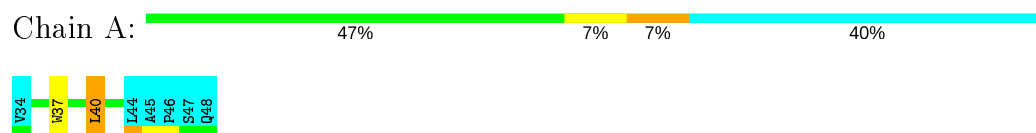


- Molecule 2: Ataxin-1

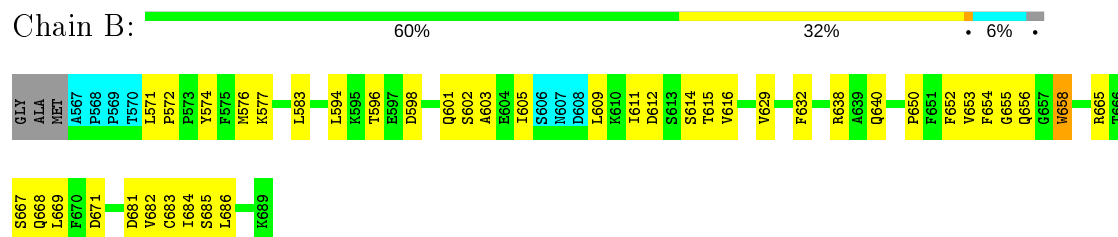


4.2.3 Score per residue for model 3

- Molecule 1: Protein capicua homolog

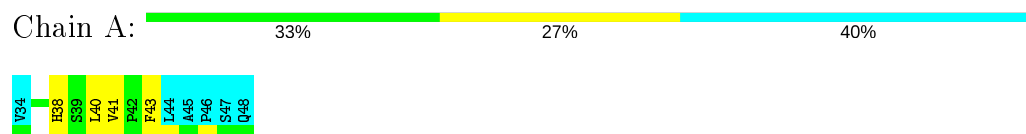


- Molecule 2: Ataxin-1

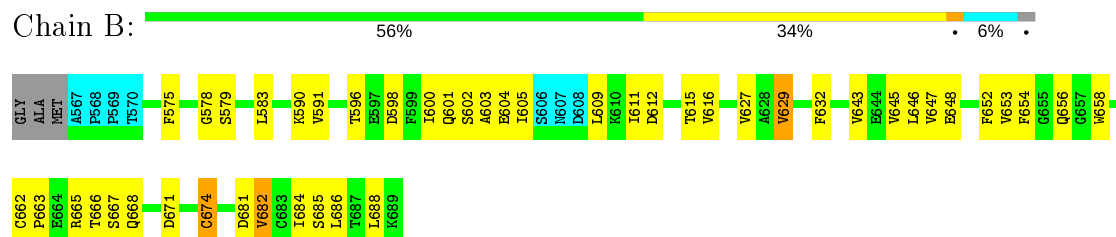


4.2.4 Score per residue for model 4

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1

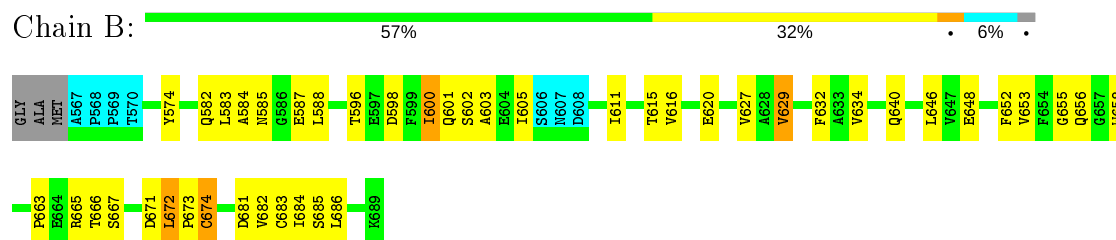


4.2.5 Score per residue for model 5

- Molecule 1: Protein capicua homolog

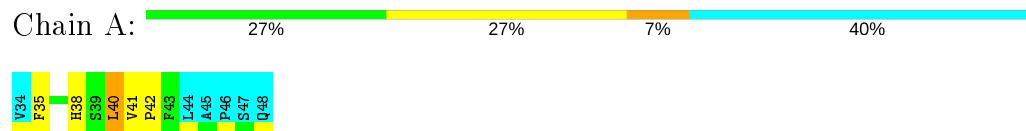


- Molecule 2: Ataxin-1

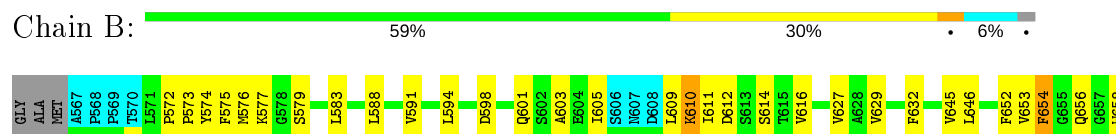


4.2.6 Score per residue for model 6

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1



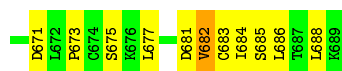


4.2.7 Score per residue for model 7

- Molecule 1: Protein capicua homolog



- Molecule 2: Ataxin-1



4.2.8 Score per residue for model 8

- Molecule 1: Protein capicua homolog



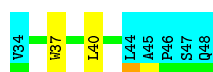
- Molecule 2: Ataxin-1



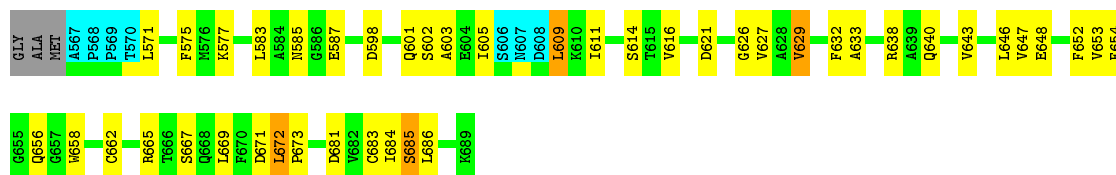
4.2.9 Score per residue for model 9

- Molecule 1: Protein capicua homolog



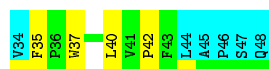


• Molecule 2: Ataxin-1

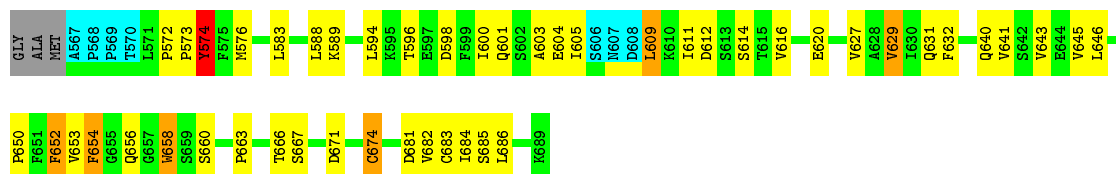


4.2.10 Score per residue for model 10

• Molecule 1: Protein capicua homolog

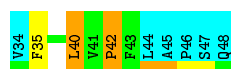
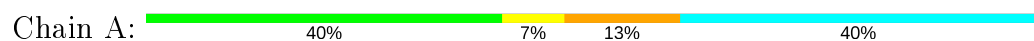


• Molecule 2: Ataxin-1

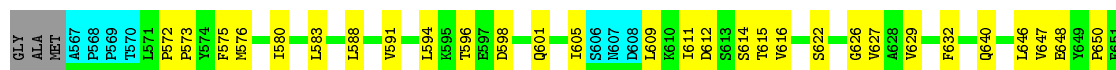


4.2.11 Score per residue for model 11

• Molecule 1: Protein capicua homolog



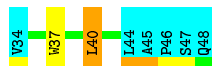
• Molecule 2: Ataxin-1



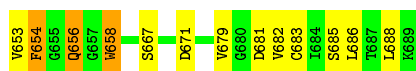


4.2.12 Score per residue for model 12

- Molecule 1: Protein capicua homolog

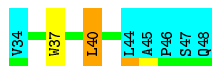


- Molecule 2: Ataxin-1



4.2.13 Score per residue for model 13

- Molecule 1: Protein capicua homolog



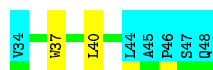
- Molecule 2: Ataxin-1



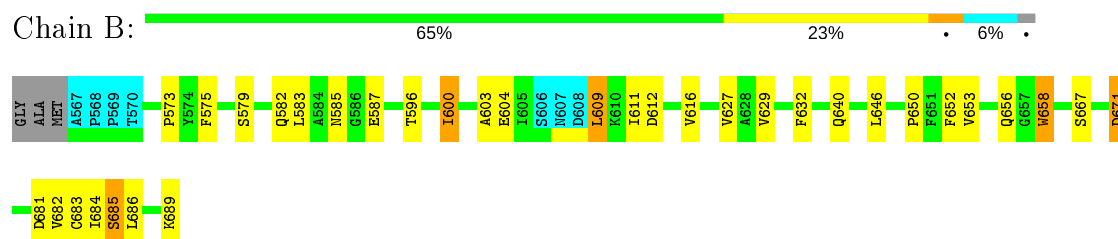
4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Protein capicua homolog



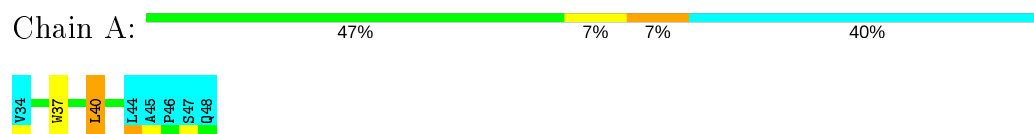


• Molecule 2: Ataxin-1

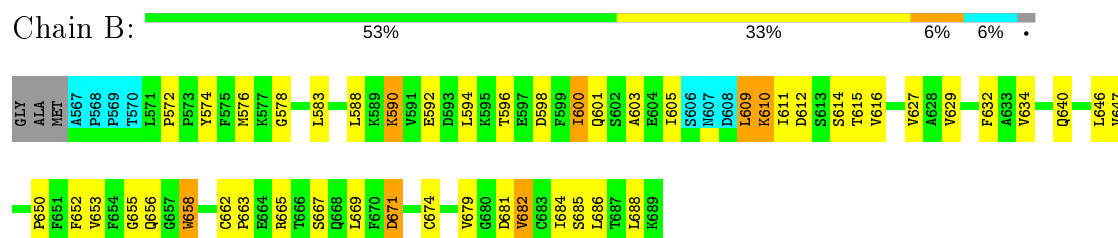


4.2.15 Score per residue for model 15

• Molecule 1: Protein capicua homolog



• Molecule 2: Ataxin-1



5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 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
ARIA	structure solution	2.3
ARIA	refinement	2.3

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

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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	81	75	74	2±1
2	B	901	902	900	30±4
All	All	14730	14655	14610	455

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:653:VAL:HG12	2:B:656:GLN:HE21	0.88	1.25	13	14
2:B:653:VAL:HG12	2:B:656:GLN:NE2	0.87	1.85	12	15
2:B:653:VAL:HG11	2:B:681:ASP:HB3	0.82	1.50	10	14
2:B:653:VAL:HG11	2:B:681:ASP:HB2	0.78	1.56	7	1
2:B:672:LEU:HD22	2:B:673:PRO:HD2	0.76	1.54	8	2
2:B:666:THR:HB	2:B:674:CYS:SG	0.74	2.22	8	5
2:B:663:PRO:HA	2:B:674:CYS:SG	0.68	2.28	4	5
2:B:632:PHE:O	2:B:640:GLN:HA	0.68	1.89	13	12
2:B:596:THR:O	2:B:600:ILE:HD13	0.67	1.89	14	3
2:B:656:GLN:NE2	2:B:682:VAL:HG13	0.67	2.04	4	6
2:B:616:VAL:HG12	2:B:681:ASP:O	0.67	1.90	6	15
2:B:653:VAL:CG1	2:B:656:GLN:HB2	0.63	2.22	5	8
2:B:600:ILE:O	2:B:604:GLU:HG3	0.62	1.94	14	5

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:632:PHE:HE1	2:B:683:CYS:HG	0.62	1.37	1	4
2:B:627:VAL:HG22	2:B:646:LEU:CD2	0.62	2.25	7	14
2:B:650:PRO:HB2	2:B:658:TRP:CH2	0.60	2.31	10	9
2:B:662:CYS:SG	2:B:665:ARG:HB3	0.60	2.36	4	1
2:B:603:ALA:HB3	2:B:611:ILE:HG12	0.60	1.72	13	12
2:B:656:GLN:NE2	2:B:682:VAL:HB	0.60	2.11	5	2
2:B:667:SER:O	2:B:671:ASP:HA	0.60	1.96	11	13
2:B:647:VAL:HB	2:B:662:CYS:SG	0.60	2.37	15	5
1:A:37:TRP:CZ2	2:B:609:LEU:HG	0.59	2.32	9	5
2:B:654:PHE:HB3	2:B:682:VAL:HG13	0.59	1.74	3	5
2:B:672:LEU:HD23	2:B:673:PRO:HD2	0.59	1.74	9	1
2:B:653:VAL:CG1	2:B:681:ASP:HB2	0.59	2.28	7	1
2:B:632:PHE:HE1	2:B:683:CYS:SG	0.58	2.22	3	5
2:B:614:SER:N	2:B:682:VAL:HG23	0.56	2.15	10	9
2:B:601:GLN:O	2:B:605:ILE:HG13	0.56	2.01	13	13
1:A:37:TRP:CZ2	2:B:609:LEU:HD13	0.56	2.36	12	5
2:B:603:ALA:CB	2:B:611:ILE:HG12	0.55	2.31	7	11
2:B:655:GLY:H	2:B:656:GLN:NE2	0.54	2.00	3	2
2:B:665:ARG:O	2:B:669:LEU:HG	0.54	2.02	9	5
2:B:620:GLU:HB2	2:B:629:VAL:HG13	0.54	1.78	5	3
2:B:582:GLN:HA	2:B:587:GLU:O	0.53	2.03	7	6
2:B:653:VAL:CG1	2:B:681:ASP:HB3	0.53	2.33	12	3
2:B:583:LEU:HB3	2:B:602:SER:OG	0.53	2.03	1	7
2:B:572:PRO:HD2	2:B:576:MET:SD	0.53	2.42	6	3
2:B:583:LEU:HD13	2:B:598:ASP:HB3	0.53	1.79	6	3
2:B:583:LEU:HB2	2:B:587:GLU:OE2	0.53	2.03	9	1
2:B:572:PRO:O	2:B:576:MET:HB2	0.52	2.05	10	6
2:B:647:VAL:HG23	2:B:662:CYS:SG	0.52	2.46	4	1
1:A:35:PHE:CD2	2:B:574:TYR:HA	0.51	2.40	10	1
2:B:651:PHE:HD2	2:B:683:CYS:HG	0.50	1.48	12	1
2:B:656:GLN:HE22	2:B:682:VAL:HG13	0.50	1.65	6	6
2:B:572:PRO:HB2	2:B:576:MET:SD	0.50	2.46	10	2
2:B:654:PHE:N	2:B:684:ILE:HG13	0.50	2.20	6	6
2:B:596:THR:OG1	2:B:684:ILE:HD11	0.50	2.07	4	9
2:B:577:LYS:HB2	2:B:671:ASP:O	0.49	2.07	9	1
2:B:573:PRO:O	2:B:579:SER:HB2	0.49	2.07	13	1
2:B:583:LEU:CD1	2:B:598:ASP:HB3	0.49	2.38	6	7
2:B:603:ALA:HB1	2:B:610:LYS:HA	0.49	1.84	13	1
2:B:653:VAL:HB	2:B:656:GLN:HB2	0.49	1.84	3	3
2:B:631:GLN:HA	2:B:641:VAL:O	0.49	2.07	10	3
2:B:577:LYS:HD2	2:B:671:ASP:O	0.49	2.08	6	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:612:ASP:HB3	2:B:685:SER:HB3	0.48	1.85	4	9
2:B:648:GLU:HB3	2:B:665:ARG:CD	0.48	2.38	5	1
2:B:583:LEU:HD11	2:B:598:ASP:HB3	0.48	1.85	9	3
2:B:612:ASP:HB3	2:B:685:SER:CB	0.48	2.38	14	1
2:B:645:VAL:HG12	2:B:646:LEU:N	0.48	2.23	4	4
2:B:591:VAL:HB	2:B:672:LEU:HD21	0.48	1.85	8	1
2:B:583:LEU:CD1	2:B:598:ASP:HB2	0.48	2.38	10	1
2:B:571:LEU:HD21	2:B:577:LYS:O	0.48	2.09	3	1
2:B:596:THR:HG21	2:B:655:GLY:HA2	0.48	1.86	15	3
2:B:571:LEU:HD11	2:B:577:LYS:O	0.47	2.09	1	1
2:B:575:PHE:O	2:B:672:LEU:HG	0.47	2.10	8	1
2:B:615:THR:HA	2:B:682:VAL:HA	0.47	1.87	15	7
1:A:40:LEU:HD11	2:B:594:LEU:CD1	0.47	2.40	2	9
2:B:653:VAL:HG12	2:B:656:GLN:HB2	0.47	1.87	5	3
1:A:38:HIS:HA	1:A:41:VAL:HG12	0.47	1.86	4	1
2:B:672:LEU:HD22	2:B:673:PRO:CD	0.46	2.35	8	1
2:B:583:LEU:HD12	2:B:587:GLU:HB2	0.46	1.87	5	1
2:B:630:ILE:HB	2:B:632:PHE:CE2	0.46	2.45	1	1
1:A:42:PRO:HD3	2:B:650:PRO:O	0.46	2.11	10	1
2:B:668:GLN:OE1	2:B:668:GLN:HA	0.46	2.11	3	3
2:B:596:THR:HA	2:B:652:PHE:CE1	0.45	2.47	10	2
1:A:37:TRP:CZ2	2:B:609:LEU:HD22	0.45	2.47	15	1
2:B:629:VAL:HA	2:B:643:VAL:O	0.45	2.11	4	6
2:B:614:SER:HB2	2:B:683:CYS:SG	0.45	2.51	9	2
2:B:664:GLU:H	2:B:664:GLU:CD	0.45	2.15	6	1
2:B:653:VAL:HG12	2:B:656:GLN:CD	0.45	2.31	12	1
2:B:626:GLY:O	2:B:646:LEU:HA	0.45	2.12	8	4
2:B:584:ALA:HB3	2:B:602:SER:HA	0.45	1.87	5	1
2:B:576:MET:N	2:B:576:MET:SD	0.45	2.89	10	2
2:B:589:LYS:NZ	2:B:594:LEU:HA	0.45	2.25	10	1
1:A:42:PRO:HG3	2:B:650:PRO:O	0.45	2.11	11	1
2:B:653:VAL:CG1	2:B:656:GLN:HE21	0.45	2.20	3	3
1:A:37:TRP:HA	2:B:581:ILE:CG2	0.45	2.42	1	1
2:B:632:PHE:CE1	2:B:683:CYS:SG	0.45	3.10	10	1
2:B:576:MET:SD	2:B:576:MET:N	0.45	2.89	12	1
2:B:677:LEU:HD21	2:B:683:CYS:SG	0.45	2.52	7	3
2:B:633:ALA:HB1	2:B:638:ARG:HB3	0.45	1.88	9	1
2:B:654:PHE:HA	2:B:684:ILE:CG1	0.44	2.42	8	2
2:B:612:ASP:CB	2:B:685:SER:HB3	0.44	2.41	12	2
2:B:578:GLY:HA2	2:B:590:LYS:CE	0.44	2.43	13	1
2:B:616:VAL:HG22	2:B:679:VAL:HA	0.44	1.90	11	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:667:SER:OG	2:B:673:PRO:HA	0.44	2.13	7	1
2:B:662:CYS:O	2:B:662:CYS:SG	0.44	2.76	4	1
2:B:583:LEU:HD11	2:B:598:ASP:HB2	0.44	1.90	10	1
2:B:688:LEU:N	2:B:688:LEU:HD22	0.44	2.28	7	2
2:B:610:LYS:NZ	2:B:610:LYS:HB3	0.43	2.27	6	2
1:A:38:HIS:CG	2:B:688:LEU:HD11	0.43	2.47	4	1
2:B:585:ASN:ND2	2:B:587:GLU:HG3	0.43	2.28	12	1
2:B:609:LEU:CD1	2:B:688:LEU:HA	0.43	2.43	11	1
1:A:37:TRP:HZ2	2:B:609:LEU:HD13	0.43	1.73	12	1
2:B:583:LEU:HB2	2:B:585:ASN:OD1	0.43	2.14	5	3
2:B:600:ILE:HD11	2:B:654:PHE:O	0.43	2.13	4	1
2:B:612:ASP:HB2	2:B:685:SER:HB3	0.43	1.89	6	1
2:B:573:PRO:HA	2:B:579:SER:OG	0.43	2.13	6	1
1:A:35:PHE:CZ	2:B:573:PRO:HG2	0.42	2.49	10	3
2:B:676:LYS:HG3	2:B:678:SER:OG	0.42	2.14	11	1
2:B:609:LEU:HD11	2:B:688:LEU:HD13	0.42	1.91	6	1
2:B:576:MET:O	2:B:591:VAL:HG21	0.42	2.15	7	1
2:B:663:PRO:HB3	2:B:674:CYS:O	0.42	2.13	8	2
2:B:615:THR:OG1	2:B:682:VAL:HG22	0.42	2.14	1	2
2:B:578:GLY:N	2:B:590:LYS:HE3	0.42	2.29	4	1
2:B:575:PHE:O	2:B:591:VAL:HG11	0.42	2.14	8	4
1:A:40:LEU:HD13	2:B:591:VAL:HG13	0.42	1.92	1	2
2:B:578:GLY:HA2	2:B:590:LYS:HE3	0.42	1.92	15	1
2:B:632:PHE:CE1	2:B:683:CYS:HB3	0.42	2.49	6	1
2:B:579:SER:HB2	2:B:591:VAL:CG2	0.42	2.44	4	1
1:A:38:HIS:HA	1:A:41:VAL:CG1	0.42	2.45	6	1
2:B:610:LYS:HB2	2:B:687:THR:OG1	0.41	2.15	2	1
2:B:672:LEU:CD2	2:B:673:PRO:HD2	0.41	2.45	5	1
2:B:579:SER:HB3	2:B:591:VAL:CG2	0.41	2.45	1	1
2:B:662:CYS:SG	2:B:664:GLU:HB2	0.41	2.56	6	1
2:B:656:GLN:OE1	2:B:682:VAL:HG12	0.41	2.15	12	1
2:B:581:ILE:HG13	2:B:594:LEU:HD11	0.41	1.92	13	2
2:B:650:PRO:HA	2:B:660:SER:CB	0.41	2.46	7	1
2:B:577:LYS:HG3	2:B:592:GLU:OE2	0.41	2.15	12	1
2:B:590:LYS:O	2:B:594:LEU:HG	0.41	2.15	15	1
2:B:580:ILE:CG2	2:B:588:LEU:HB3	0.41	2.46	11	1
2:B:600:ILE:O	2:B:604:GLU:HG2	0.41	2.16	8	1
2:B:612:ASP:HB3	2:B:685:SER:HB2	0.41	1.92	14	1
2:B:659:SER:OG	2:B:675:SER:HB2	0.40	2.16	7	1
2:B:672:LEU:HD12	2:B:673:PRO:HD2	0.40	1.92	11	1
2:B:585:ASN:HB3	2:B:587:GLU:OE2	0.40	2.16	9	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:650:PRO:HA	2:B:660:SER:OG	0.40	2.15	10	1
2:B:611:ILE:HG23	2:B:684:ILE:HG23	0.40	1.94	11	1
2:B:573:PRO:O	2:B:579:SER:HB3	0.40	2.16	14	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	9/15 (60%)	7±1 (77±10%)	2±1 (21±10%)	0±0 (1±4%)	14	59
2	B	115/126 (91%)	110±1 (95±1%)	4±2 (4±1%)	1±1 (1±1%)	20	68
All	All	1860/2115 (88%)	1748 (94%)	93 (5%)	19 (1%)	20	68

All 5 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	574	TYR	9
2	B	654	PHE	6
1	A	42	PRO	2
2	B	575	PHE	1
2	B	571	LEU	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	9/14 (64%)	8±0 (89±0%)	1±0 (11±0%)	9	53
2	B	104/111 (94%)	97±2 (93±2%)	7±2 (7±2%)	18	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1695/1875 (90%)	1568 (93%)	127 (7%)	17 65

All 27 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	686	LEU	15
2	B	652	PHE	15
2	B	658	TRP	15
2	B	629	VAL	15
1	A	40	LEU	15
2	B	682	VAL	7
2	B	609	LEU	6
2	B	671	ASP	5
2	B	674	CYS	5
2	B	575	PHE	4
2	B	648	GLU	3
2	B	600	ILE	3
2	B	610	LYS	2
2	B	685	SER	2
2	B	571	LEU	2
2	B	672	LEU	2
2	B	688	LEU	1
2	B	668	GLN	1
2	B	592	GLU	1
2	B	623	HIS	1
2	B	638	ARG	1
2	B	590	LYS	1
2	B	614	SER	1
2	B	574	TYR	1
2	B	656	GLN	1
2	B	621	ASP	1
2	B	622	SER	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 77% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1420
Number of shifts mapped to atoms	1420
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	26

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	90	-0.21 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	119	0.16 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	115	-0.33 ± 0.44	None needed (< 0.5 ppm)

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 77%, i.e. 1173 atoms were assigned a chemical shift out of a possible 1526. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	432/609 (71%)	236/242 (98%)	86/250 (34%)	110/117 (94%)
Sidechain	670/772 (87%)	415/454 (91%)	248/295 (84%)	7/23 (30%)

Continued on next page...

Continued from previous page...

	Total	¹H	¹³C	¹⁵N
Aromatic	71/145 (49%)	45/77 (58%)	25/60 (42%)	1/8 (12%)
Overall	1173/1526 (77%)	696/773 (90%)	359/605 (59%)	118/148 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1249 atoms were assigned a chemical shift out of a possible 1662. 27 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	462/668 (69%)	257/265 (97%)	90/276 (33%)	115/127 (91%)
Sidechain	716/849 (84%)	443/500 (89%)	265/324 (82%)	8/25 (32%)
Aromatic	71/145 (49%)	45/77 (58%)	25/60 (42%)	1/8 (12%)
Overall	1249/1662 (75%)	745/842 (88%)	380/660 (58%)	124/160 (78%)

7.1.4 Statistically unusual chemical shifts ⓘ

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	43	PHE	CD2	7.16	137.34 – 125.84	-108.2
1	A	35	PHE	CD2	7.34	137.34 – 125.84	-108.0
1	A	43	PHE	CD1	7.16	137.63 – 125.43	-101.9
1	A	35	PHE	CE2	7.47	136.81 – 124.71	-101.9
1	A	35	PHE	CD1	7.34	137.63 – 125.43	-101.8
1	A	35	PHE	CE1	7.47	137.92 – 123.42	-85.0
1	A	39	SER	CB	3.85	71.24 – 56.34	-40.2
1	A	47	SER	CB	3.91	71.24 – 56.34	-40.2
1	A	48	GLN	CG	2.29	39.38 – 28.18	-28.1
1	A	41	VAL	CG1	0.72	28.40 – 14.60	-15.1
1	A	34	VAL	CG1	0.86	28.40 – 14.60	-15.0
1	A	44	LEU	CD1	0.68	32.77 – 16.57	-14.8
1	A	40	LEU	CD1	0.91	32.77 – 16.57	-14.7
1	A	44	LEU	CD2	0.28	32.60 – 15.60	-14.0
1	A	40	LEU	CD2	0.47	32.60 – 15.60	-13.9
1	A	41	VAL	CG2	0.63	29.20 – 13.40	-13.1
1	A	34	VAL	CG2	0.83	29.20 – 13.40	-13.0
1	A	45	ALA	CB	1.33	28.03 – 9.93	-9.7
2	B	602	SER	HB3	1.47	5.25 – 2.45	-8.5
2	B	652	PHE	HD2	5.22	8.56 – 5.56	-6.1
2	B	652	PHE	HD1	5.22	8.56 – 5.56	-6.1
2	B	657	GLY	HA3	1.57	5.80 – 2.00	-6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	650	PRO	HD3	1.34	5.52 – 1.72	-6.0
2	B	575	PHE	HB3	0.78	4.85 – 1.05	-5.7
2	B	650	PRO	HG3	0.13	3.56 – 0.26	-5.4
2	B	650	PRO	HG2	0.33	3.48 – 0.38	-5.2

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

The images below report *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:



Random coil index (RCI) for chain B:

