



Full wwPDB NMR Structure Validation Report ⓘ

Feb 13, 2017 – 02:31 am GMT

PDB ID : 4B2R
Title : Solution structure of CCP modules 10-11 of complement factor H
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Deposited on : 2012-07-17

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

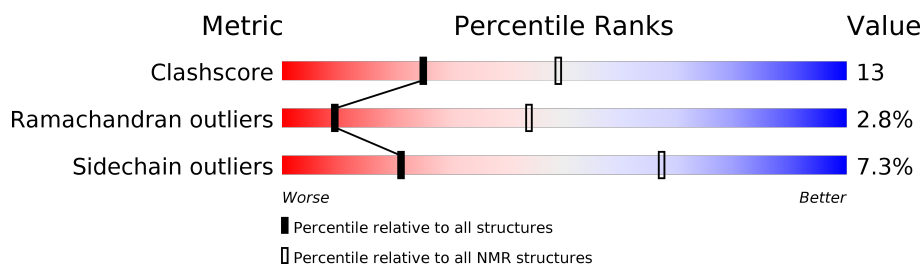
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	126	

2 Ensemble composition and analysis

This entry contains 20 models. Model 11 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:568-A:687 (120)	0.61	11

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1967 atoms, of which 975 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called COMPLEMENT FACTOR H.

Mol	Chain	Residues	Atoms						Trace
1	A	126	Total	C	H	N	O	S	0
			1967	630	975	164	189	9	

There are 4 discrepancies between the modelled and reference sequences:

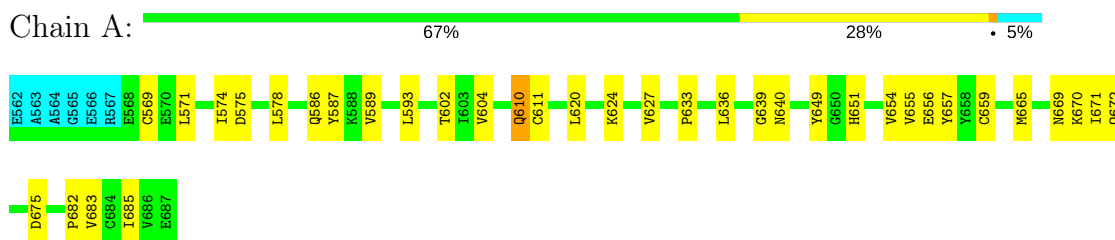
Chain	Residue	Modelled	Actual	Comment	Reference
A	562	GLU	-	EXPRESSION TAG	UNP P08603
A	563	ALA	-	EXPRESSION TAG	UNP P08603
A	564	ALA	-	EXPRESSION TAG	UNP P08603
A	565	GLY	-	EXPRESSION TAG	UNP P08603

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: COMPLEMENT FACTOR H

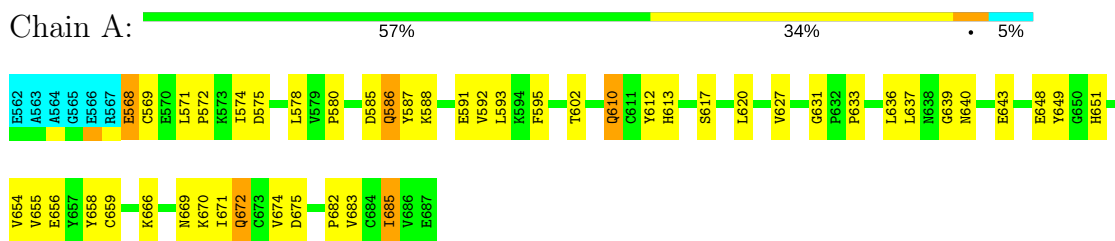


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: COMPLEMENT FACTOR H



4.2.2 Score per residue for model 2

• Molecule 1: COMPLEMENT FACTOR H

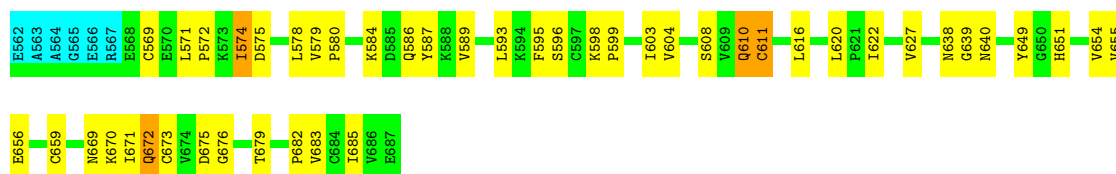




4.2.3 Score per residue for model 3

- Molecule 1: COMPLEMENT FACTOR H

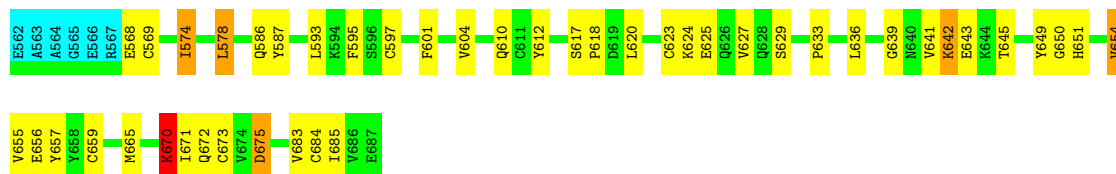
Chain A: 59% 33% 5%



4.2.4 Score per residue for model 4

- Molecule 1: COMPLEMENT FACTOR H

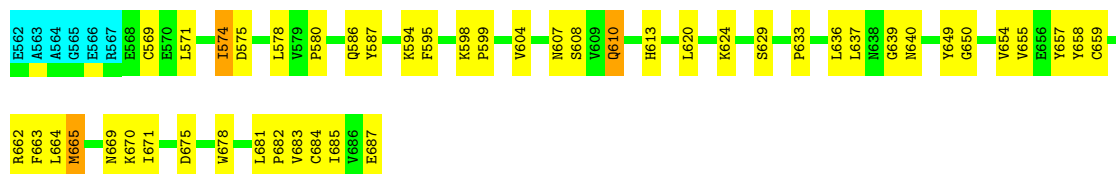
Chain A: 60% 31% 5%



4.2.5 Score per residue for model 5

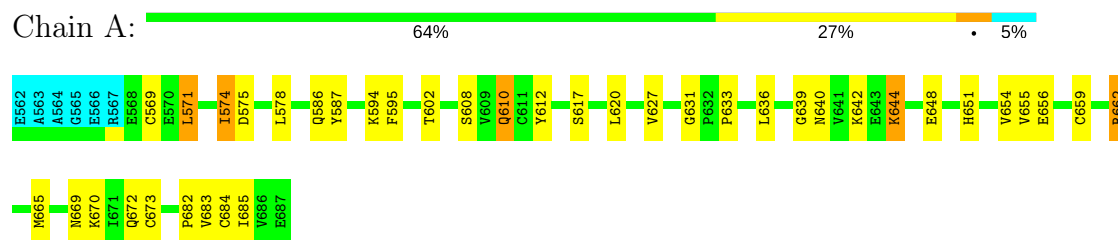
- Molecule 1: COMPLEMENT FACTOR H

Chain A: 58% 35% 5%



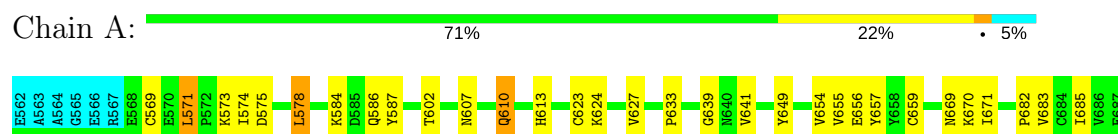
4.2.6 Score per residue for model 6

- Molecule 1: COMPLEMENT FACTOR H



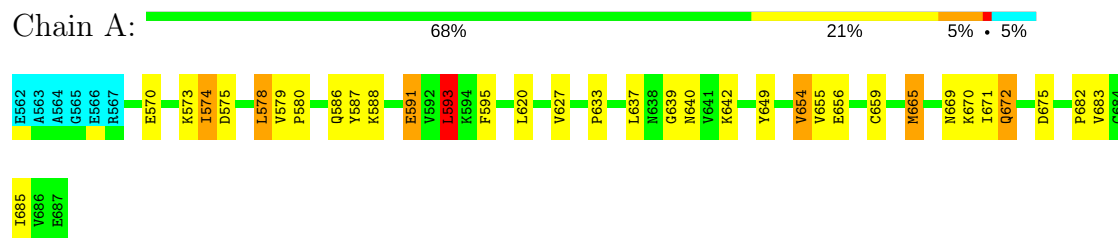
4.2.7 Score per residue for model 7

- Molecule 1: COMPLEMENT FACTOR H



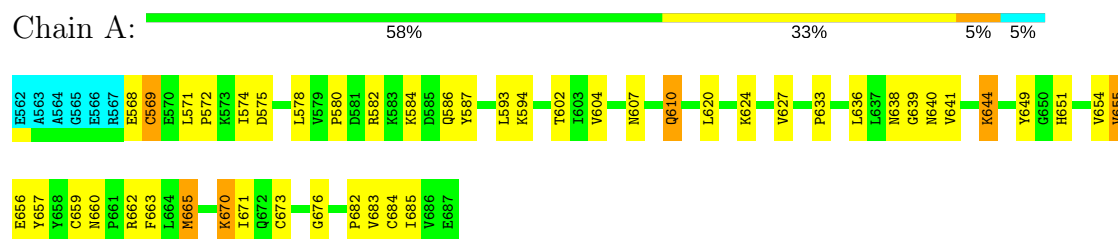
4.2.8 Score per residue for model 8

- Molecule 1: COMPLEMENT FACTOR H



4.2.9 Score per residue for model 9

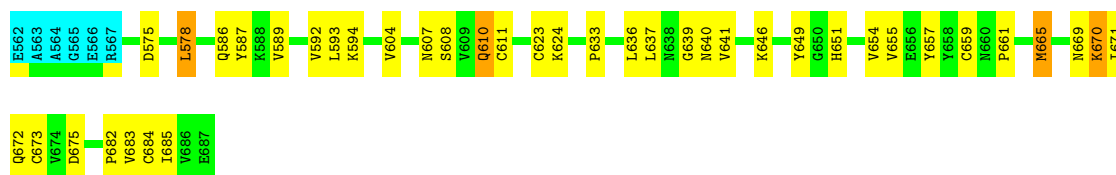
- Molecule 1: COMPLEMENT FACTOR H



4.2.10 Score per residue for model 10

- Molecule 1: COMPLEMENT FACTOR H

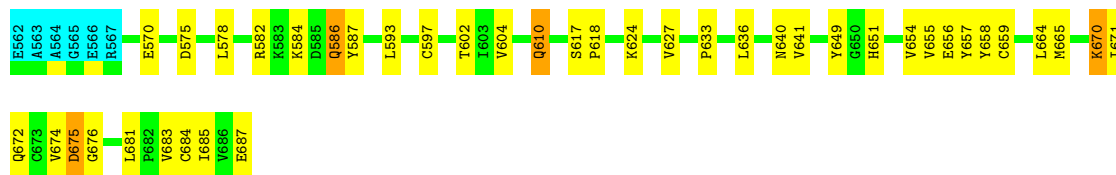




4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: COMPLEMENT FACTOR H

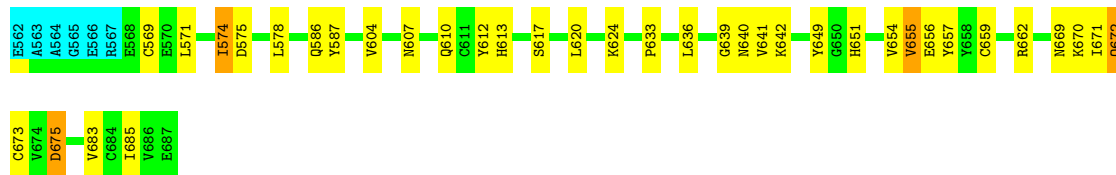
Chain A: 63% 29% 5%



4.2.12 Score per residue for model 12

- Molecule 1: COMPLEMENT FACTOR H

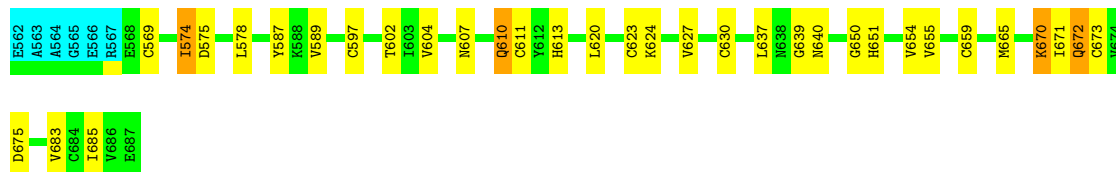
Chain A: 66% 26% 5%



4.2.13 Score per residue for model 13

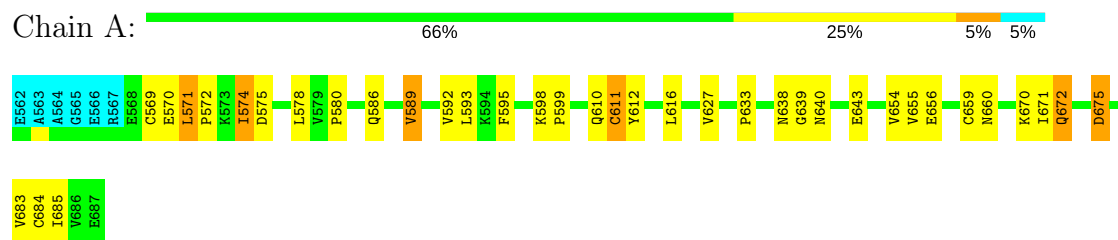
- Molecule 1: COMPLEMENT FACTOR H

Chain A: 68% 24% 5%



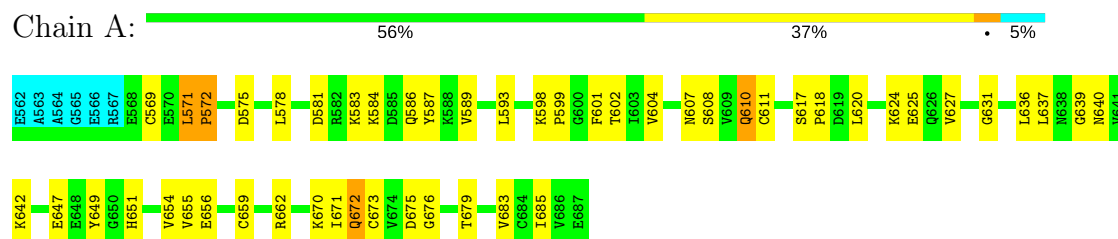
4.2.14 Score per residue for model 14

- Molecule 1: COMPLEMENT FACTOR H



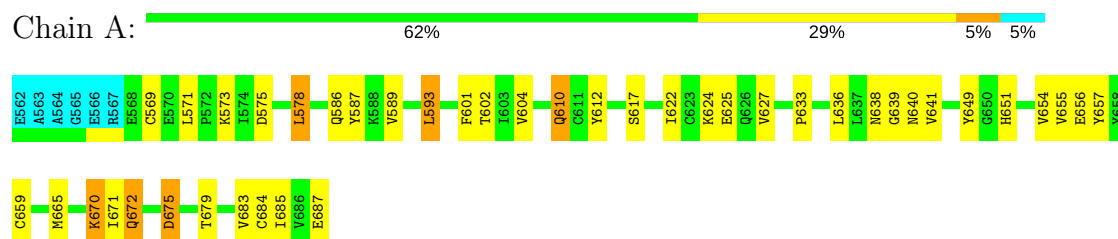
4.2.15 Score per residue for model 15

- Molecule 1: COMPLEMENT FACTOR H



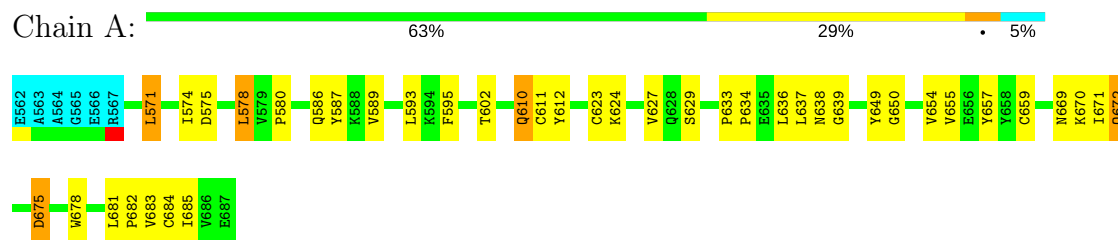
4.2.16 Score per residue for model 16

- Molecule 1: COMPLEMENT FACTOR H



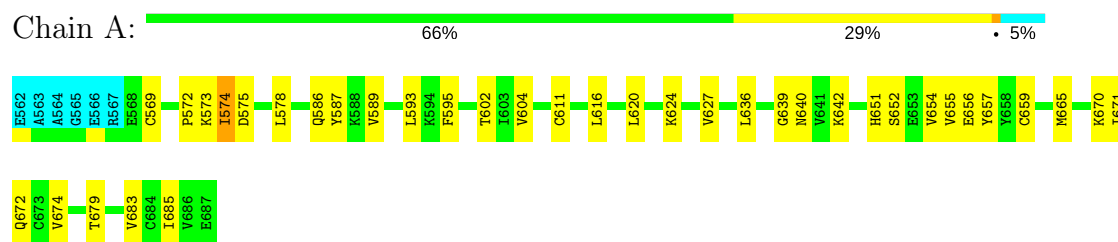
4.2.17 Score per residue for model 17

- Molecule 1: COMPLEMENT FACTOR H



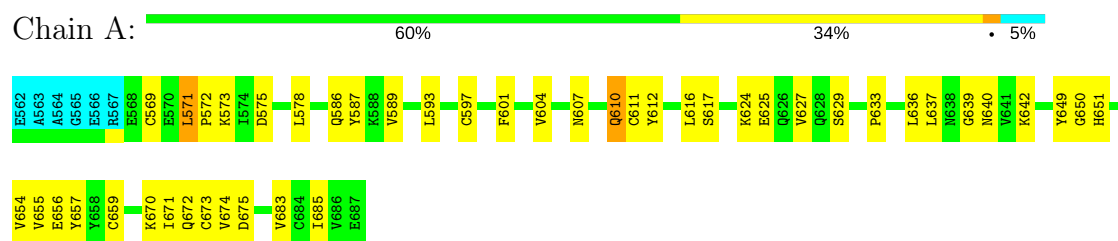
4.2.18 Score per residue for model 18

- Molecule 1: COMPLEMENT FACTOR H



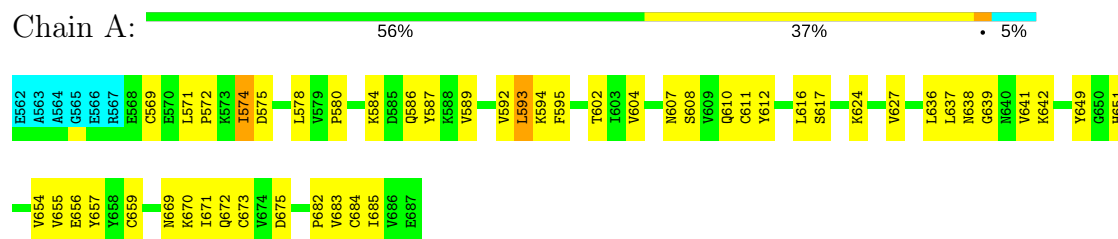
4.2.19 Score per residue for model 19

- Molecule 1: COMPLEMENT FACTOR H



4.2.20 Score per residue for model 20

- Molecule 1: COMPLEMENT FACTOR H



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY*.

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

Software name	Classification	Version
CNS	refinement	1.2
CNS	structure solution	1.2
PROCHECKNMR	structure solution	3.4.3
TOPSPIN	structure solution	1.3
MOLMOL	structure solution	2
AZARA	structure solution	2.0
CCPNMR ANALYSIS	structure solution	2.0
CCPNMR ANALYSIS	structure solution	2.1
CCPNMR ANALYSIS	structure solution	2.2

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)	4b2r_cs.str
Number of chemical shift lists	1
Total number of shifts	1574
Number of shifts mapped to atoms	1572
Number of unparsed shifts	2
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.93±0.02	0±0/974 (0.0±0.0%)	0.72±0.02	0±0/1320 (0.0±0.0%)
All	All	0.93	2/19480 (0.0%)	0.72	1/26400 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.3
All	All	0	2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	670	LYS	N-CA	-6.47	1.33	1.46	4	1
1	A	654	VAL	CB-CG2	-5.59	1.41	1.52	4	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	593	LEU	CB-CG-CD1	5.09	119.65	111.00	8	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	662	ARG	Sidechain	2

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	949	935	932	25±4
All	All	18980	18700	18640	497

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:636:LEU:HD21	1:A:659:CYS:SG	0.94	2.03	6	11
1:A:604:VAL:HG21	1:A:622:ILE:HG12	0.84	1.47	16	1
1:A:575:ASP:HB3	1:A:578:LEU:HB2	0.77	1.56	18	19
1:A:636:LEU:HD21	1:A:684:CYS:SG	0.71	2.24	17	3
1:A:655:VAL:O	1:A:670:LYS:HA	0.70	1.86	12	19
1:A:604:VAL:HG21	1:A:624:LYS:HD3	0.70	1.64	11	10
1:A:669:ASN:HA	1:A:682:PRO:HB3	0.69	1.64	17	10
1:A:665:MET:HG3	1:A:684:CYS:SG	0.69	2.27	11	3
1:A:578:LEU:HD11	1:A:595:PHE:HB3	0.68	1.63	3	8
1:A:569:CYS:HB3	1:A:616:LEU:HD11	0.68	1.66	14	1
1:A:589:VAL:HA	1:A:611:CYS:SG	0.66	2.31	17	9
1:A:654:VAL:HG21	1:A:670:LYS:HB2	0.66	1.68	4	1
1:A:574:ILE:HG13	1:A:575:ASP:H	0.65	1.51	5	5
1:A:665:MET:HG3	1:A:682:PRO:HB2	0.65	1.69	5	2
1:A:666:LYS:HG2	1:A:685:ILE:HD11	0.64	1.68	1	1
1:A:639:GLY:HA3	1:A:659:CYS:HA	0.63	1.69	15	18
1:A:571:LEU:HD11	1:A:580:PRO:HG3	0.63	1.70	1	7
1:A:638:ASN:HB2	1:A:684:CYS:HB2	0.62	1.69	16	4
1:A:644:LYS:HD3	1:A:644:LYS:H	0.61	1.55	2	3
1:A:651:HIS:HA	1:A:673:CYS:O	0.61	1.95	4	10
1:A:636:LEU:HD23	1:A:639:GLY:HA3	0.60	1.71	6	6
1:A:582:ARG:HD2	1:A:584:LYS:HE3	0.60	1.73	9	1
1:A:642:LYS:HD3	1:A:656:GLU:HB3	0.60	1.74	19	8
1:A:570:GLU:HG2	1:A:586:GLN:HG3	0.60	1.72	11	1
1:A:574:ILE:HG22	1:A:620:LEU:HD23	0.59	1.72	3	6
1:A:569:CYS:HB2	1:A:587:TYR:HB2	0.58	1.75	16	14
1:A:574:ILE:HG22	1:A:620:LEU:HG	0.58	1.75	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:571:LEU:HB2	1:A:587:TYR:CE2	0.58	2.34	15	3
1:A:633:PRO:HD3	1:A:649:TYR:CE1	0.57	2.34	9	6
1:A:587:TYR:CE1	1:A:593:LEU:HG	0.56	2.35	10	6
1:A:651:HIS:ND1	1:A:674:VAL:HA	0.56	2.15	18	1
1:A:636:LEU:CD2	1:A:659:CYS:SG	0.56	2.93	15	1
1:A:654:VAL:HA	1:A:671:ILE:O	0.55	2.01	9	14
1:A:654:VAL:HG11	1:A:670:LYS:HE3	0.55	1.78	8	2
1:A:654:VAL:CG2	1:A:670:LYS:HB2	0.55	2.31	4	3
1:A:654:VAL:HG21	1:A:670:LYS:HE2	0.55	1.78	10	3
1:A:643:GLU:HG2	1:A:656:GLU:HB2	0.55	1.78	1	3
1:A:664:LEU:HG	1:A:687:GLU:HG2	0.55	1.77	5	1
1:A:571:LEU:HB2	1:A:587:TYR:CE1	0.55	2.37	3	2
1:A:572:PRO:HD3	1:A:616:LEU:HD13	0.54	1.79	14	1
1:A:655:VAL:HG22	1:A:657:TYR:CE1	0.54	2.38	12	1
1:A:572:PRO:HD2	1:A:616:LEU:HD12	0.54	1.79	2	2
1:A:665:MET:HG2	1:A:682:PRO:HB2	0.54	1.78	9	2
1:A:587:TYR:CZ	1:A:593:LEU:HG	0.54	2.38	8	1
1:A:633:PRO:HD3	1:A:649:TYR:CE2	0.54	2.38	17	6
1:A:627:VAL:CG2	1:A:675:ASP:HA	0.53	2.33	19	7
1:A:610:GLN:HB2	1:A:612:TYR:CE1	0.53	2.38	2	2
1:A:641:VAL:HG22	1:A:657:TYR:CE2	0.53	2.38	7	3
1:A:572:PRO:HG2	1:A:620:LEU:HD11	0.53	1.81	9	2
1:A:633:PRO:HB3	1:A:655:VAL:HG11	0.53	1.80	12	2
1:A:587:TYR:CD1	1:A:593:LEU:HD22	0.53	2.39	16	1
1:A:604:VAL:CG1	1:A:624:LYS:HG2	0.53	2.34	16	1
1:A:656:GLU:HG2	1:A:670:LYS:HG2	0.52	1.80	14	5
1:A:610:GLN:N	1:A:610:GLN:HE21	0.52	2.02	9	4
1:A:575:ASP:CB	1:A:578:LEU:HB2	0.52	2.32	8	4
1:A:656:GLU:HA	1:A:669:ASN:O	0.52	2.05	7	3
1:A:588:LYS:O	1:A:591:GLU:HB2	0.52	2.05	8	1
1:A:636:LEU:HD22	1:A:657:TYR:HB3	0.52	1.80	5	6
1:A:672:GLN:N	1:A:672:GLN:HE21	0.52	2.02	15	1
1:A:640:ASN:HB3	1:A:658:TYR:CE2	0.51	2.40	11	2
1:A:584:LYS:HG2	1:A:587:TYR:CE1	0.51	2.39	2	4
1:A:610:GLN:HE21	1:A:610:GLN:N	0.51	2.04	13	8
1:A:656:GLU:CG	1:A:670:LYS:HG2	0.51	2.36	19	7
1:A:641:VAL:HG22	1:A:657:TYR:CE1	0.51	2.40	10	3
1:A:651:HIS:CE1	1:A:674:VAL:HA	0.51	2.41	11	2
1:A:671:ILE:HD13	1:A:681:LEU:CD2	0.50	2.36	5	1
1:A:638:ASN:HB2	1:A:684:CYS:SG	0.50	2.46	9	1
1:A:665:MET:CG	1:A:682:PRO:HB2	0.50	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:654:VAL:HG22	1:A:671:ILE:N	0.50	2.22	8	3
1:A:610:GLN:HB2	1:A:612:TYR:CE2	0.50	2.42	12	3
1:A:574:ILE:HA	1:A:620:LEU:HG	0.50	1.83	8	1
1:A:604:VAL:HG21	1:A:624:LYS:HG3	0.50	1.84	13	1
1:A:594:LYS:HA	1:A:607:ASN:O	0.49	2.08	20	1
1:A:578:LEU:HD12	1:A:597:CYS:SG	0.49	2.48	13	5
1:A:654:VAL:HG21	1:A:670:LYS:HE3	0.49	1.83	2	6
1:A:612:TYR:CD1	1:A:617:SER:HB2	0.49	2.42	19	1
1:A:645:THR:HA	1:A:649:TYR:OH	0.49	2.07	4	1
1:A:664:LEU:HG	1:A:687:GLU:HB3	0.49	1.83	11	1
1:A:592:VAL:HG12	1:A:610:GLN:HG3	0.49	1.85	20	4
1:A:594:LYS:HG2	1:A:608:SER:HB3	0.49	1.84	20	3
1:A:659:CYS:SG	1:A:665:MET:HG3	0.49	2.47	16	1
1:A:574:ILE:HD13	1:A:580:PRO:HD3	0.49	1.83	1	3
1:A:633:PRO:HG3	1:A:655:VAL:HG11	0.49	1.84	2	3
1:A:596:SER:HA	1:A:603:ILE:HD12	0.49	1.83	3	1
1:A:671:ILE:HD12	1:A:678:TRP:HB3	0.48	1.85	5	1
1:A:602:THR:HB	1:A:624:LYS:O	0.48	2.09	7	4
1:A:602:THR:HG21	1:A:627:VAL:HG11	0.48	1.85	11	9
1:A:636:LEU:HD23	1:A:639:GLY:CA	0.48	2.37	17	2
1:A:587:TYR:CD1	1:A:593:LEU:HD21	0.48	2.44	1	2
1:A:587:TYR:CD2	1:A:593:LEU:HD21	0.48	2.44	19	1
1:A:584:LYS:HG2	1:A:587:TYR:CE2	0.48	2.44	9	2
1:A:639:GLY:CA	1:A:659:CYS:HA	0.48	2.39	15	1
1:A:612:TYR:CD2	1:A:617:SER:HB3	0.48	2.44	6	4
1:A:655:VAL:HG22	1:A:657:TYR:CE2	0.47	2.43	9	1
1:A:583:LYS:HA	1:A:587:TYR:OH	0.47	2.10	2	1
1:A:641:VAL:HG23	1:A:655:VAL:HG23	0.47	1.85	9	2
1:A:598:LYS:HB3	1:A:599:PRO:HD2	0.47	1.87	14	4
1:A:644:LYS:HD3	1:A:644:LYS:N	0.47	2.25	2	2
1:A:612:TYR:CD2	1:A:617:SER:HB2	0.47	2.45	16	2
1:A:654:VAL:HG22	1:A:670:LYS:HB3	0.47	1.86	6	2
1:A:570:GLU:O	1:A:571:LEU:HB2	0.46	2.10	14	1
1:A:578:LEU:HD12	1:A:623:CYS:SG	0.46	2.50	4	3
1:A:572:PRO:HD2	1:A:616:LEU:HD22	0.46	1.87	3	1
1:A:663:PHE:HB3	1:A:684:CYS:HB2	0.46	1.86	5	1
1:A:672:GLN:H	1:A:672:GLN:NE2	0.46	2.08	1	4
1:A:587:TYR:CD1	1:A:593:LEU:HD11	0.46	2.45	18	1
1:A:636:LEU:HD23	1:A:659:CYS:SG	0.46	2.50	15	1
1:A:654:VAL:CG2	1:A:670:LYS:HB3	0.46	2.41	6	1
1:A:655:VAL:HG23	1:A:678:TRP:CZ3	0.46	2.45	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:582:ARG:HG2	1:A:584:LYS:HE3	0.45	1.87	11	1
1:A:627:VAL:HG11	1:A:651:HIS:HB2	0.45	1.88	19	1
1:A:654:VAL:HG11	1:A:670:LYS:CE	0.45	2.41	19	1
1:A:636:LEU:CD2	1:A:684:CYS:SG	0.45	3.05	10	1
1:A:610:GLN:HG2	1:A:612:TYR:CE1	0.45	2.46	17	1
1:A:642:LYS:NZ	1:A:642:LYS:HB2	0.45	2.26	4	1
1:A:578:LEU:CD1	1:A:595:PHE:HB3	0.45	2.42	17	1
1:A:649:TYR:CE2	1:A:655:VAL:HG22	0.45	2.47	1	2
1:A:601:PHE:HA	1:A:625:GLU:HA	0.45	1.87	4	2
1:A:666:LYS:CG	1:A:685:ILE:HD11	0.45	2.38	1	1
1:A:636:LEU:HB3	1:A:639:GLY:C	0.45	2.33	19	2
1:A:601:PHE:CE1	1:A:625:GLU:HB2	0.45	2.46	15	2
1:A:636:LEU:HG	1:A:637:LEU:N	0.45	2.27	15	2
1:A:672:GLN:NE2	1:A:672:GLN:H	0.44	2.10	14	4
1:A:656:GLU:HA	1:A:670:LYS:HB3	0.44	1.88	4	3
1:A:601:PHE:CD2	1:A:625:GLU:HB2	0.44	2.47	16	1
1:A:649:TYR:CE1	1:A:655:VAL:HG22	0.44	2.47	7	1
1:A:588:LYS:O	1:A:591:GLU:HG2	0.44	2.12	1	1
1:A:631:GLY:HA2	1:A:648:GLU:HA	0.44	1.89	1	2
1:A:660:ASN:HB2	1:A:663:PHE:CE1	0.44	2.48	9	1
1:A:671:ILE:HG21	1:A:681:LEU:HD23	0.44	1.90	17	1
1:A:640:ASN:HB3	1:A:658:TYR:CE1	0.43	2.48	5	1
1:A:649:TYR:CE1	1:A:655:VAL:HG12	0.43	2.48	3	3
1:A:593:LEU:HD23	1:A:593:LEU:N	0.43	2.28	16	1
1:A:617:SER:HA	1:A:618:PRO:C	0.43	2.34	15	2
1:A:671:ILE:HB	1:A:679:THR:OG1	0.43	2.13	16	1
1:A:654:VAL:HG21	1:A:670:LYS:CB	0.43	2.43	17	1
1:A:572:PRO:HG2	1:A:620:LEU:HD21	0.43	1.90	18	1
1:A:610:GLN:CG	1:A:612:TYR:HE1	0.43	2.26	17	1
1:A:650:GLY:O	1:A:673:CYS:HB3	0.43	2.14	13	1
1:A:671:ILE:HD13	1:A:681:LEU:HD12	0.43	1.91	11	1
1:A:627:VAL:HG23	1:A:675:ASP:HA	0.43	1.89	3	1
1:A:602:THR:O	1:A:623:CYS:HA	0.43	2.13	13	1
1:A:629:SER:HA	1:A:650:GLY:HA2	0.42	1.89	19	4
1:A:671:ILE:HD13	1:A:681:LEU:HD23	0.42	1.91	5	1
1:A:649:TYR:CE2	1:A:655:VAL:HG12	0.42	2.49	11	2
1:A:604:VAL:HB	1:A:622:ILE:HG13	0.42	1.90	3	1
1:A:656:GLU:CG	1:A:670:LYS:HD2	0.42	2.44	3	1
1:A:654:VAL:HG22	1:A:670:LYS:HB2	0.42	1.92	5	1
1:A:656:GLU:CG	1:A:670:LYS:HB3	0.42	2.44	8	1
1:A:572:PRO:HD3	1:A:616:LEU:HD23	0.42	1.89	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:651:HIS:CE1	1:A:675:ASP:H	0.42	2.33	16	1
1:A:624:LYS:HE2	1:A:675:ASP:OD2	0.42	2.14	11	1
1:A:587:TYR:CE2	1:A:593:LEU:HG	0.42	2.50	9	1
1:A:646:LYS:HE3	1:A:649:TYR:HA	0.41	1.92	10	1
1:A:593:LEU:O	1:A:608:SER:HA	0.41	2.16	15	2
1:A:611:CYS:HA	1:A:616:LEU:HD13	0.41	1.91	19	1
1:A:642:LYS:HE3	1:A:643:GLU:OE1	0.41	2.15	4	1
1:A:578:LEU:HD13	1:A:579:VAL:N	0.41	2.30	8	2
1:A:651:HIS:HD1	1:A:674:VAL:HA	0.41	1.74	19	1
1:A:593:LEU:HD22	1:A:595:PHE:CZ	0.41	2.50	8	1
1:A:627:VAL:HG11	1:A:651:HIS:CB	0.41	2.44	19	1
1:A:656:GLU:HG2	1:A:670:LYS:HB3	0.41	1.92	4	1
1:A:617:SER:OG	1:A:618:PRO:HA	0.41	2.16	11	1
1:A:568:GLU:HB3	1:A:587:TYR:O	0.41	2.16	9	1
1:A:631:GLY:HA2	1:A:647:GLU:O	0.41	2.16	15	1
1:A:654:VAL:HG23	1:A:671:ILE:N	0.41	2.31	4	1
1:A:569:CYS:HB3	1:A:616:LEU:CD2	0.41	2.46	20	1
1:A:637:LEU:H	1:A:637:LEU:HD23	0.41	1.76	20	1
1:A:568:GLU:HG3	1:A:586:GLN:HB3	0.41	1.91	1	1
1:A:587:TYR:HD1	1:A:593:LEU:HD21	0.41	1.74	1	1
1:A:624:LYS:HE2	1:A:675:ASP:OD1	0.41	2.16	12	1
1:A:651:HIS:O	1:A:672:GLN:HB2	0.41	2.16	3	1
1:A:569:CYS:CB	1:A:587:TYR:HB2	0.41	2.45	9	1
1:A:654:VAL:HG22	1:A:655:VAL:N	0.40	2.31	4	1
1:A:641:VAL:HG11	1:A:645:THR:HG21	0.40	1.92	2	1
1:A:595:PHE:CZ	1:A:620:LEU:HD12	0.40	2.52	4	1
1:A:578:LEU:HD21	1:A:595:PHE:HB3	0.40	1.92	5	1
1:A:569:CYS:HB3	1:A:616:LEU:CD1	0.40	2.46	3	1
1:A:654:VAL:HG11	1:A:670:LYS:HE2	0.40	1.93	17	1
1:A:594:LYS:HD2	1:A:608:SER:HB3	0.40	1.92	10	1
1:A:578:LEU:HD22	1:A:623:CYS:SG	0.40	2.57	17	1
1:A:636:LEU:HB2	1:A:657:TYR:CD2	0.40	2.52	17	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	119/126 (94%)	104±3 (87±3%)	12±3 (10±3%)	3±1 (3±1%)	9	44
All	All	2380/2520 (94%)	2076 (87%)	238 (10%)	66 (3%)	9	44

All 14 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	683	VAL	20
1	A	574	ILE	13
1	A	675	ASP	11
1	A	571	LEU	7
1	A	676	GLY	4
1	A	572	PRO	3
1	A	634	PRO	1
1	A	661	PRO	1
1	A	652	SER	1
1	A	583	LYS	1
1	A	569	CYS	1
1	A	630	CYS	1
1	A	585	ASP	1
1	A	570	GLU	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	111/114 (97%)	103±2 (93±2%)	8±2 (7±2%)	21	67
All	All	2220/2280 (97%)	2058 (93%)	162 (7%)	21	67

All 30 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	685	ILE	20
1	A	586	GLN	19
1	A	672	GLN	17
1	A	610	GLN	13

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Mol	Chain	Res	Type	Models (Total)
1	A	640	ASN	13
1	A	607	ASN	9
1	A	637	LEU	8
1	A	665	MET	6
1	A	573	LYS	6
1	A	670	LYS	6
1	A	578	LEU	6
1	A	613	HIS	5
1	A	662	ARG	4
1	A	593	LEU	4
1	A	679	THR	3
1	A	571	LEU	3
1	A	644	LYS	3
1	A	611	CYS	2
1	A	568	GLU	2
1	A	655	VAL	2
1	A	589	VAL	2
1	A	660	ASN	1
1	A	687	GLU	1
1	A	628	GLN	1
1	A	581	ASP	1
1	A	591	GLU	1
1	A	654	VAL	1
1	A	594	LYS	1
1	A	638	ASN	1
1	A	642	LYS	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 carbohydrates 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 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: 4b2r_cs.str

Chemical shift list name: *assigned_chem_shift_list*

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	1574
Number of shifts mapped to atoms	1572
Number of unparsed shifts	2
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 2 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1147	A	654	VAL	N	124.445	?	1
1154	A	655	VAL	H	8.655	0.002	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
$^{13}\text{C}_\alpha$	126	0.11 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	116	-0.21 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	124	0.49 ± 0.17	None needed (< 0.5 ppm)
^{15}N	113	0.35 ± 0.37	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 93%, i.e. 1379 atoms were assigned a chemical shift out of a possible 1483. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	572/576 (99%)	227/228 (100%)	238/240 (99%)	107/108 (99%)
Sidechain	717/795 (90%)	446/472 (94%)	261/295 (88%)	10/28 (36%)
Aromatic	90/112 (80%)	45/58 (78%)	44/47 (94%)	1/7 (14%)
Overall	1379/1483 (93%)	718/758 (95%)	543/582 (93%)	118/143 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1433 atoms were assigned a chemical shift out of a possible 1549. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	601/606 (99%)	238/240 (99%)	250/252 (99%)	113/114 (99%)
Sidechain	742/831 (89%)	462/493 (94%)	270/307 (88%)	10/31 (32%)
Aromatic	90/112 (80%)	45/58 (78%)	44/47 (94%)	1/7 (14%)
Overall	1433/1549 (93%)	745/791 (94%)	564/606 (93%)	124/152 (82%)

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, ppm	Expected range, ppm	Z-score
1	A	638	ASN	HB2	1.05	4.36 – 1.26	-5.7

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:

