



Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 6MWM
Title : Bat coronavirus HKU4 SUD-C
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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 : 2.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

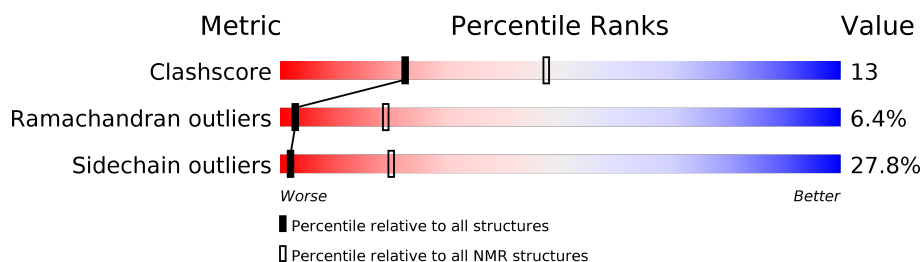
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 67%.

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	81	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:1445-A:1518 (74)	0.26	3

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

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

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

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1258 atoms, of which 617 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Non-structural protein 3.

Mol	Chain	Residues	Atoms						Trace
1	A	81	Total	C	H	N	O	S	0
			1258	409	617	109	119	4	

There are 3 discrepancies between the modelled and reference sequences:

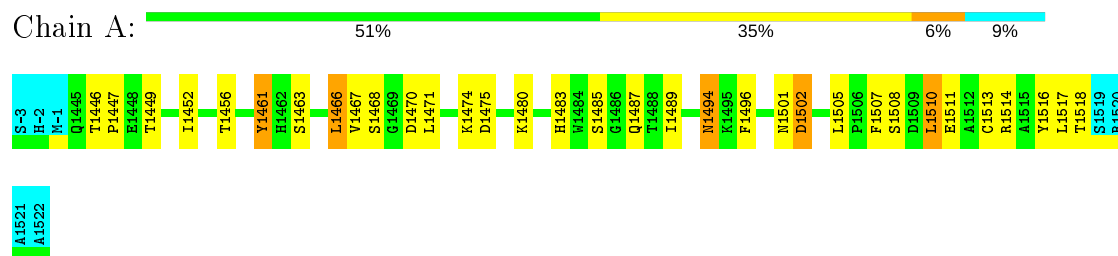
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP P0C6W3
A	-2	HIS	-	expression tag	UNP P0C6W3
A	-1	MET	-	expression tag	UNP P0C6W3

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: Non-structural protein 3

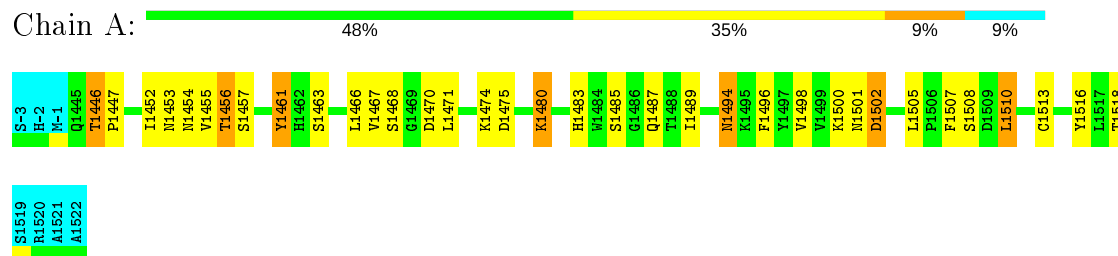


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

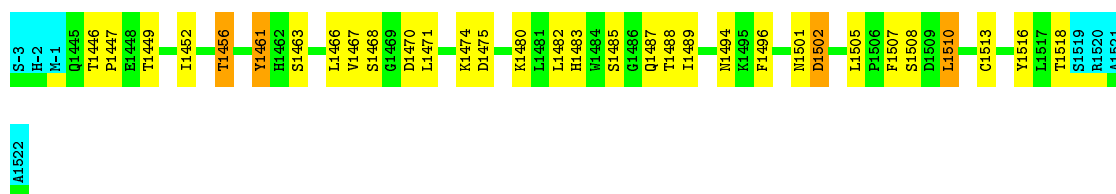
- Molecule 1: Non-structural protein 3



4.2.2 Score per residue for model 2

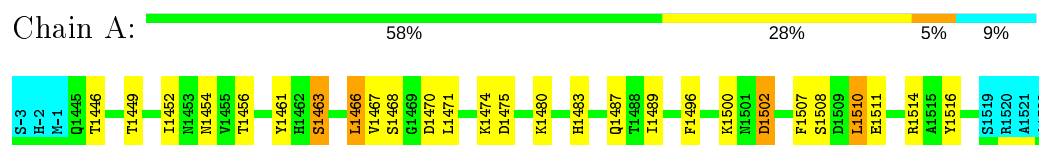
- Molecule 1: Non-structural protein 3





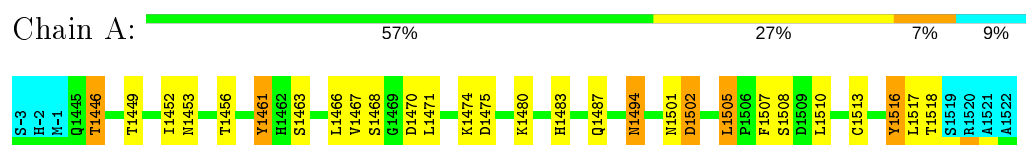
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Non-structural protein 3



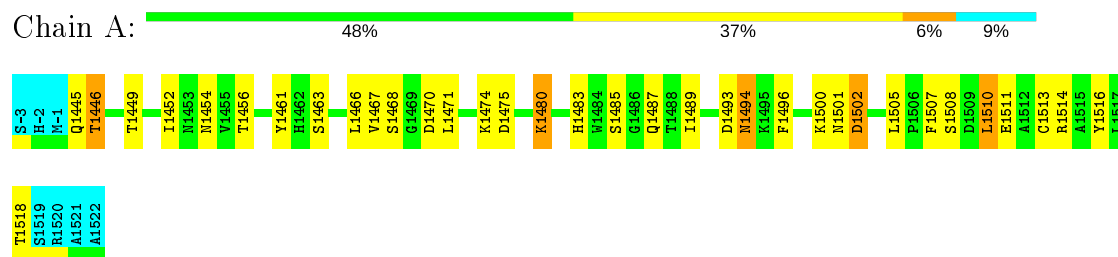
4.2.4 Score per residue for model 4

- Molecule 1: Non-structural protein 3



4.2.5 Score per residue for model 5

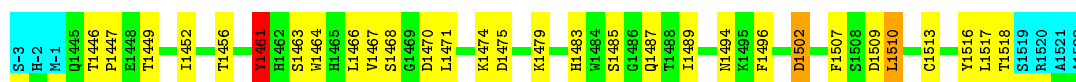
- Molecule 1: Non-structural protein 3



4.2.6 Score per residue for model 6

- Molecule 1: Non-structural protein 3

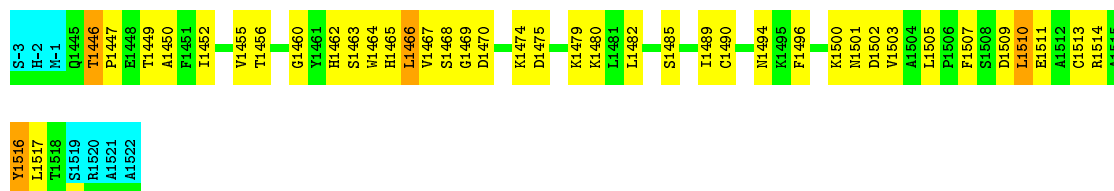




4.2.7 Score per residue for model 7

- Molecule 1: Non-structural protein 3

Chain A: 42% 44% 5% 9%



4.2.8 Score per residue for model 8

- Molecule 1: Non-structural protein 3

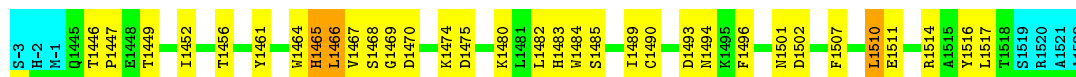
Chain A: 53% 30% 7% 9%



4.2.9 Score per residue for model 9

- Molecule 1: Non-structural protein 3

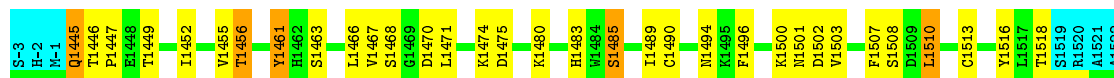
Chain A: 51% 37% 9%



4.2.10 Score per residue for model 10

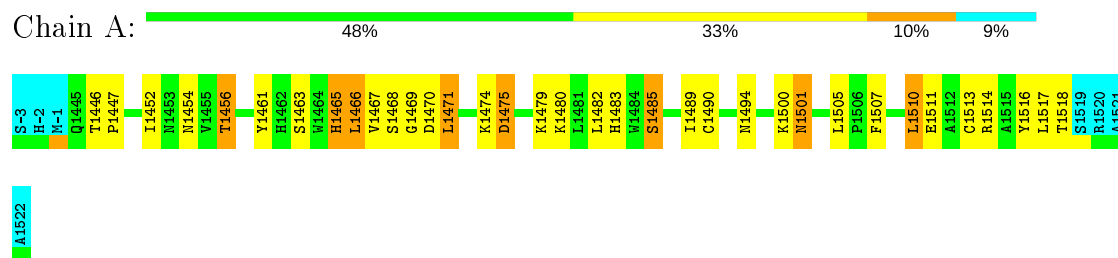
- Molecule 1: Non-structural protein 3

Chain A: 51% 35% 6% 9%



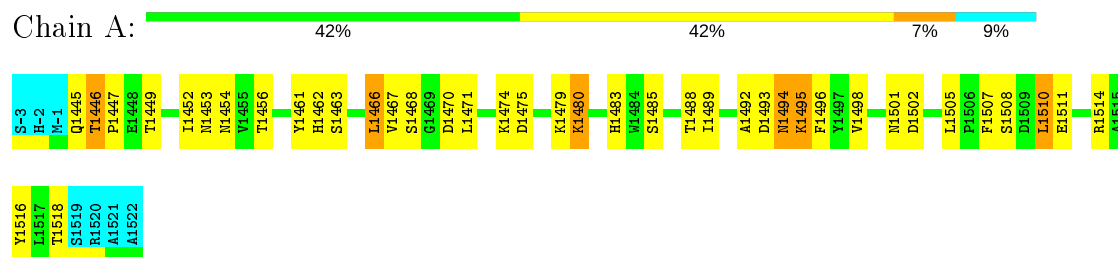
4.2.11 Score per residue for model 11

- Molecule 1: Non-structural protein 3



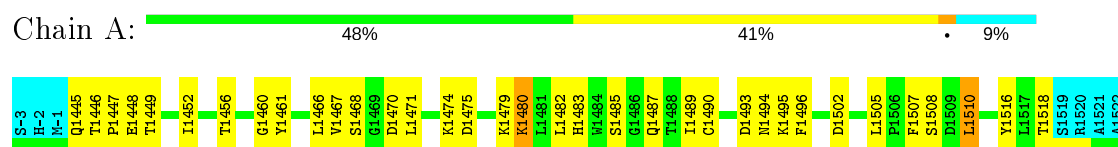
4.2.12 Score per residue for model 12

- Molecule 1: Non-structural protein 3



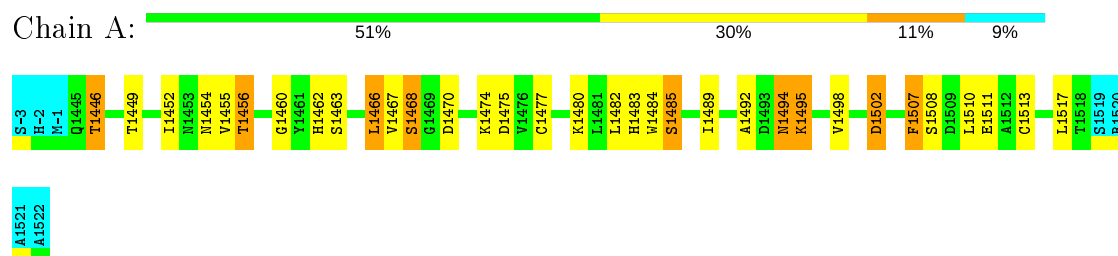
4.2.13 Score per residue for model 13

- Molecule 1: Non-structural protein 3



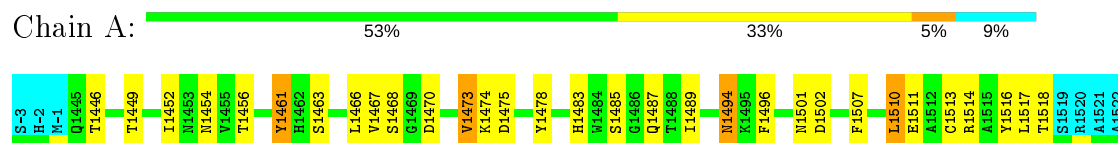
4.2.14 Score per residue for model 14

- Molecule 1: Non-structural protein 3



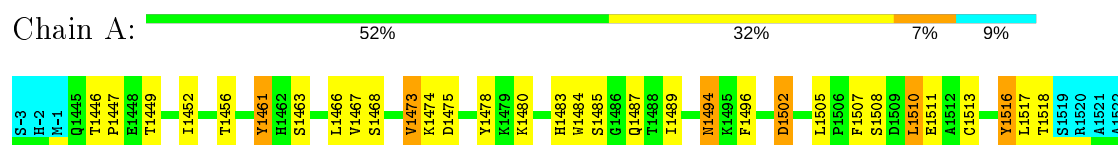
4.2.15 Score per residue for model 15

- Molecule 1: Non-structural protein 3



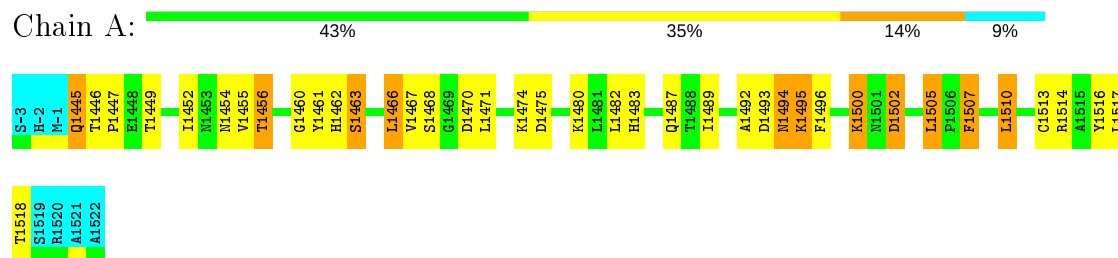
4.2.16 Score per residue for model 16

- Molecule 1: Non-structural protein 3



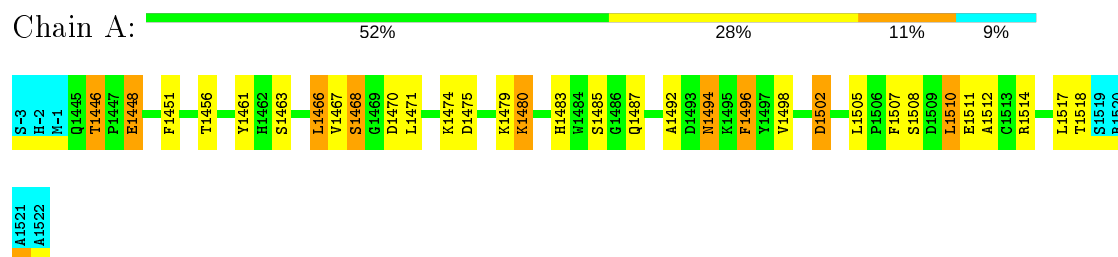
4.2.17 Score per residue for model 17

- Molecule 1: Non-structural protein 3



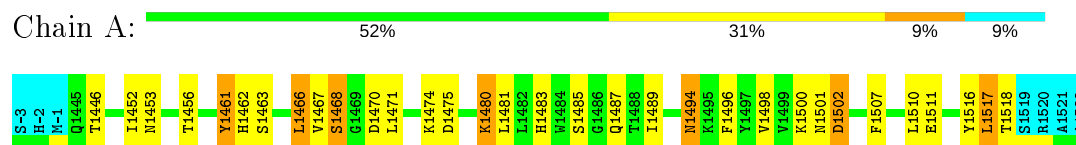
4.2.18 Score per residue for model 18

- Molecule 1: Non-structural protein 3



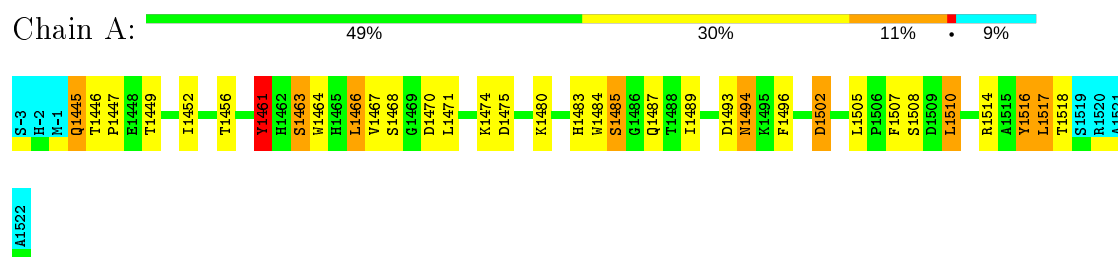
4.2.19 Score per residue for model 19

- Molecule 1: Non-structural protein 3



4.2.20 Score per residue for model 20

- Molecule 1: Non-structural protein 3



5 Refinement protocol and experimental data overview

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

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CYANA	refinement	
CYANA	structure calculation	

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	944
Number of shifts mapped to atoms	625
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	319
Assignment completeness (well-defined parts)	67%

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	590	568	568	15±3
All	All	11800	11360	11360	295

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1456:THR:HG22	1:A:1466:LEU:HD13	0.88	1.46	2	3
1:A:1456:THR:HG22	1:A:1466:LEU:HD23	0.79	1.53	11	15
1:A:1456:THR:CG2	1:A:1466:LEU:HD23	0.69	2.17	20	15
1:A:1456:THR:HG23	1:A:1466:LEU:HD23	0.69	1.63	19	2
1:A:1498:VAL:HG11	1:A:1516:TYR:CE1	0.67	2.24	19	1
1:A:1467:VAL:HG23	1:A:1480:LYS:O	0.67	1.90	7	15
1:A:1466:LEU:HD22	1:A:1467:VAL:N	0.66	2.06	20	17
1:A:1492:ALA:HB3	1:A:1495:LYS:HG2	0.65	1.68	17	3
1:A:1489:ILE:HG23	1:A:1496:PHE:CE2	0.64	2.28	17	9
1:A:1489:ILE:HG23	1:A:1496:PHE:CE1	0.63	2.28	15	6
1:A:1456:THR:HG22	1:A:1466:LEU:CD1	0.62	2.22	2	3
1:A:1505:LEU:HD22	1:A:1516:TYR:OH	0.62	1.95	16	4
1:A:1464:TRP:CB	1:A:1482:LEU:HD22	0.61	2.24	7	1
1:A:1465:HIS:O	1:A:1482:LEU:HD23	0.60	1.96	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1456:THR:O	1:A:1466:LEU:HD22	0.60	1.96	2	3
1:A:1498:VAL:HG11	1:A:1516:TYR:CZ	0.59	2.32	19	1
1:A:1447:PRO:O	1:A:1510:LEU:HD11	0.59	1.98	20	13
1:A:1467:VAL:HG21	1:A:1483:HIS:HB2	0.57	1.75	16	14
1:A:1510:LEU:HD23	1:A:1514:ARG:HD3	0.57	1.77	12	3
1:A:1467:VAL:HG21	1:A:1483:HIS:HB3	0.56	1.77	17	1
1:A:1452:ILE:HD11	1:A:1513:CYS:SG	0.56	2.40	2	13
1:A:1446:THR:HG21	1:A:1494:ASN:HA	0.56	1.78	5	4
1:A:1500:LYS:HD3	1:A:1505:LEU:HD12	0.55	1.78	1	1
1:A:1449:THR:HA	1:A:1452:ILE:HD12	0.55	1.78	13	12
1:A:1455:VAL:HG12	1:A:1460:GLY:O	0.54	2.03	7	3
1:A:1492:ALA:HB3	1:A:1495:LYS:CG	0.53	2.33	12	2
1:A:1473:VAL:HG12	1:A:1478:TYR:HE2	0.53	1.63	16	1
1:A:1483:HIS:CD2	1:A:1488:THR:HG23	0.53	2.39	2	2
1:A:1466:LEU:HD13	1:A:1466:LEU:O	0.53	2.03	20	8
1:A:1466:LEU:HD13	1:A:1466:LEU:C	0.53	2.24	20	10
1:A:1510:LEU:HD23	1:A:1514:ARG:NE	0.53	2.19	15	3
1:A:1448:GLU:HA	1:A:1510:LEU:HD12	0.52	1.81	18	1
1:A:1461:TYR:CD2	1:A:1517:LEU:HD13	0.52	2.39	8	5
1:A:1473:VAL:HG12	1:A:1478:TYR:HE1	0.52	1.63	15	1
1:A:1500:LYS:HB2	1:A:1503:VAL:HG12	0.51	1.81	10	2
1:A:1466:LEU:C	1:A:1466:LEU:HD13	0.51	2.27	17	7
1:A:1466:LEU:O	1:A:1466:LEU:HD13	0.50	2.07	19	7
1:A:1517:LEU:HD22	1:A:1517:LEU:H	0.50	1.67	19	1
1:A:1452:ILE:HG22	1:A:1456:THR:OG1	0.50	2.07	11	9
1:A:1517:LEU:N	1:A:1517:LEU:CD2	0.50	2.74	20	1
1:A:1517:LEU:N	1:A:1517:LEU:HD22	0.49	2.22	19	1
1:A:1510:LEU:HD23	1:A:1514:ARG:CD	0.48	2.39	11	4
1:A:1464:TRP:CE2	1:A:1517:LEU:HD23	0.48	2.43	8	3
1:A:1456:THR:HG22	1:A:1466:LEU:CD2	0.48	2.37	7	2
1:A:1461:TYR:CD2	1:A:1517:LEU:HD12	0.48	2.43	20	1
1:A:1461:TYR:CD1	1:A:1517:LEU:HD13	0.48	2.44	16	1
1:A:1517:LEU:N	1:A:1517:LEU:HD13	0.48	2.24	19	1
1:A:1494:ASN:O	1:A:1494:ASN:CG	0.48	2.53	14	1
1:A:1516:TYR:C	1:A:1517:LEU:HD13	0.47	2.29	19	1
1:A:1446:THR:O	1:A:1450:ALA:HB2	0.47	2.09	7	1
1:A:1445:GLN:HE21	1:A:1449:THR:HG23	0.47	1.69	10	4
1:A:1489:ILE:CD1	1:A:1517:LEU:HD21	0.47	2.39	14	3
1:A:1464:TRP:HB3	1:A:1482:LEU:HD22	0.46	1.87	7	1
1:A:1466:LEU:HA	1:A:1482:LEU:HD23	0.45	1.88	17	1
1:A:1496:PHE:CD2	1:A:1496:PHE:C	0.45	2.90	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1452:ILE:HD13	1:A:1481:LEU:HD23	0.45	1.89	19	1
1:A:1498:VAL:O	1:A:1498:VAL:HG13	0.44	2.12	18	3
1:A:1467:VAL:HG11	1:A:1483:HIS:HB3	0.44	1.88	18	2
1:A:1510:LEU:HD23	1:A:1514:ARG:HD2	0.44	1.89	17	3
1:A:1464:TRP:HB2	1:A:1482:LEU:HD22	0.44	1.86	7	1
1:A:1456:THR:HG23	1:A:1482:LEU:HD21	0.43	1.88	14	2
1:A:1489:ILE:HG23	1:A:1496:PHE:HE2	0.43	1.73	9	5
1:A:1445:GLN:HE22	1:A:1453:ASN:ND2	0.43	2.11	12	1
1:A:1500:LYS:HD2	1:A:1505:LEU:HD12	0.43	1.90	17	1
1:A:1471:LEU:HD22	1:A:1490:CYS:SG	0.43	2.53	11	1
1:A:1484:TRP:C	1:A:1484:TRP:CD1	0.43	2.91	16	1
1:A:1455:VAL:HG11	1:A:1461:TYR:HA	0.43	1.91	10	2
1:A:1498:VAL:HG13	1:A:1498:VAL:O	0.42	2.14	1	1
1:A:1484:TRP:O	1:A:1484:TRP:CG	0.42	2.71	9	1
1:A:1466:LEU:HD12	1:A:1467:VAL:N	0.42	2.29	1	2
1:A:1489:ILE:HG23	1:A:1496:PHE:HE1	0.42	1.75	13	3
1:A:1446:THR:OG1	1:A:1449:THR:HG22	0.42	2.14	7	1
1:A:1464:TRP:CD1	1:A:1517:LEU:HD13	0.42	2.50	20	1
1:A:1460:GLY:HA2	1:A:1482:LEU:HD21	0.42	1.91	13	1
1:A:1501:ASN:ND2	1:A:1501:ASN:H	0.41	2.13	11	1
1:A:1446:THR:HG21	1:A:1494:ASN:ND2	0.41	2.31	12	1
1:A:1445:GLN:NE2	1:A:1449:THR:HG23	0.41	2.30	5	1
1:A:1484:TRP:CD1	1:A:1484:TRP:C	0.41	2.94	20	1
1:A:1507:PHE:CD2	1:A:1512:ALA:CB	0.41	3.04	18	1
1:A:1466:LEU:HD22	1:A:1466:LEU:C	0.41	2.37	20	1
1:A:1475:ASP:O	1:A:1475:ASP:CG	0.40	2.59	11	1
1:A:1451:PHE:CZ	1:A:1517:LEU:HD12	0.40	2.51	18	1
1:A:1461:TYR:CD2	1:A:1517:LEU:CG	0.40	3.05	20	1
1:A:1501:ASN:H	1:A:1501:ASN:ND2	0.40	2.13	7	1
1:A:1446:THR:HG21	1:A:1492:ALA:O	0.40	2.16	18	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	74/81 (91%)	57±2 (76±2%)	13±2 (17±3%)	5±1 (6±2%)	3	19
All	All	1480/1620 (91%)	1132 (76%)	253 (17%)	95 (6%)	3	19

All 12 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	1468	SER	20
1	A	1502	ASP	19
1	A	1470	ASP	16
1	A	1485	SER	13
1	A	1494	ASN	7
1	A	1462	HIS	5
1	A	1461	TYR	5
1	A	1469	GLY	3
1	A	1445	GLN	3
1	A	1507	PHE	2
1	A	1477	CYS	1
1	A	1471	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	65/70 (93%)	47±2 (72±4%)	18±2 (28±4%)	2	20
All	All	1300/1400 (93%)	939 (72%)	361 (28%)	2	20

All 39 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	1446	THR	20
1	A	1474	LYS	20
1	A	1510	LEU	20
1	A	1475	ASP	20
1	A	1494	ASN	19
1	A	1507	PHE	19

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Mol	Chain	Res	Type	Models (Total)
1	A	1516	TYR	17
1	A	1461	TYR	17
1	A	1463	SER	17
1	A	1518	THR	15
1	A	1471	LEU	14
1	A	1502	ASP	13
1	A	1508	SER	13
1	A	1487	GLN	13
1	A	1511	GLU	12
1	A	1466	LEU	11
1	A	1501	ASN	10
1	A	1485	SER	9
1	A	1454	ASN	9
1	A	1480	LYS	8
1	A	1505	LEU	8
1	A	1479	LYS	7
1	A	1456	THR	6
1	A	1493	ASP	6
1	A	1500	LYS	5
1	A	1468	SER	4
1	A	1490	CYS	4
1	A	1495	LYS	4
1	A	1453	ASN	3
1	A	1470	ASP	3
1	A	1473	VAL	2
1	A	1465	HIS	2
1	A	1448	GLU	2
1	A	1509	ASP	2
1	A	1517	LEU	2
1	A	1483	HIS	2
1	A	1496	PHE	1
1	A	1457	SER	1
1	A	1449	THR	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 67% for the well-defined parts and 63% 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	944
Number of shifts mapped to atoms	625
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	319
Number of shift outliers (ShiftChecker)	3

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atoms found in structure. All 319 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1510	LEU	3HB	1.313	0.0	1
A	1447	PRO	2HD	3.84	0.0	1
A	1467	VAL	1HG2	0.694	0.0	1
A	1516	TYR	3HB	3.005	0.0	1
A	1480	LYS	2HG	1.05	0.0	1
A	1472	ILE	1HG2	0.585	0.0	1
A	1481	LEU	2HD2	0.797	0.0	1
A	1448	GLU	2HG	2.146	0.0	1
A	1505	LEU	3HB	1.497	0.0	1
A	1445	GLN	2HB	2.05	0.0	1
A	1512	ALA	3HB	1.574	0.0	1
A	1519	SER	2HB	3.822	0.0	1
A	1489	ILE	1HD1	0.529	0.0	1
A	1512	ALA	2HB	1.574	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1510	LEU	3HD2	0.409	0.0	1
A	1456	THR	2HG2	1.19	0.0	1
A	1489	ILE	2HG1	0.74	0.0	1
A	1488	THR	1HG2	1.27	0.0	1
A	1445	GLN	2HE2	6.779	0.0	1
A	1475	ASP	2HB	2.726	0.0	1
A	1503	VAL	2HG1	0.852	0.0	1
A	1517	LEU	1HD2	0.08	0.0	1
A	1452	ILE	2HG1	0.624	0.0	1
A	1452	ILE	3HG2	0.687	0.0	1
A	1521	ALA	2HB	1.095	0.0	1
A	1480	LYS	2HE	2.698	0.0	1
A	1504	ALA	2HB	0.61	0.0	1
A	1467	VAL	2HG2	0.694	0.0	1
A	1512	ALA	1HB	1.574	0.0	1
A	1510	LEU	1HD1	0.832	0.0	1
A	1463	SER	3HB	2.846	0.0	1
A	1468	SER	2HB	3.728	0.0	1
A	1489	ILE	2HD1	0.529	0.0	1
A	1500	LYS	3HD	1.546	0.0	1
A	1474	LYS	2HG	1.472	0.0	1
A	1481	LEU	2HD1	0.797	0.0	1
A	1451	PHE	3HB	2.972	0.0	1
A	1479	LYS	2HE	2.828	0.0	1
A	1467	VAL	3HG2	0.694	0.0	1
A	1472	ILE	2HG1	1.392	0.0	1
A	1446	THR	1HG2	1.297	0.0	1
A	1474	LYS	3HD	1.679	0.0	1
A	1505	LEU	1HD1	0.753	0.0	1
A	1474	LYS	3HB	1.777	0.0	1
A	1488	THR	2HG2	1.27	0.0	1
A	1482	LEU	2HD2	0.56	0.0	1
A	1466	LEU	3HD2	1.092	0.0	1
A	1514	ARG	3HB	1.306	0.0	1
A	1460	GLY	3HA	4.853	0.0	1
A	1490	CYS	2HB	2.729	0.0	1
A	1520	ARG	3HD	2.805	0.0	1
A	1445	GLN	2HG	2.302	0.0	1
A	1487	GLN	2HB	2.414	0.0	1
A	1505	LEU	3HD2	0.687	0.0	1
A	1476	VAL	3HG2	-0.04	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1493	ASP	2HB	2.857	0.0	1
A	1489	ILE	3HD1	0.529	0.0	1
A	1480	LYS	3HG	1.29	0.0	1
A	1503	VAL	2HG2	0.808	0.0	1
A	1511	GLU	3HB	1.82	0.0	1
A	1450	ALA	3HB	1.367	0.0	1
A	1467	VAL	2HG1	0.946	0.0	1
A	1476	VAL	3HG1	0.716	0.0	1
A	1453	ASN	3HB	2.781	0.0	1
A	1510	LEU	2HD1	0.832	0.0	1
A	1466	LEU	1HD1	1.036	0.0	1
A	1480	LYS	2HD	1.42	0.0	1
A	1473	VAL	3HG1	0.644	0.0	1
A	1500	LYS	3HG	1.274	0.0	1
A	1482	LEU	1HD1	0.786	0.0	1
A	1491	TYR	3HB	2.442	0.0	1
A	1476	VAL	2HG2	-0.04	0.0	1
A	1481	LEU	2HB	1.74	0.0	1
A	1448	GLU	3HG	2.839	0.0	1
A	1494	ASN	2HD2	7.481	0.0	1
A	1489	ILE	3HG2	1.018	0.0	1
A	1474	LYS	3HG	1.393	0.0	1
A	1472	ILE	1HD1	0.717	0.0	1
A	1492	ALA	3HB	1.217	0.0	1
A	1487	GLN	2HE2	7.641	0.0	1
A	1491	TYR	2HB	2.329	0.0	1
A	1471	LEU	3HD2	0.685	0.0	1
A	1482	LEU	3HD1	0.786	0.0	1
A	1520	ARG	2HG	1.314	0.0	1
A	1495	LYS	2HD	1.643	0.0	1
A	1498	VAL	3HG1	0.964	0.0	1
A	1466	LEU	3HD1	1.036	0.0	1
A	1487	GLN	3HB	2.248	0.0	1
A	1494	ASN	2HB	2.848	0.0	1
A	1447	PRO	2HG	1.944	0.0	1
A	1506	PRO	3HG	2.019	0.0	1
A	1479	LYS	2HG	1.231	0.0	1
A	1453	ASN	2HB	2.781	0.0	1
A	1511	GLU	2HG	2.143	0.0	1
A	1460	GLY	2HA	3.23	0.0	1
A	1509	ASP	2HB	3.085	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1487	GLN	3HG	2.148	0.0	1
A	1505	LEU	1HD2	0.687	0.0	1
A	1472	ILE	3HD1	0.717	0.0	1
A	1516	TYR	2HB	3.005	0.0	1
A	1502	ASP	3HB	2.715	0.0	1
A	1505	LEU	3HD1	0.753	0.0	1
A	1489	ILE	1HG2	1.018	0.0	1
A	1506	PRO	2HG	1.944	0.0	1
A	1471	LEU	1HD2	0.685	0.0	1
A	1478	TYR	3HB	2.402	0.0	1
A	1494	ASN	3HB	2.886	0.0	1
A	1499	VAL	2HG1	0.384	0.0	1
A	1511	GLU	3HG	2.143	0.0	1
A	1452	ILE	2HD1	0.07	0.0	1
A	1494	ASN	1HD2	6.672	0.0	1
A	1501	ASN	2HD2	6.873	0.0	1
A	1503	VAL	1HG2	0.808	0.0	1
A	1449	THR	3HG2	1.165	0.0	1
A	1504	ALA	1HB	0.61	0.0	1
A	1471	LEU	3HB	1.073	0.0	1
A	1481	LEU	1HD1	0.797	0.0	1
A	1462	HIS	2HB	3.198	0.0	1
A	1486	GLY	3HA	4.133	0.0	1
A	1502	ASP	2HB	2.811	0.0	1
A	1445	GLN	3HG	2.302	0.0	1
A	1489	ILE	3HG1	1.54	0.0	1
A	1518	THR	3HG2	0.98	0.0	1
A	1455	VAL	1HG2	0.37	0.0	1
A	1446	THR	3HG2	1.297	0.0	1
A	1484	TRP	3HB	1.014	0.0	1
A	1481	LEU	3HD1	0.797	0.0	1
A	1456	THR	3HG2	1.19	0.0	1
A	1448	GLU	3HB	1.847	0.0	1
A	1499	VAL	3HG1	0.384	0.0	1
A	1447	PRO	3HD	3.894	0.0	1
A	1492	ALA	2HB	1.217	0.0	1
A	1499	VAL	2HG2	0.622	0.0	1
A	1479	LYS	3HB	0.625	0.0	1
A	1458	ASN	2HB	2.871	0.0	1
A	1473	VAL	2HG1	0.644	0.0	1
A	1482	LEU	2HB	1.919	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1501	ASN	2HB	2.923	0.0	1
A	1514	ARG	2HG	1.036	0.0	1
A	1471	LEU	3HD1	0.812	0.0	1
A	1490	CYS	3HB	2.334	0.0	1
A	1520	ARG	2HD	2.805	0.0	1
A	1499	VAL	1HG2	0.622	0.0	1
A	1471	LEU	2HD1	0.812	0.0	1
A	1461	TYR	2HB	2.682	0.0	1
A	1465	HIS	3HB	3.403	0.0	1
A	1498	VAL	2HG2	0.428	0.0	1
A	1485	SER	2HB	2.764	0.0	1
A	1477	CYS	2HB	2.396	0.0	1
A	1448	GLU	2HB	2.338	0.0	1
A	1506	PRO	3HD	3.723	0.0	1
A	1521	ALA	3HB	1.095	0.0	1
A	1479	LYS	2HB	1.206	0.0	1
A	1499	VAL	3HG2	0.622	0.0	1
A	1467	VAL	1HG1	0.946	0.0	1
A	1521	ALA	1HB	1.095	0.0	1
A	1517	LEU	1HD1	-0.598	0.0	1
A	1455	VAL	3HG2	0.37	0.0	1
A	1475	ASP	3HB	2.809	0.0	1
A	1453	ASN	2HD2	6.799	0.0	1
A	1500	LYS	3HE	2.867	0.0	1
A	1454	ASN	2HB	2.752	0.0	1
A	1489	ILE	2HG2	1.018	0.0	1
A	1456	THR	1HG2	1.19	0.0	1
A	1505	LEU	2HB	1.265	0.0	1
A	1445	GLN	1HE2	7.445	0.0	1
A	1498	VAL	3HG2	0.428	0.0	1
A	1483	HIS	2HB	3.07	0.0	1
A	1446	THR	2HG2	1.297	0.0	1
A	1464	TRP	3HB	3.174	0.0	1
A	1452	ILE	2HG2	0.687	0.0	1
A	1452	ILE	3HG1	1.807	0.0	1
A	1449	THR	2HG2	1.165	0.0	1
A	1507	PHE	3HB	2.948	0.0	1
A	1445	GLN	3HB	1.931	0.0	1
A	1481	LEU	1HD2	0.797	0.0	1
A	1447	PRO	3HG	2.154	0.0	1
A	1505	LEU	2HD1	0.753	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1476	VAL	1HG1	0.716	0.0	1
A	1474	LYS	2HD	1.679	0.0	1
A	1474	LYS	2HB	1.92	0.0	1
A	1488	THR	3HG2	1.27	0.0	1
A	1469	GLY	3HA	4.533	0.0	1
A	1479	LYS	3HE	2.913	0.0	1
A	1480	LYS	2HB	1.423	0.0	1
A	1498	VAL	2HG1	0.964	0.0	1
A	1514	ARG	2HB	1.533	0.0	1
A	1482	LEU	3HB	1.579	0.0	1
A	1450	ALA	1HB	1.367	0.0	1
A	1510	LEU	1HD2	0.409	0.0	1
A	1459	GLY	2HA	3.672	0.0	1
A	1453	ASN	1HD2	7.43	0.0	1
A	1466	LEU	2HD1	1.036	0.0	1
A	1486	GLY	2HA	3.82	0.0	1
A	1452	ILE	3HD1	0.07	0.0	1
A	1471	LEU	2HB	1.619	0.0	1
A	1449	THR	1HG2	1.165	0.0	1
A	1482	LEU	2HD1	0.786	0.0	1
A	1471	LEU	2HD2	0.685	0.0	1
A	1455	VAL	2HG1	0.37	0.0	1
A	1514	ARG	3HG	0.793	0.0	1
A	1470	ASP	2HB	2.433	0.0	1
A	1493	ASP	3HB	2.544	0.0	1
A	1479	LYS	3HD	1.474	0.0	1
A	1495	LYS	3HG	1.363	0.0	1
A	1515	ALA	1HB	1.331	0.0	1
A	1450	ALA	2HB	1.367	0.0	1
A	1452	ILE	1HD1	0.07	0.0	1
A	1520	ARG	3HB	1.504	0.0	1
A	1519	SER	3HB	3.87	0.0	1
A	1472	ILE	3HG2	0.585	0.0	1
A	1472	ILE	2HG2	0.585	0.0	1
A	1464	TRP	2HB	3.67	0.0	1
A	1480	LYS	3HB	1.423	0.0	1
A	1503	VAL	3HG2	0.808	0.0	1
A	1455	VAL	3HG1	0.37	0.0	1
A	1461	TYR	3HB	2.79	0.0	1
A	1487	GLN	2HG	2.458	0.0	1
A	1517	LEU	3HB	1.014	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1463	SER	2HB	3.07	0.0	1
A	1473	VAL	3HG2	0.729	0.0	1
A	1517	LEU	3HD1	-0.598	0.0	1
A	1515	ALA	2HB	1.331	0.0	1
A	1495	LYS	2HE	2.981	0.0	1
A	1507	PHE	2HB	2.506	0.0	1
A	1480	LYS	3HD	1.352	0.0	1
A	1517	LEU	2HD1	-0.598	0.0	1
A	1458	ASN	1HD2	7.49	0.0	1
A	1495	LYS	2HG	1.42	0.0	1
A	1447	PRO	3HB	1.69	0.0	1
A	1477	CYS	3HB	2.645	0.0	1
A	1478	TYR	2HB	2.66	0.0	1
A	1508	SER	3HB	3.796	0.0	1
A	1517	LEU	2HB	1.78	0.0	1
A	1510	LEU	2HD2	0.409	0.0	1
A	1466	LEU	1HD2	1.092	0.0	1
A	1505	LEU	2HD2	0.687	0.0	1
A	1506	PRO	2HB	1.785	0.0	1
A	1476	VAL	1HG2	-0.04	0.0	1
A	1500	LYS	3HB	1.795	0.0	1
A	1496	PHE	3HB	2.772	0.0	1
A	1474	LYS	2HE	2.998	0.0	1
A	1482	LEU	1HD2	0.56	0.0	1
A	1476	VAL	2HG1	0.716	0.0	1
A	1520	ARG	3HG	1.398	0.0	1
A	1473	VAL	2HG2	0.729	0.0	1
A	1503	VAL	3HG1	0.852	0.0	1
A	1504	ALA	3HB	0.61	0.0	1
A	1468	SER	3HB	3.728	0.0	1
A	1510	LEU	2HB	1.576	0.0	1
A	1466	LEU	2HD2	1.092	0.0	1
A	1481	LEU	3HB	1.532	0.0	1
A	1482	LEU	3HD2	0.56	0.0	1
A	1520	ARG	2HB	1.634	0.0	1
A	1466	LEU	2HB	1.668	0.0	1
A	1451	PHE	2HB	3.05	0.0	1
A	1509	ASP	3HB	2.986	0.0	1
A	1514	ARG	3HD	2.748	0.0	1
A	1485	SER	3HB	1.903	0.0	1
A	1518	THR	1HG2	0.98	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1495	LYS	3HB	1.821	0.0	1
A	1447	PRO	2HB	2.242	0.0	1
A	1458	ASN	2HD2	6.849	0.0	1
A	1506	PRO	3HB	1.478	0.0	1
A	1472	ILE	2HD1	0.717	0.0	1
A	1501	ASN	1HD2	7.569	0.0	1
A	1472	ILE	3HG1	0.932	0.0	1
A	1511	GLU	2HB	1.885	0.0	1
A	1499	VAL	1HG1	0.384	0.0	1
A	1517	LEU	3HD2	0.08	0.0	1
A	1454	ASN	2HD2	7.464	0.0	1
A	1471	LEU	1HD1	0.812	0.0	1
A	1506	PRO	2HD	3.828	0.0	1
A	1492	ALA	1HB	1.217	0.0	1
A	1483	HIS	3HB	2.911	0.0	1
A	1498	VAL	1HG2	0.428	0.0	1
A	1495	LYS	2HB	1.762	0.0	1
A	1480	LYS	3HE	2.614	0.0	1
A	1503	VAL	1HG1	0.852	0.0	1
A	1500	LYS	2HD	1.546	0.0	1
A	1500	LYS	2HE	2.867	0.0	1
A	1455	VAL	2HG2	0.37	0.0	1
A	1498	VAL	1HG1	0.964	0.0	1
A	1518	THR	2HG2	0.98	0.0	1
A	1500	LYS	2HG	1.351	0.0	1
A	1517	LEU	2HD2	0.08	0.0	1
A	1459	GLY	3HA	4.184	0.0	1
A	1514	ARG	2HD	2.748	0.0	1
A	1465	HIS	2HB	3.403	0.0	1
A	1454	ASN	1HD2	6.912	0.0	1
A	1455	VAL	1HG1	0.37	0.0	1
A	1473	VAL	1HG1	0.644	0.0	1
A	1497	TYR	3HB	2.087	0.0	1
A	1457	SER	2HB	3.885	0.0	1
A	1481	LEU	3HD2	0.797	0.0	1
A	1470	ASP	3HB	2.339	0.0	1
A	1501	ASN	3HB	2.782	0.0	1
A	1467	VAL	3HG1	0.946	0.0	1
A	1473	VAL	1HG2	0.729	0.0	1
A	1479	LYS	3HG	1.231	0.0	1
A	1474	LYS	3HE	2.998	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	1497	TYR	2HB	2.144	0.0	1
A	1454	ASN	3HB	2.891	0.0	1
A	1510	LEU	3HD1	0.832	0.0	1
A	1508	SER	2HB	3.796	0.0	1
A	1484	TRP	2HB	2.286	0.0	1
A	1466	LEU	3HB	1.042	0.0	1
A	1457	SER	3HB	3.937	0.0	1
A	1496	PHE	2HB	3.132	0.0	1
A	1469	GLY	2HA	3.708	0.0	1
A	1487	GLN	1HE2	7.146	0.0	1
A	1452	ILE	1HG2	0.687	0.0	1
A	1500	LYS	2HB	1.661	0.0	1
A	1479	LYS	2HD	1.547	0.0	1
A	1495	LYS	3HD	1.643	0.0	1
A	1515	ALA	3HB	1.331	0.0	1
A	1458	ASN	3HB	2.871	0.0	1
A	1495	LYS	3HE	2.981	0.0	1
A	1462	HIS	3HB	3.198	0.0	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	76	-0.17 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	72	0.38 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}'$	74	0.27 ± 0.17	None needed (< 0.5 ppm)
^{15}N	76	0.45 ± 0.46	None needed (< 0.5 ppm)

7.1.3 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 67%, i.e. 597 atoms were assigned a chemical shift out of a possible 893. 12 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	358/366 (98%)	141/146 (97%)	145/148 (98%)	72/72 (100%)
Sidechain	165/415 (40%)	22/241 (9%)	136/159 (86%)	7/15 (47%)
Aromatic	74/112 (66%)	46/59 (78%)	26/48 (54%)	2/5 (40%)
Overall	597/893 (67%)	209/446 (47%)	307/355 (86%)	81/92 (88%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 63%, i.e. 618 atoms were assigned a chemical shift out of a possible 974. 12 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	374/401 (93%)	148/160 (92%)	150/162 (93%)	76/79 (96%)
Sidechain	170/454 (37%)	22/265 (8%)	141/171 (82%)	7/18 (39%)
Aromatic	74/119 (62%)	46/63 (73%)	26/50 (52%)	2/6 (33%)
Overall	618/974 (63%)	216/488 (44%)	317/383 (83%)	85/103 (83%)

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.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	1510	LEU	HG	-0.36	3.16 – -0.14	-5.7
1	A	1478	TYR	HE2	5.49	7.86 – 5.56	-5.3
1	A	1478	TYR	HE1	5.49	7.86 – 5.56	-5.3

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.

Random coil index (RCI) for chain A:

