



Full wwPDB NMR Structure Validation Report ⓘ

Mar 12, 2026 – 02:35 AM UTC

PDB ID : 7NT7 / pdb_00007nt7
BMRB ID : 34610
Title : Solution structure of toll like receptor 1 (TLR1) TIR domain
Authors : Mineev, K.S.; Lushpa, V.A.; Goncharuk, M.V.
Deposited on : 2021-03-09

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

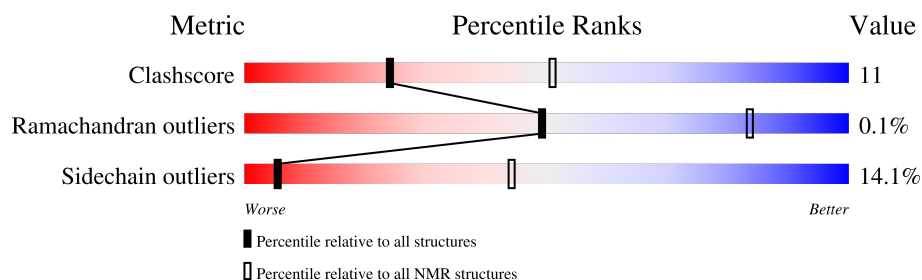
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 92%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	163	53% 18% • 27%

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: *fewest violations*.

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:634-A:668, A:682-A:713, A:724-A:775 (119)	0.61	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 3 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2710 atoms, of which 1354 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Toll-like receptor 1.

Mol	Chain	Residues	Atoms						Trace
1	A	163	Total	C	H	N	O	S	0
			2710	882	1354	231	238	5	

There is a discrepancy between the modelled and reference sequences:

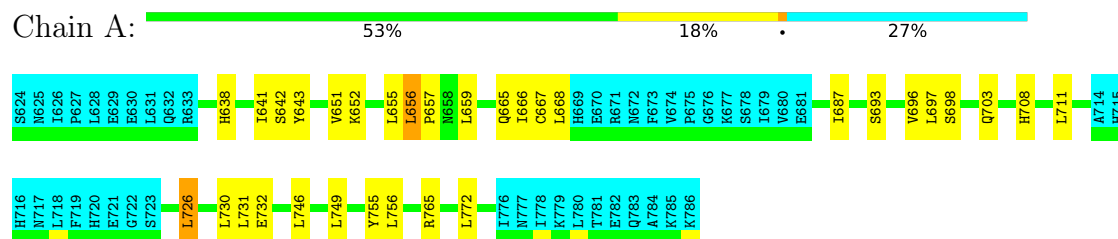
Chain	Residue	Modelled	Actual	Comment	Reference
A	624	SER	-	expression tag	UNP Q15399

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Toll-like receptor 1

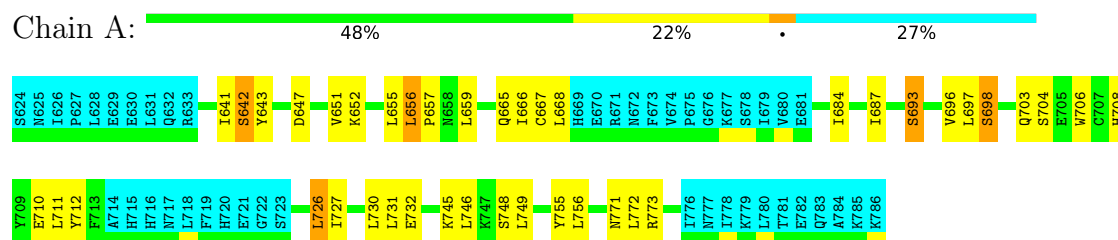


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

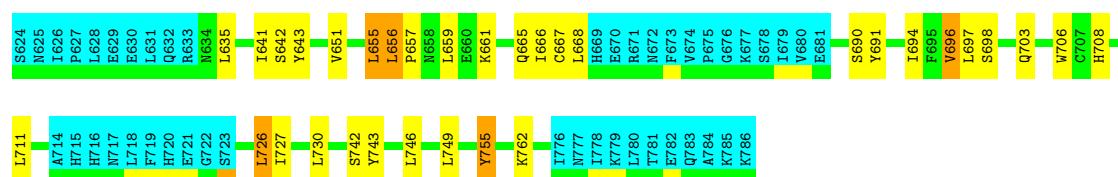
- Molecule 1: Toll-like receptor 1



4.2.2 Score per residue for model 2

- Molecule 1: Toll-like receptor 1

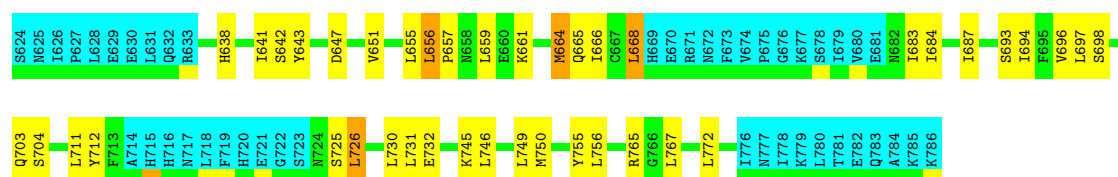




4.2.3 Score per residue for model 3

- Molecule 1: Toll-like receptor 1

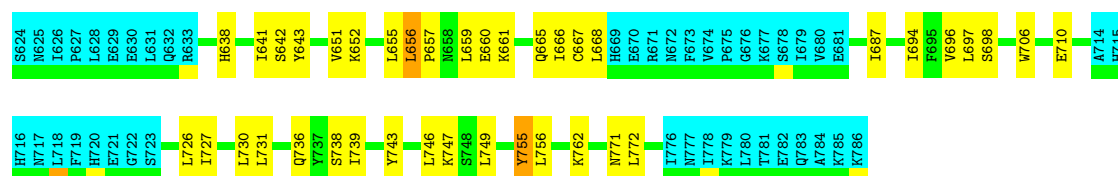
Chain A: 48% 23% 27%



4.2.4 Score per residue for model 4

- Molecule 1: Toll-like receptor 1

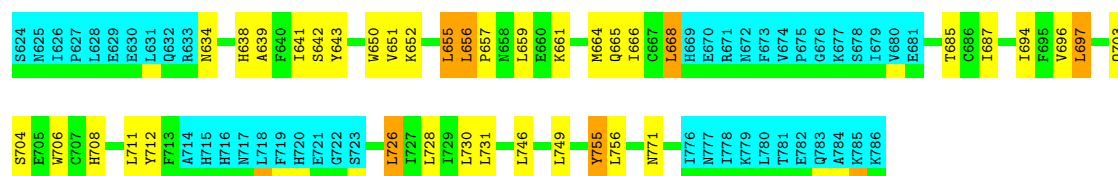
Chain A: 49% 23% 27%



4.2.5 Score per residue for model 5 (medoid)

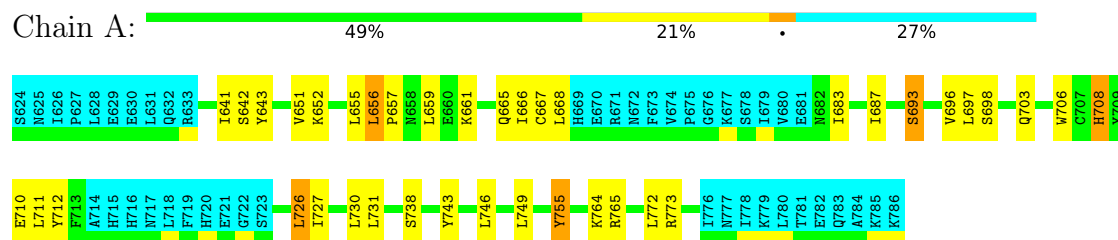
- Molecule 1: Toll-like receptor 1

Chain A: 50% 20% 27%



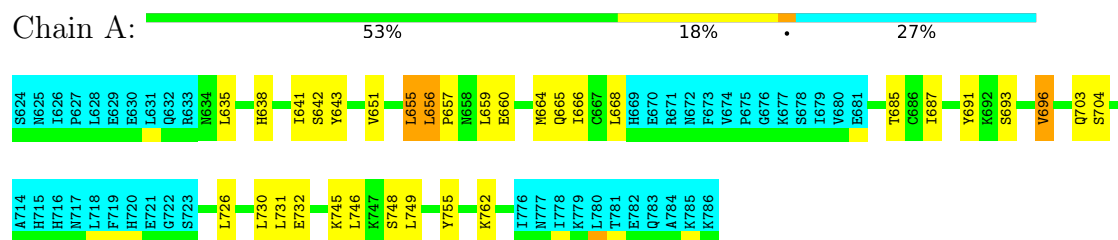
4.2.6 Score per residue for model 6

- Molecule 1: Toll-like receptor 1



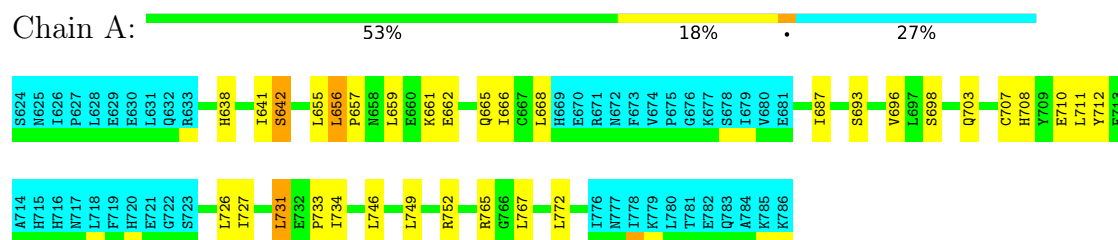
4.2.7 Score per residue for model 7

- Molecule 1: Toll-like receptor 1



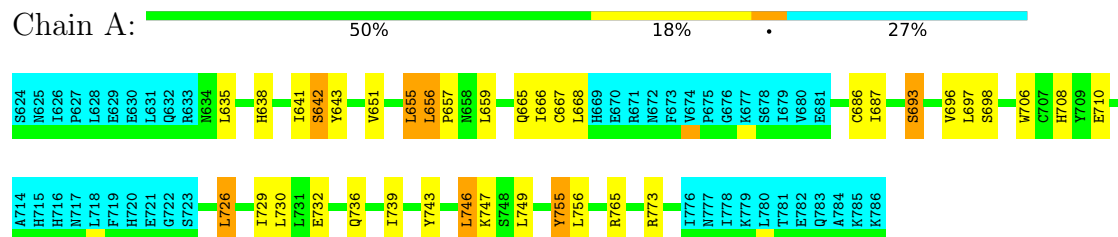
4.2.8 Score per residue for model 8

- Molecule 1: Toll-like receptor 1



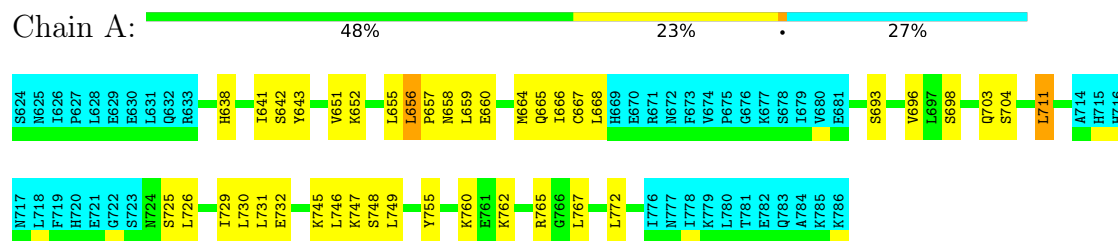
4.2.9 Score per residue for model 9

- Molecule 1: Toll-like receptor 1



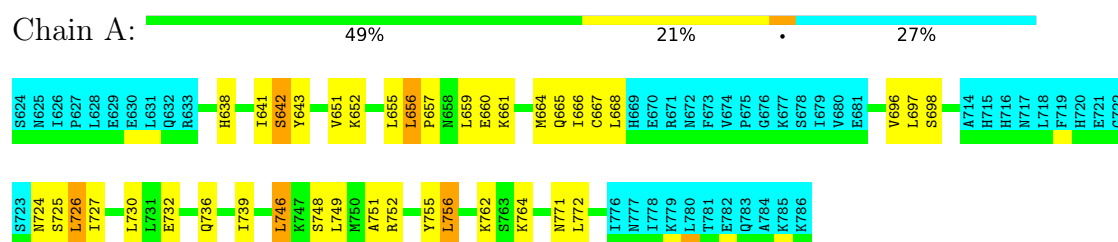
4.2.10 Score per residue for model 10

- Molecule 1: Toll-like receptor 1



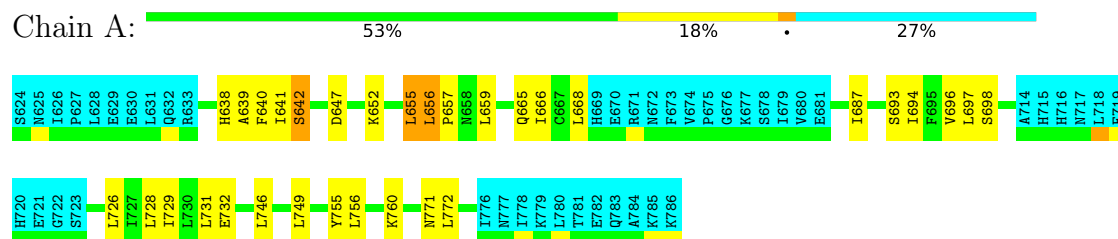
4.2.11 Score per residue for model 11

- Molecule 1: Toll-like receptor 1



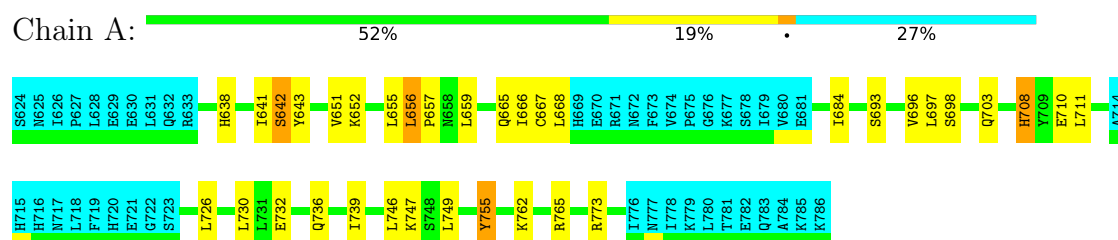
4.2.12 Score per residue for model 12

- Molecule 1: Toll-like receptor 1



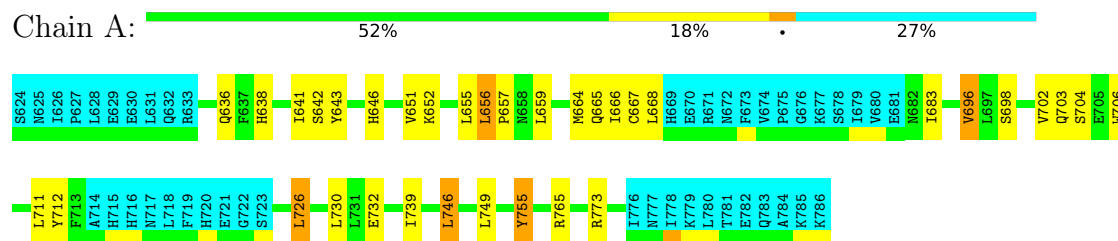
4.2.13 Score per residue for model 13

- Molecule 1: Toll-like receptor 1



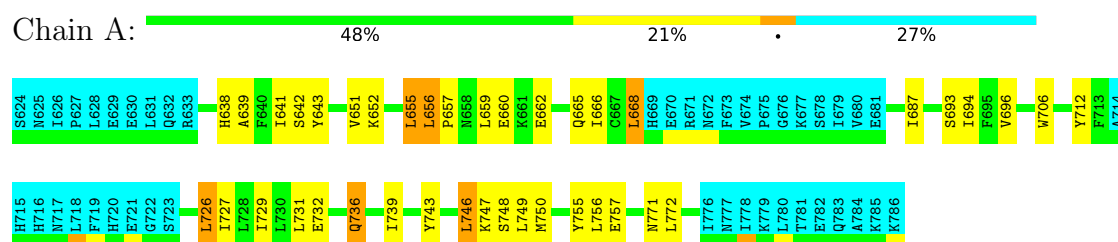
4.2.14 Score per residue for model 14

- Molecule 1: Toll-like receptor 1



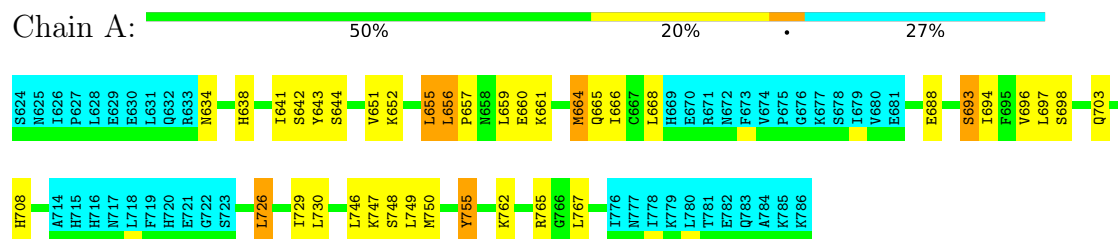
4.2.15 Score per residue for model 15

- Molecule 1: Toll-like receptor 1



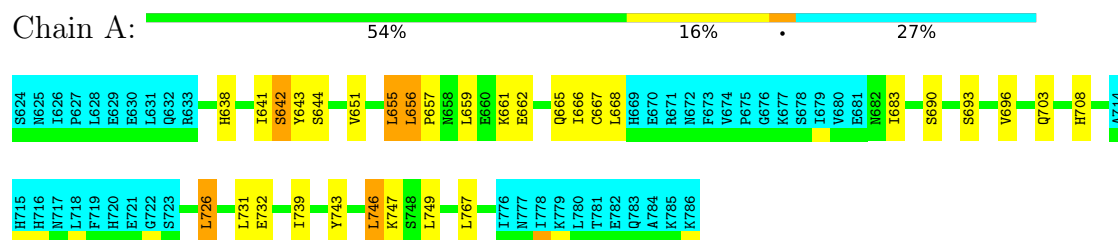
4.2.16 Score per residue for model 16

- Molecule 1: Toll-like receptor 1



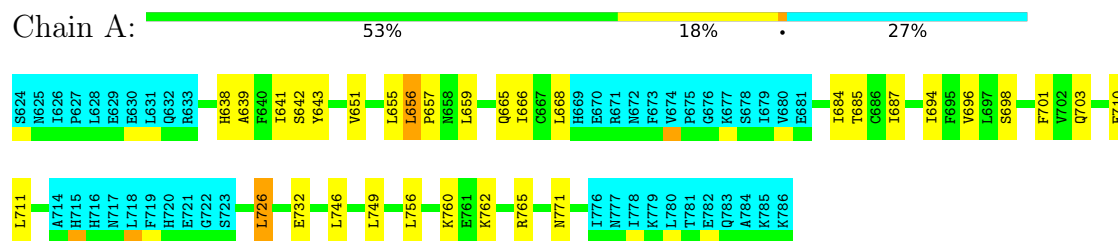
4.2.17 Score per residue for model 17

- Molecule 1: Toll-like receptor 1



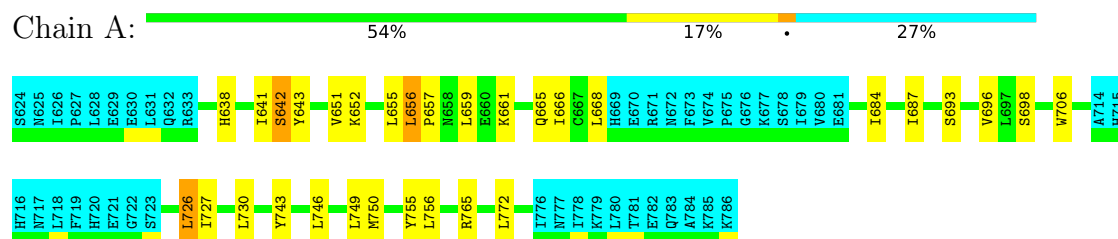
4.2.18 Score per residue for model 18

- Molecule 1: Toll-like receptor 1



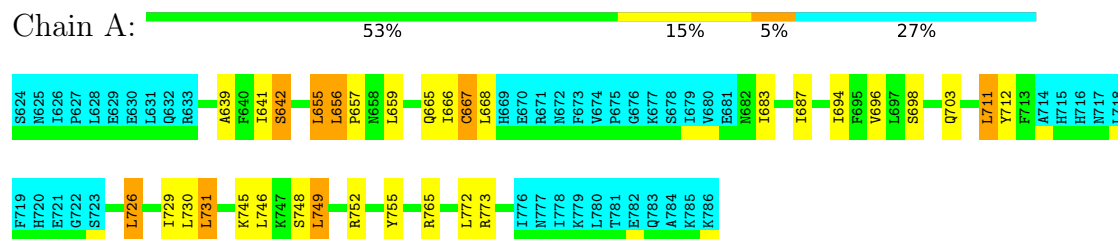
4.2.19 Score per residue for model 19

- Molecule 1: Toll-like receptor 1



4.2.20 Score per residue for model 20

- Molecule 1: Toll-like receptor 1



5 Refinement protocol and experimental data overview

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

Of the 200 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
CYANA	structure calculation	3.98.13

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2081
Number of shifts mapped to atoms	2081
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	92%

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	997	996	996	22±3
All	All	19940	19920	19920	430

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:641:ILE:HD13	1:A:655:LEU:HD23	0.98	1.35	20	9
1:A:641:ILE:HD13	1:A:655:LEU:HD13	0.92	1.41	18	10
1:A:641:ILE:HD12	1:A:668:LEU:HD21	0.85	1.48	17	19
1:A:655:LEU:HD11	1:A:729:ILE:HD13	0.72	1.60	15	3
1:A:641:ILE:HG21	1:A:655:LEU:HD23	0.71	1.60	12	6
1:A:643:TYR:CD2	1:A:651:VAL:HG11	0.70	2.22	19	12
1:A:730:LEU:HD13	1:A:755:TYR:CZ	0.69	2.22	14	12
1:A:659:LEU:HD13	1:A:666:ILE:HD12	0.69	1.63	20	19
1:A:641:ILE:HD11	1:A:659:LEU:HD12	0.67	1.65	1	14
1:A:643:TYR:CD1	1:A:651:VAL:HG11	0.65	2.27	9	4
1:A:693:SER:O	1:A:726:LEU:HD13	0.63	1.92	10	8
1:A:641:ILE:HD11	1:A:659:LEU:CD1	0.62	2.24	9	20
1:A:706:TRP:CD1	1:A:743:TYR:HH	0.62	2.12	2	6
1:A:756:LEU:HD23	1:A:772:LEU:HD12	0.62	1.70	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:739:ILE:HG12	1:A:746:LEU:HD13	0.62	1.71	14	1
1:A:639:ALA:HB1	1:A:694:ILE:HD11	0.62	1.70	12	3
1:A:641:ILE:HG21	1:A:655:LEU:HD13	0.61	1.71	14	6
1:A:664:MET:HE3	1:A:666:ILE:HD11	0.61	1.72	11	5
1:A:655:LEU:HD11	1:A:729:ILE:CD1	0.61	2.25	15	1
1:A:727:ILE:CG2	1:A:772:LEU:HD11	0.60	2.27	6	7
1:A:652:LYS:O	1:A:656:LEU:HD23	0.60	1.96	1	10
1:A:697:LEU:CB	1:A:730:LEU:HD12	0.60	2.27	4	2
1:A:641:ILE:HD12	1:A:668:LEU:CD2	0.59	2.28	5	14
1:A:733:PRO:O	1:A:734:ILE:HD13	0.59	1.97	8	1
1:A:736:GLN:HA	1:A:739:ILE:HD12	0.58	1.75	4	4
1:A:697:LEU:HD11	1:A:728:LEU:HD12	0.58	1.76	5	1
1:A:641:ILE:HD13	1:A:668:LEU:CD2	0.56	2.30	3	1
1:A:642:SER:O	1:A:696:VAL:HG12	0.56	2.00	11	20
1:A:751:ALA:HB3	1:A:752:ARG:CZ	0.56	2.30	11	1
1:A:731:LEU:HD13	1:A:732:GLU:HG2	0.56	1.77	3	1
1:A:756:LEU:HD11	1:A:771:ASN:HB3	0.55	1.78	4	4
1:A:683:ILE:HG21	1:A:712:TYR:CD2	0.55	2.36	6	3
1:A:639:ALA:HB1	1:A:694:ILE:CD1	0.55	2.32	18	4
1:A:731:LEU:HD13	1:A:732:GLU:HG3	0.55	1.77	17	1
1:A:746:LEU:HD12	1:A:749:LEU:HD23	0.55	1.79	5	2
1:A:730:LEU:HD22	1:A:755:TYR:CE2	0.54	2.37	9	1
1:A:656:LEU:N	1:A:657:PRO:HD2	0.53	2.18	18	20
1:A:652:LYS:HA	1:A:656:LEU:HD12	0.53	1.79	5	1
1:A:698:SER:OG	1:A:731:LEU:HD22	0.53	2.03	10	3
1:A:739:ILE:HD12	1:A:746:LEU:HG	0.53	1.79	13	2
1:A:729:ILE:HD11	1:A:772:LEU:HD11	0.52	1.81	12	3
1:A:696:VAL:HG13	1:A:701:PHE:CE1	0.52	2.40	18	1
1:A:697:LEU:HD22	1:A:755:TYR:CE1	0.52	2.39	6	1
1:A:727:ILE:HG23	1:A:772:LEU:HD11	0.51	1.81	6	1
1:A:711:LEU:HD23	1:A:711:LEU:O	0.51	2.05	18	1
1:A:683:ILE:HG21	1:A:712:TYR:CD1	0.51	2.40	20	1
1:A:697:LEU:HB2	1:A:730:LEU:HD12	0.51	1.81	4	3
1:A:659:LEU:HD22	1:A:664:MET:HE1	0.51	1.81	3	1
1:A:730:LEU:HD13	1:A:755:TYR:CE1	0.51	2.41	2	1
1:A:659:LEU:HD13	1:A:666:ILE:CD1	0.51	2.35	20	2
1:A:697:LEU:HB3	1:A:730:LEU:HD12	0.50	1.83	2	3
1:A:664:MET:CE	1:A:666:ILE:HD11	0.50	2.36	3	1
1:A:659:LEU:HD22	1:A:664:MET:CE	0.49	2.37	10	3
1:A:643:TYR:CE2	1:A:651:VAL:HG11	0.49	2.43	1	10
1:A:641:ILE:HD13	1:A:668:LEU:HD21	0.48	1.83	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:635:LEU:HD21	1:A:691:TYR:HB2	0.48	1.84	7	2
1:A:697:LEU:HD11	1:A:728:LEU:CD2	0.48	2.38	12	1
1:A:694:ILE:HG23	1:A:727:ILE:HB	0.48	1.84	2	1
1:A:687:ILE:HG23	1:A:693:SER:OG	0.48	2.08	7	1
1:A:730:LEU:HD13	1:A:755:TYR:OH	0.47	2.08	4	2
1:A:730:LEU:HD13	1:A:755:TYR:CE2	0.47	2.42	14	1
1:A:749:LEU:C	1:A:749:LEU:HD12	0.47	2.35	20	20
1:A:707:CYS:O	1:A:711:LEU:HD12	0.47	2.08	8	1
1:A:641:ILE:HG12	1:A:655:LEU:HD13	0.47	1.85	3	1
1:A:767:LEU:C	1:A:767:LEU:HD13	0.47	2.34	3	3
1:A:731:LEU:C	1:A:731:LEU:HD13	0.47	2.34	7	1
1:A:746:LEU:O	1:A:749:LEU:HD23	0.47	2.10	18	18
1:A:641:ILE:HG12	1:A:694:ILE:HD12	0.47	1.86	16	1
1:A:697:LEU:HD12	1:A:755:TYR:CE1	0.47	2.45	9	1
1:A:641:ILE:HG13	1:A:694:ILE:HD12	0.46	1.87	3	1
1:A:652:LYS:CA	1:A:656:LEU:HD12	0.46	2.40	5	1
1:A:731:LEU:O	1:A:731:LEU:HD12	0.46	2.11	4	1
1:A:641:ILE:HG21	1:A:655:LEU:CD1	0.46	2.39	8	1
1:A:711:LEU:HD12	1:A:712:TYR:N	0.46	2.25	6	1
1:A:664:MET:HE1	1:A:666:ILE:HD11	0.46	1.87	3	1
1:A:641:ILE:HD13	1:A:655:LEU:CD2	0.45	2.25	2	2
1:A:702:VAL:HG11	1:A:746:LEU:HD11	0.45	1.88	14	1
1:A:641:ILE:CD1	1:A:668:LEU:HD21	0.45	2.40	6	2
1:A:731:LEU:HD13	1:A:731:LEU:C	0.45	2.36	3	2
1:A:729:ILE:HD11	1:A:772:LEU:CD1	0.45	2.42	12	1
1:A:743:TYR:CD1	1:A:746:LEU:HD23	0.45	2.47	17	1
1:A:656:LEU:CB	1:A:657:PRO:CD	0.45	2.94	8	17
1:A:666:ILE:HG22	1:A:668:LEU:HG	0.45	1.88	3	6
1:A:643:TYR:CE1	1:A:651:VAL:HG11	0.45	2.45	9	1
1:A:659:LEU:HB3	1:A:664:MET:HE1	0.44	1.88	3	2
1:A:650:TRP:CE2	1:A:731:LEU:HD13	0.44	2.47	5	1
1:A:730:LEU:C	1:A:730:LEU:HD13	0.44	2.37	7	3
1:A:664:MET:SD	1:A:666:ILE:HD11	0.44	2.53	16	1
1:A:767:LEU:HD23	1:A:767:LEU:O	0.44	2.12	16	1
1:A:641:ILE:HD11	1:A:659:LEU:HD11	0.44	1.89	11	1
1:A:697:LEU:HD13	1:A:755:TYR:CD1	0.43	2.49	6	1
1:A:730:LEU:HD22	1:A:755:TYR:HE2	0.43	1.74	9	1
1:A:756:LEU:HD12	1:A:771:ASN:HB3	0.43	1.89	11	1
1:A:725:SER:O	1:A:726:LEU:HD22	0.43	2.13	10	2
1:A:656:LEU:N	1:A:657:PRO:CD	0.43	2.81	18	3
1:A:641:ILE:HG21	1:A:655:LEU:CD2	0.43	2.42	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:647:ASP:CG	1:A:731:LEU:HD21	0.43	2.38	12	1
1:A:756:LEU:HD11	1:A:772:LEU:HA	0.43	1.90	3	1
1:A:756:LEU:HD11	1:A:772:LEU:CA	0.42	2.44	3	1
1:A:697:LEU:HD11	1:A:728:LEU:HD22	0.42	1.91	12	1
1:A:652:LYS:CB	1:A:656:LEU:HD12	0.42	2.44	5	1
1:A:667:CYS:O	1:A:668:LEU:HD23	0.42	2.15	20	1
1:A:683:ILE:HG21	1:A:712:TYR:HD2	0.42	1.75	14	1
1:A:640:PHE:O	1:A:694:ILE:HD12	0.42	2.15	12	1
1:A:641:ILE:HB	1:A:668:LEU:HD23	0.41	1.93	5	1
1:A:652:LYS:O	1:A:656:LEU:HD22	0.41	2.15	16	1
1:A:731:LEU:HD13	1:A:732:GLU:CG	0.41	2.45	17	1
1:A:683:ILE:HG21	1:A:712:TYR:CE1	0.41	2.50	20	1
1:A:694:ILE:HD12	1:A:727:ILE:HB	0.41	1.91	4	1
1:A:756:LEU:HD11	1:A:771:ASN:CB	0.41	2.46	1	2
1:A:756:LEU:HD12	1:A:771:ASN:CB	0.41	2.46	11	1
1:A:698:SER:HB2	1:A:731:LEU:HD22	0.41	1.93	1	1
1:A:684:ILE:O	1:A:687:ILE:HD12	0.41	2.15	18	1
1:A:697:LEU:HD13	1:A:755:TYR:CD2	0.41	2.49	5	1
1:A:656:LEU:HB3	1:A:657:PRO:HD3	0.41	1.93	9	3

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	119/163 (73%)	113±1 (95±1%)	6±1 (5±1%)	0±0 (0±0%)	49	83
All	All	2380/3260 (73%)	2260 (95%)	118 (5%)	2 (0%)	49	83

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	697	LEU	2

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	111/151 (74%)	95±3 (86±2%)	16±3 (14±2%)	5	44
All	All	2220/3020 (74%)	1908 (86%)	312 (14%)	5	44

All 57 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	656	LEU	20
1	A	665	GLN	20
1	A	726	LEU	19
1	A	638	HIS	16
1	A	703	GLN	14
1	A	698	SER	13
1	A	755	TYR	13
1	A	667	CYS	11
1	A	765	ARG	11
1	A	732	GLU	10
1	A	661	LYS	10
1	A	642	SER	9
1	A	655	LEU	9
1	A	693	SER	8
1	A	708	HIS	8
1	A	762	LYS	8
1	A	710	GLU	7
1	A	748	SER	7
1	A	747	LYS	7
1	A	704	SER	6
1	A	773	ARG	6
1	A	660	GLU	6
1	A	745	LYS	5
1	A	746	LEU	5
1	A	750	MET	4
1	A	731	LEU	4
1	A	706	TRP	3
1	A	696	VAL	3
1	A	668	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	662	GLU	3
1	A	756	LEU	3
1	A	711	LEU	3
1	A	760	LYS	3
1	A	647	ASP	2
1	A	684	ILE	2
1	A	690	SER	2
1	A	664	MET	2
1	A	738	SER	2
1	A	634	ASN	2
1	A	685	THR	2
1	A	764	LYS	2
1	A	752	ARG	2
1	A	736	GLN	2
1	A	644	SER	2
1	A	742	SER	1
1	A	697	LEU	1
1	A	635	LEU	1
1	A	686	CYS	1
1	A	658	ASN	1
1	A	725	SER	1
1	A	771	ASN	1
1	A	636	GLN	1
1	A	646	HIS	1
1	A	757	GLU	1
1	A	688	GLU	1
1	A	767	LEU	1
1	A	749	LEU	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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

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 92% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	2081
Number of shifts mapped to atoms	2081
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	158	0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	153	0.57 ± 0.07	Should be checked
$^{13}\text{C}'$	152	0.32 ± 0.10	None needed (< 0.5 ppm)
^{15}N	142	0.52 ± 0.41	None needed (imprecise)

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 92%, i.e. 1582 atoms were assigned a chemical shift out of a possible 1728. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	573/586 (98%)	230/235 (98%)	235/238 (99%)	108/113 (96%)
Sidechain	860/933 (92%)	584/610 (96%)	266/291 (91%)	10/32 (31%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	149/209 (71%)	90/103 (87%)	55/98 (56%)	4/8 (50%)
Overall	1582/1728 (92%)	904/948 (95%)	556/627 (89%)	122/153 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 2080 atoms were assigned a chemical shift out of a possible 2355. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	756/804 (94%)	304/323 (94%)	310/326 (95%)	142/155 (92%)
Sidechain	1159/1294 (90%)	787/842 (93%)	358/404 (89%)	14/48 (29%)
Aromatic	165/257 (64%)	100/129 (78%)	61/116 (53%)	4/12 (33%)
Overall	2080/2355 (88%)	1191/1294 (92%)	729/846 (86%)	160/215 (74%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	731	LEU	HD21	-1.05	-0.65 – 2.13	-6.4
1	A	731	LEU	HD22	-1.05	-0.65 – 2.13	-6.4
1	A	731	LEU	HD23	-1.05	-0.65 – 2.13	-6.4
1	A	654	GLU	HB2	0.71	1.00 – 3.05	-6.4
1	A	650	TRP	HE1	6.14	6.88 – 13.28	-6.2
1	A	665	GLN	H	11.69	5.39 – 11.05	6.1
1	A	705	GLU	HB2	0.92	1.00 – 3.05	-5.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

