



Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 08:47 AM EDT

PDB ID : 2LM0
BMRB ID : 18094
Title : Solution structure of the AF4-AF9 complex
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Deposited on : 2011-11-18

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 : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.36.2

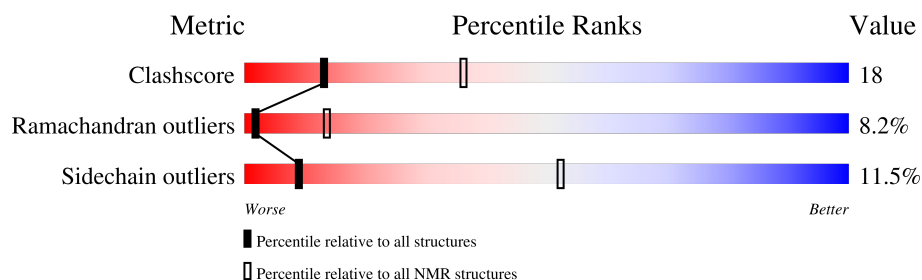
1 Overall quality at a glance

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	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	125	

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:760-A:774, A:1502-A:1563 (77)	0.93	6

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 4 single-model clusters were found.

Cluster number	Models
1	1, 3, 8, 9
2	6, 7
Single-model clusters	2; 4; 5; 10

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2050 atoms, of which 1046 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AF4/FMR2 family member 1/Protein AF-9 chimera.

Mol	Chain	Residues	Atoms						Trace
1	A	125	Total	C	H	N	O	S	0
			2050	632	1046	177	190	5	

There are 4 discrepancies between the modelled and reference sequences:

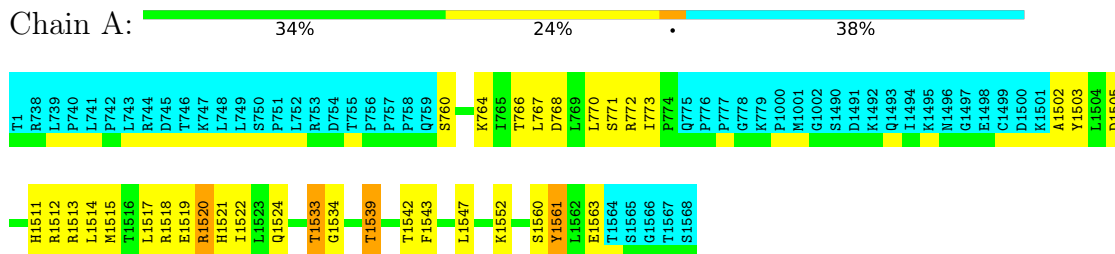
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	THR	-	expression tag	UNP P51825
A	1000	PRO	-	linker	UNP P51825
A	1001	MET	-	linker	UNP P51825
A	1002	GLY	-	linker	UNP P51825

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: AF4/FMR2 family member 1/Protein AF-9 chimera

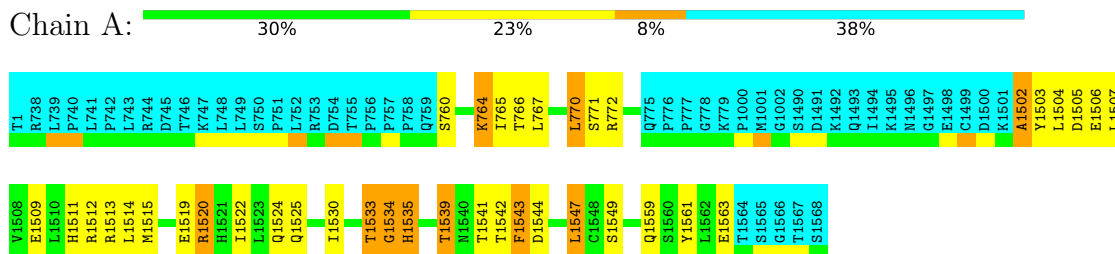


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

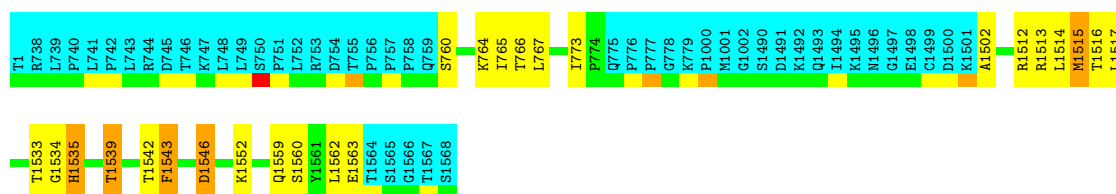
- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera



4.2.2 Score per residue for model 2

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera

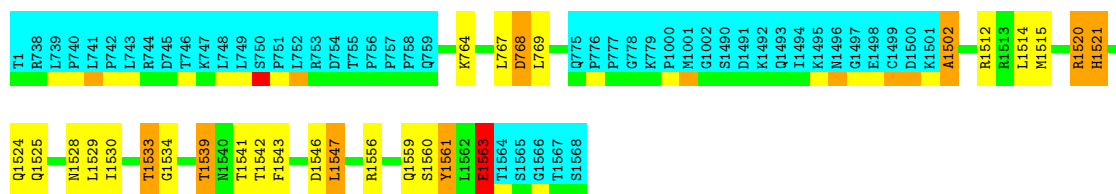




4.2.3 Score per residue for model 3

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera

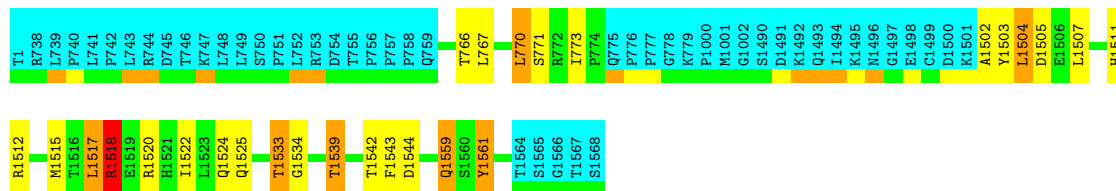
Chain A: 39% 15% 6% • 38%



4.2.4 Score per residue for model 4

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera

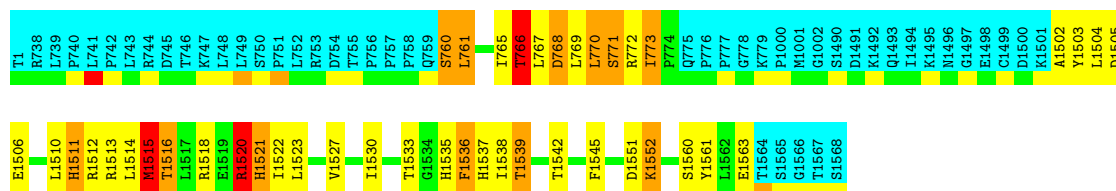
Chain A: 40% 15% 6% • 38%



4.2.5 Score per residue for model 5

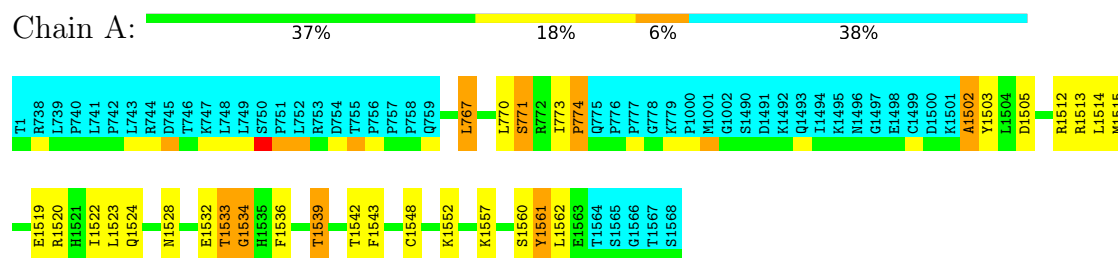
- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera

Chain A: 27% 22% 10% • 38%



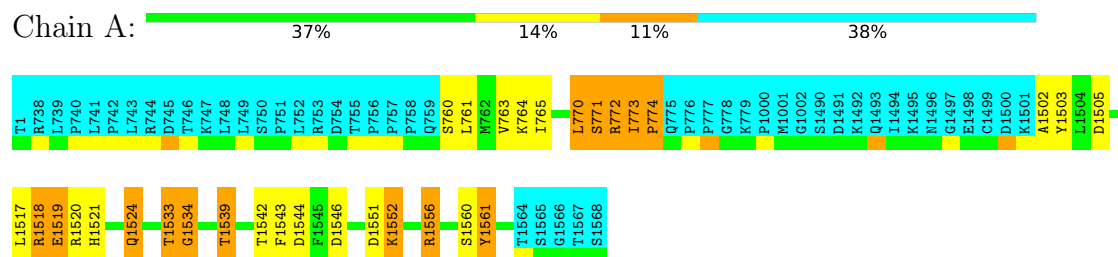
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera



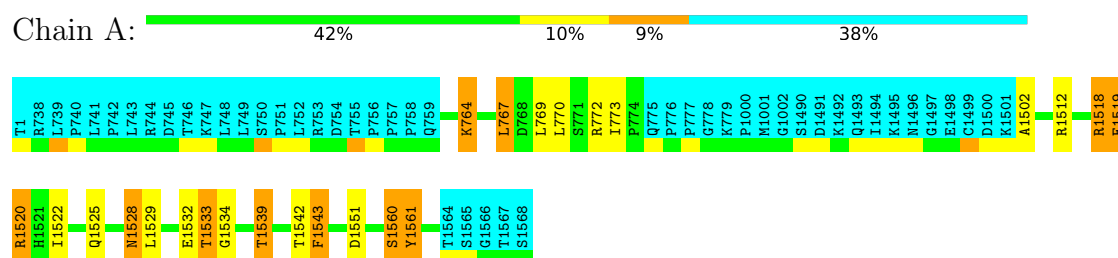
4.2.7 Score per residue for model 7

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera



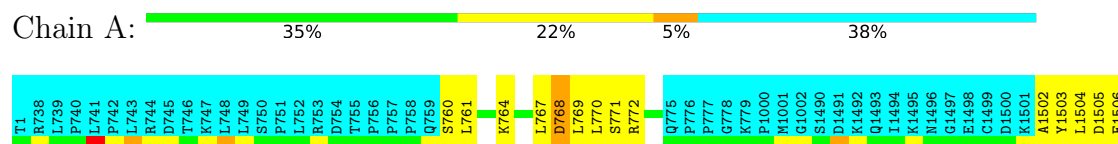
4.2.8 Score per residue for model 8

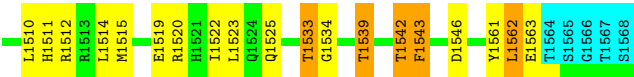
- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera



4.2.9 Score per residue for model 9

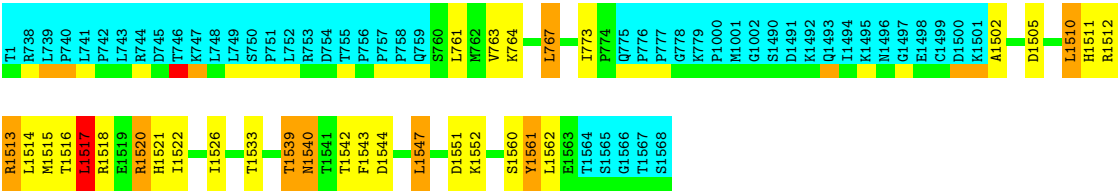
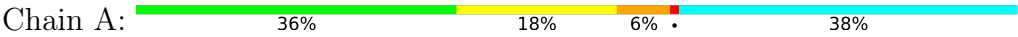
- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera





4.2.10 Score per residue for model 10

- Molecule 1: AF4/FMR2 family member 1/Protein AF-9 chimera



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 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
XPLOR-NIH	refinement	2.27
XPLOR-NIH	structure solution	2.27

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	1285
Number of shifts mapped to atoms	1285
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%

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	641	667	663	24±7
All	All	6410	6670	6630	239

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 18.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:770:LEU:HD23	1:A:771:SER:H	0.70	1.44	4	1
1:A:1518:ARG:NE	1:A:1518:ARG:N	0.67	2.43	4	1
1:A:770:LEU:C	1:A:770:LEU:HD22	0.66	2.11	7	1
1:A:773:ILE:HD12	1:A:773:ILE:N	0.65	2.07	5	2
1:A:767:LEU:O	1:A:770:LEU:HD22	0.64	1.93	4	1
1:A:1536:PHE:CZ	1:A:1545:PHE:CG	0.62	2.88	5	1
1:A:1503:TYR:CE1	1:A:1552:LYS:NZ	0.61	2.67	6	1
1:A:770:LEU:HD23	1:A:771:SER:N	0.61	2.10	4	1
1:A:1561:TYR:CD1	1:A:1561:TYR:C	0.59	2.75	10	3
1:A:764:LYS:N	1:A:764:LYS:CD	0.59	2.65	8	2
1:A:1560:SER:OG	1:A:1561:TYR:CD1	0.58	2.56	6	1
1:A:1534:GLY:O	1:A:1535:HIS:CB	0.58	2.50	1	2
1:A:1518:ARG:N	1:A:1518:ARG:HE	0.58	1.96	4	1
1:A:765:ILE:HD12	1:A:765:ILE:N	0.57	2.14	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:765:ILE:HG21	1:A:770:LEU:HD23	0.57	1.77	5	1
1:A:770:LEU:O	1:A:771:SER:C	0.57	2.41	7	2
1:A:1530:ILE:O	1:A:1533:THR:HG23	0.56	1.99	5	1
1:A:771:SER:OG	1:A:772:ARG:N	0.56	2.38	9	3
1:A:1504:LEU:HD12	1:A:1505:ASP:N	0.56	2.15	9	1
1:A:1520:ARG:O	1:A:1521:HIS:CG	0.56	2.59	3	1
1:A:770:LEU:O	1:A:770:LEU:HD13	0.56	2.01	7	2
1:A:1521:HIS:O	1:A:1523:LEU:N	0.55	2.38	5	1
1:A:1560:SER:OG	1:A:1561:TYR:N	0.55	2.37	6	2
1:A:1507:LEU:O	1:A:1511:HIS:CE1	0.55	2.59	1	1
1:A:1528:ASN:HD22	1:A:1528:ASN:N	0.55	1.99	8	1
1:A:1544:ASP:N	1:A:1544:ASP:OD1	0.54	2.39	1	2
1:A:1518:ARG:C	1:A:1520:ARG:H	0.54	2.06	8	1
1:A:1517:LEU:C	1:A:1517:LEU:HD12	0.54	2.23	4	1
1:A:1525:GLN:O	1:A:1529:LEU:HD13	0.54	2.03	8	2
1:A:1535:HIS:NE2	1:A:1549:SER:CB	0.54	2.70	1	1
1:A:1512:ARG:O	1:A:1515:MET:N	0.53	2.41	6	8
1:A:772:ARG:CZ	1:A:1524:GLN:NE2	0.53	2.72	1	1
1:A:1505:ASP:OD1	1:A:1506:GLU:N	0.53	2.42	5	2
1:A:768:ASP:N	1:A:768:ASP:OD1	0.52	2.41	5	1
1:A:1504:LEU:HD12	1:A:1504:LEU:C	0.52	2.24	9	1
1:A:1512:ARG:O	1:A:1514:LEU:N	0.52	2.42	5	7
1:A:1561:TYR:CD1	1:A:1561:TYR:N	0.52	2.74	4	4
1:A:769:LEU:HD22	1:A:769:LEU:N	0.52	2.19	5	1
1:A:769:LEU:N	1:A:769:LEU:CD2	0.52	2.72	5	1
1:A:1547:LEU:HD12	1:A:1547:LEU:H	0.52	1.63	1	2
1:A:1509:GLU:OE2	1:A:1512:ARG:NH2	0.51	2.43	1	1
1:A:1551:ASP:OD1	1:A:1552:LYS:N	0.51	2.43	5	2
1:A:1515:MET:SD	1:A:1515:MET:O	0.51	2.68	5	1
1:A:1533:THR:OG1	1:A:1534:GLY:N	0.51	2.44	7	7
1:A:1548:CYS:SG	1:A:1548:CYS:O	0.51	2.69	6	1
1:A:1514:LEU:O	1:A:1516:THR:N	0.51	2.43	2	2
1:A:770:LEU:O	1:A:771:SER:CB	0.50	2.60	1	3
1:A:1546:ASP:N	1:A:1546:ASP:OD1	0.50	2.44	7	2
1:A:760:SER:OG	1:A:761:LEU:N	0.50	2.42	9	2
1:A:1512:ARG:C	1:A:1514:LEU:N	0.50	2.65	10	5
1:A:1522:ILE:HG21	1:A:1561:TYR:CE1	0.50	2.41	10	2
1:A:1502:ALA:O	1:A:1504:LEU:N	0.50	2.44	5	2
1:A:1551:ASP:OD1	1:A:1551:ASP:N	0.50	2.44	7	1
1:A:1539:THR:CB	1:A:1542:THR:O	0.49	2.60	3	10
1:A:1546:ASP:OD1	1:A:1546:ASP:N	0.49	2.42	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1530:ILE:CD1	1:A:1530:ILE:N	0.49	2.75	1	1
1:A:1526:ILE:HG22	1:A:1526:ILE:O	0.49	2.07	10	1
1:A:766:THR:HG22	1:A:767:LEU:N	0.49	2.22	2	1
1:A:1518:ARG:NE	1:A:1518:ARG:H	0.49	2.05	4	1
1:A:1503:TYR:O	1:A:1505:ASP:N	0.49	2.45	4	1
1:A:1505:ASP:N	1:A:1505:ASP:OD1	0.49	2.44	6	1
1:A:1517:LEU:HD22	1:A:1517:LEU:N	0.49	2.22	7	1
1:A:1524:GLN:H	1:A:1524:GLN:CD	0.49	2.11	7	1
1:A:1530:ILE:O	1:A:1533:THR:OG1	0.49	2.23	3	1
1:A:1560:SER:OG	1:A:1561:TYR:CE1	0.49	2.65	6	1
1:A:1523:LEU:CD2	1:A:1523:LEU:N	0.49	2.75	6	1
1:A:773:ILE:HD12	1:A:773:ILE:H	0.48	1.66	5	1
1:A:1523:LEU:N	1:A:1523:LEU:HD22	0.48	2.23	6	1
1:A:770:LEU:C	1:A:770:LEU:CD2	0.48	2.82	7	1
1:A:1530:ILE:N	1:A:1530:ILE:HD12	0.48	2.22	1	1
1:A:773:ILE:N	1:A:773:ILE:CD1	0.48	2.73	5	1
1:A:772:ARG:NH1	1:A:1524:GLN:CD	0.48	2.66	1	1
1:A:1524:GLN:O	1:A:1528:ASN:ND2	0.48	2.46	3	1
1:A:1552:LYS:CD	1:A:1552:LYS:H	0.48	2.20	7	1
1:A:1528:ASN:N	1:A:1528:ASN:OD1	0.48	2.46	3	2
1:A:765:ILE:CG2	1:A:770:LEU:HD23	0.47	2.38	5	1
1:A:1503:TYR:C	1:A:1505:ASP:N	0.47	2.68	4	1
1:A:763:VAL:O	1:A:1544:ASP:CB	0.47	2.62	10	2
1:A:1522:ILE:O	1:A:1525:GLN:N	0.47	2.44	9	3
1:A:1533:THR:O	1:A:1534:GLY:O	0.47	2.31	1	1
1:A:1518:ARG:HE	1:A:1518:ARG:H	0.47	1.53	4	1
1:A:767:LEU:C	1:A:769:LEU:N	0.47	2.68	9	3
1:A:1502:ALA:C	1:A:1504:LEU:N	0.46	2.69	5	2
1:A:771:SER:OG	1:A:1524:GLN:N	0.46	2.48	6	1
1:A:1517:LEU:N	1:A:1517:LEU:CD2	0.46	2.79	7	1
1:A:767:LEU:HD13	1:A:767:LEU:O	0.46	2.10	10	2
1:A:1518:ARG:N	1:A:1518:ARG:CD	0.46	2.78	4	1
1:A:1543:PHE:CD2	1:A:1543:PHE:O	0.46	2.68	2	1
1:A:1517:LEU:HD13	1:A:1518:ARG:N	0.46	2.26	10	1
1:A:1530:ILE:O	1:A:1533:THR:N	0.46	2.41	1	1
1:A:1518:ARG:C	1:A:1520:ARG:N	0.46	2.69	8	1
1:A:1519:GLU:O	1:A:1520:ARG:O	0.45	2.34	8	2
1:A:1520:ARG:C	1:A:1522:ILE:H	0.45	2.15	4	3
1:A:1536:PHE:CE1	1:A:1545:PHE:CB	0.45	3.00	5	1
1:A:773:ILE:O	1:A:774:PRO:O	0.45	2.35	7	2
1:A:767:LEU:C	1:A:769:LEU:H	0.45	2.14	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1502:ALA:O	1:A:1505:ASP:OD2	0.45	2.35	5	1
1:A:1520:ARG:O	1:A:1521:HIS:O	0.45	2.35	5	1
1:A:1510:LEU:O	1:A:1511:HIS:C	0.45	2.55	5	3
1:A:1518:ARG:O	1:A:1520:ARG:N	0.44	2.50	8	1
1:A:1515:MET:SD	1:A:1515:MET:C	0.44	2.96	5	1
1:A:1556:ARG:O	1:A:1560:SER:OG	0.44	2.36	7	2
1:A:1515:MET:O	1:A:1516:THR:OG1	0.44	2.36	2	1
1:A:765:ILE:O	1:A:766:THR:O	0.44	2.36	5	1
1:A:1559:GLN:HA	1:A:1562:LEU:HD12	0.43	1.88	2	1
1:A:1541:THR:O	1:A:1542:THR:OG1	0.43	2.36	3	2
1:A:772:ARG:CZ	1:A:1524:GLN:CD	0.43	2.87	1	1
1:A:1532:GLU:O	1:A:1533:THR:O	0.43	2.36	6	2
1:A:1520:ARG:C	1:A:1521:HIS:CG	0.43	2.91	7	2
1:A:1502:ALA:O	1:A:1505:ASP:OD1	0.43	2.37	7	3
1:A:1543:PHE:CD1	1:A:1543:PHE:C	0.43	2.92	8	1
1:A:770:LEU:HD11	1:A:773:ILE:HG13	0.43	1.91	4	1
1:A:1557:LYS:O	1:A:1560:SER:OG	0.43	2.33	6	1
1:A:1523:LEU:O	1:A:1527:VAL:HG23	0.43	2.14	5	1
1:A:767:LEU:O	1:A:769:LEU:N	0.43	2.52	9	1
1:A:1543:PHE:CD1	1:A:1543:PHE:O	0.43	2.72	9	1
1:A:1530:ILE:O	1:A:1533:THR:CG2	0.42	2.66	5	1
1:A:770:LEU:O	1:A:1524:GLN:OE1	0.42	2.37	4	1
1:A:1545:PHE:N	1:A:1545:PHE:CD1	0.42	2.87	5	1
1:A:764:LYS:CB	1:A:764:LYS:NZ	0.42	2.82	9	1
1:A:1516:THR:OG1	1:A:1516:THR:O	0.42	2.38	2	1
1:A:1559:GLN:O	1:A:1563:GLU:OE2	0.42	2.37	3	1
1:A:1517:LEU:C	1:A:1517:LEU:CD1	0.42	2.88	4	1
1:A:1521:HIS:C	1:A:1523:LEU:H	0.42	2.15	5	1
1:A:1563:GLU:CD	1:A:1563:GLU:N	0.42	2.72	5	1
1:A:770:LEU:CD2	1:A:771:SER:N	0.42	2.81	4	1
1:A:1502:ALA:O	1:A:1505:ASP:N	0.42	2.46	5	1
1:A:1512:ARG:C	1:A:1514:LEU:H	0.42	2.17	10	1
1:A:768:ASP:OD1	1:A:768:ASP:N	0.42	2.52	9	2
1:A:1528:ASN:N	1:A:1528:ASN:ND2	0.42	2.66	8	1
1:A:1559:GLN:O	1:A:1559:GLN:OE1	0.41	2.38	4	1
1:A:1513:ARG:O	1:A:1516:THR:OG1	0.41	2.38	10	1
1:A:1518:ARG:O	1:A:1519:GLU:O	0.41	2.38	7	1
1:A:770:LEU:O	1:A:771:SER:OG	0.41	2.38	9	1
1:A:765:ILE:O	1:A:766:THR:C	0.41	2.58	1	1
1:A:1539:THR:OG1	1:A:1542:THR:O	0.41	2.35	2	2
1:A:1533:THR:C	1:A:1534:GLY:O	0.41	2.58	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1542:THR:HG22	1:A:1543:PHE:N	0.41	2.30	1	1
1:A:1511:HIS:O	1:A:1511:HIS:ND1	0.41	2.54	4	1
1:A:1537:HIS:C	1:A:1538:ILE:HD12	0.41	2.36	5	1
1:A:1524:GLN:N	1:A:1524:GLN:NE2	0.41	2.67	7	1
1:A:1517:LEU:HD12	1:A:1517:LEU:O	0.41	2.15	4	1
1:A:1528:ASN:O	1:A:1532:GLU:OE1	0.41	2.39	8	1
1:A:1526:ILE:O	1:A:1526:ILE:CG2	0.41	2.68	10	1
1:A:765:ILE:N	1:A:765:ILE:CD1	0.41	2.83	2	2
1:A:1510:LEU:O	1:A:1512:ARG:N	0.41	2.53	5	1
1:A:770:LEU:N	1:A:770:LEU:CD1	0.41	2.84	7	1
1:A:1511:HIS:ND1	1:A:1511:HIS:N	0.40	2.69	1	1
1:A:1561:TYR:C	1:A:1563:GLU:N	0.40	2.74	1	1
1:A:1530:ILE:O	1:A:1533:THR:O	0.40	2.40	1	1
1:A:770:LEU:HD12	1:A:772:ARG:O	0.40	2.17	5	1
1:A:1506:GLU:CD	1:A:1506:GLU:N	0.40	2.74	9	1
1:A:1540:ASN:HD22	1:A:1540:ASN:N	0.40	2.13	10	1
1:A:1561:TYR:C	1:A:1563:GLU:H	0.40	2.20	1	1
1:A:1547:LEU:H	1:A:1547:LEU:HD12	0.40	1.76	3	1
1:A:1536:PHE:CD1	1:A:1536:PHE:N	0.40	2.90	6	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	77/125 (62%)	57±2 (74±3%)	13±3 (17±4%)	6±2 (8±3%)	2	13
All	All	770/1250 (62%)	573 (74%)	134 (17%)	63 (8%)	2	13

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	1533	THR	7
1	A	1513	ARG	5
1	A	760	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	1502	ALA	4
1	A	1520	ARG	4
1	A	1518	ARG	4
1	A	1519	GLU	4
1	A	1534	GLY	3
1	A	1517	LEU	3
1	A	1563	GLU	3
1	A	771	SER	3
1	A	1503	TYR	2
1	A	1535	HIS	2
1	A	1515	MET	2
1	A	1521	HIS	2
1	A	766	THR	2
1	A	774	PRO	2
1	A	1560	SER	2
1	A	1504	LEU	1
1	A	1511	HIS	1
1	A	1516	THR	1
1	A	1522	ILE	1
1	A	1551	ASP	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	75/119 (63%)	66±3 (89±4%)	9±3 (11±4%)	9	52	
All	All	750/1190 (63%)	664 (89%)	86 (11%)	9	52	

All 36 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	1539	THR	10
1	A	1543	PHE	9
1	A	764	LYS	6
1	A	1561	TYR	6
1	A	767	LEU	5

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Mol	Chain	Res	Type	Models (Total)
1	A	770	LEU	5
1	A	1547	LEU	3
1	A	1552	LYS	3
1	A	768	ASP	3
1	A	761	LEU	3
1	A	773	ILE	3
1	A	1562	LEU	3
1	A	1559	GLN	2
1	A	1520	ARG	2
1	A	772	ARG	2
1	A	1533	THR	1
1	A	1546	ASP	1
1	A	1563	GLU	1
1	A	1504	LEU	1
1	A	1507	LEU	1
1	A	1518	ARG	1
1	A	766	THR	1
1	A	1515	MET	1
1	A	1535	HIS	1
1	A	1536	PHE	1
1	A	1524	GLN	1
1	A	1556	ARG	1
1	A	1512	ARG	1
1	A	1528	ASN	1
1	A	1503	TYR	1
1	A	1523	LEU	1
1	A	1542	THR	1
1	A	1505	ASP	1
1	A	1510	LEU	1
1	A	1517	LEU	1
1	A	1540	ASN	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 monosaccharides 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 72% for the entire structure.

7.1 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *shiftFile_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	1285
Number of shifts mapped to atoms	1285
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	114	-0.18 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	0.18 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	98	-0.47 ± 0.10	None needed (< 0.5 ppm)
^{15}N	104	-0.15 ± 0.33	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 86%, i.e. 997 atoms were assigned a chemical shift out of a possible 1153. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	378/384 (98%)	153/154 (99%)	150/154 (97%)	75/76 (99%)
Sidechain	587/689 (85%)	407/450 (90%)	177/213 (83%)	3/26 (12%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	32/80 (40%)	27/39 (69%)	5/33 (15%)	0/8 (0%)
Overall	997/1153 (86%)	587/643 (91%)	332/400 (83%)	78/110 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1285 atoms were assigned a chemical shift out of a possible 1785. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	525/610 (86%)	209/245 (85%)	212/250 (85%)	104/115 (90%)
Sidechain	728/1095 (66%)	495/711 (70%)	229/340 (67%)	4/44 (9%)
Aromatic	32/80 (40%)	27/39 (69%)	5/33 (15%)	0/8 (0%)
Overall	1285/1785 (72%)	731/995 (73%)	446/623 (72%)	108/167 (65%)

7.1.4 Statistically unusual chemical shifts [i](#)

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
2	A	1512	ARG	NE	94.69	76.53 – 92.65	6.3

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. 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:

