



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 08:32 PM UTC

PDB ID : 2KMS / pdb_00002kms
BMRB ID : 16439
Title : Combined high- and low-resolution techniques reveal compact structure in central portion of factor H despite long inter-modular linkers
Authors : Schmidt, C.Q.; Herbert, A.P.; Guariento, M.; Mertens, H.D.T.; Soares, D.C.; Uhrin, D.; Rowe, A.J.; Svergun, D.I.; Barlow, P.N.
Deposited on : 2009-08-04

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

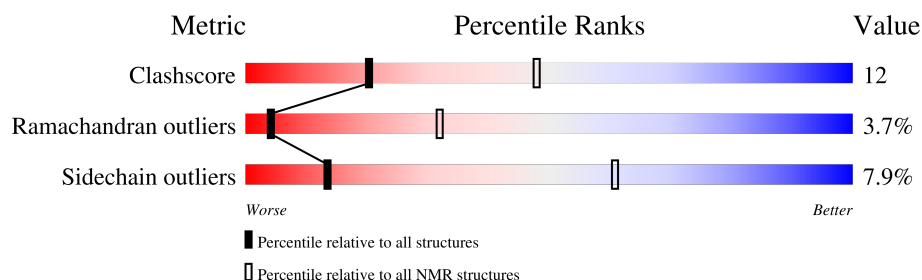
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	115	 65% 30% . .

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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:690-A:750 (61)	0.45	7
2	A:751-A:801 (51)	0.48	8

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 5 clusters. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1815 atoms, of which 887 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Complement factor H.

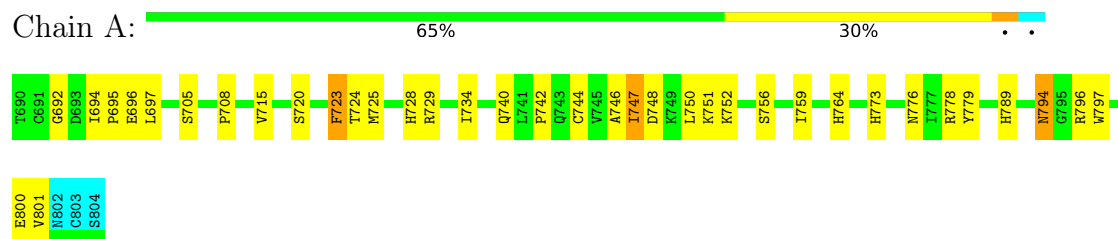
Mol	Chain	Residues	Atoms						Trace
1	A	115	Total	C	H	N	O	S	0
			1815	582	887	164	173	9	

4 Residue-property plots [i](#)

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: Complement factor H

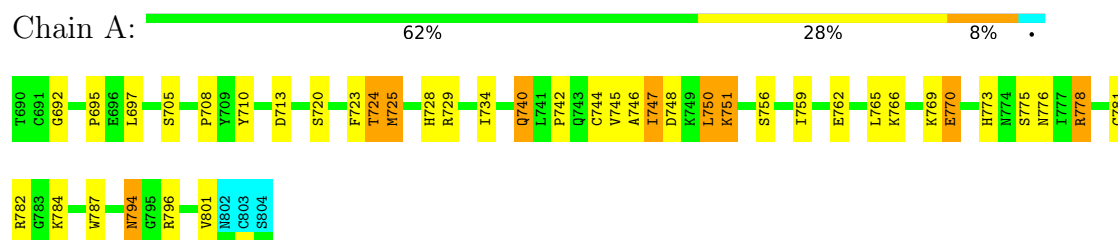


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

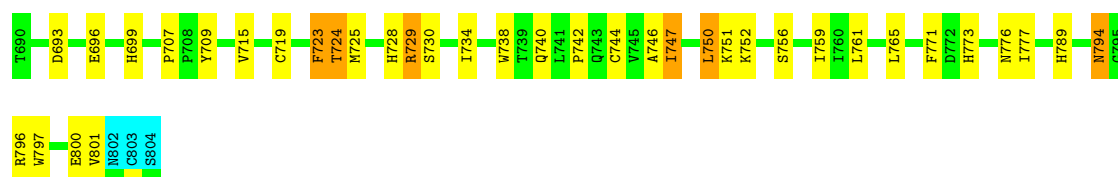
- Molecule 1: Complement factor H



4.2.2 Score per residue for model 2

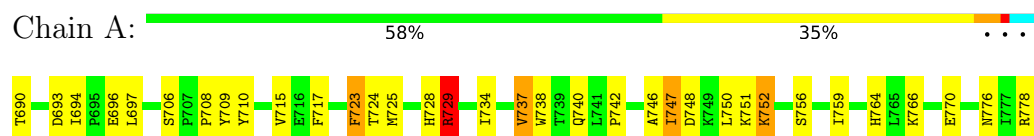
- Molecule 1: Complement factor H





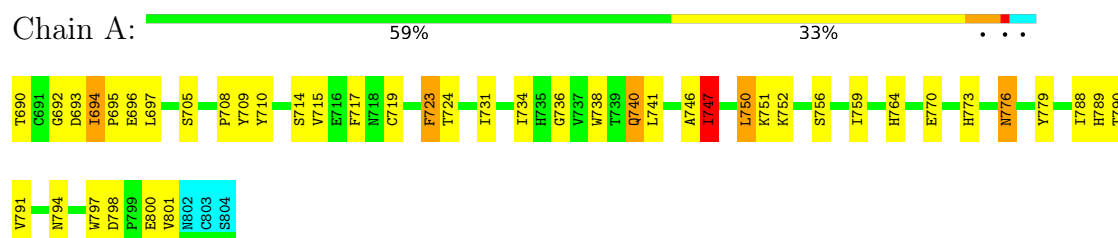
4.2.3 Score per residue for model 3

- Molecule 1: Complement factor H



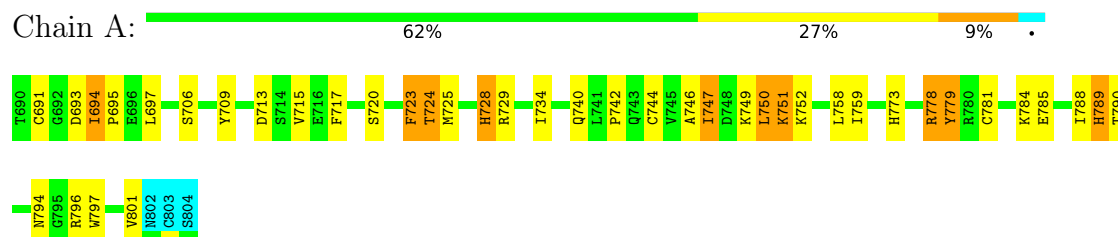
4.2.4 Score per residue for model 4

- Molecule 1: Complement factor H



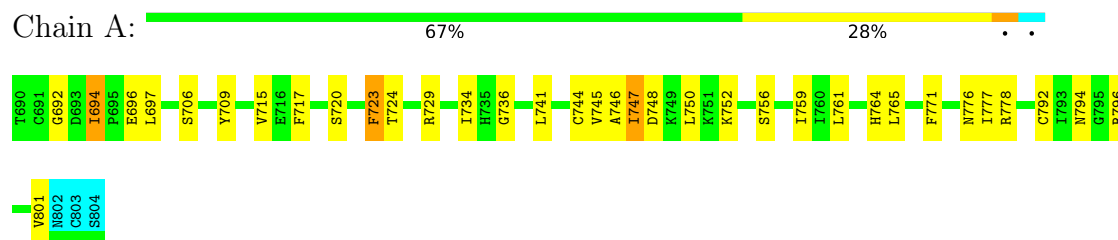
4.2.5 Score per residue for model 5

- Molecule 1: Complement factor H



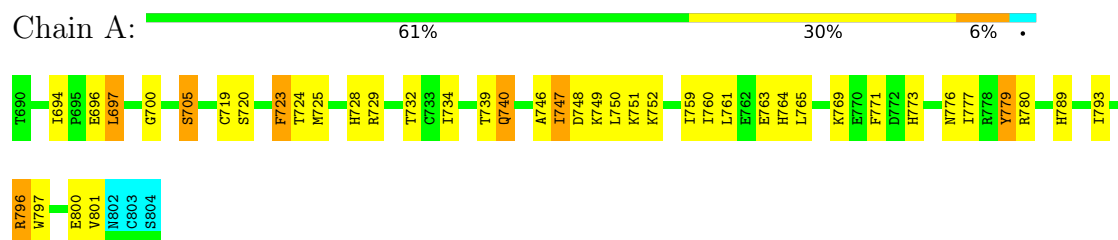
4.2.6 Score per residue for model 6

- Molecule 1: Complement factor H



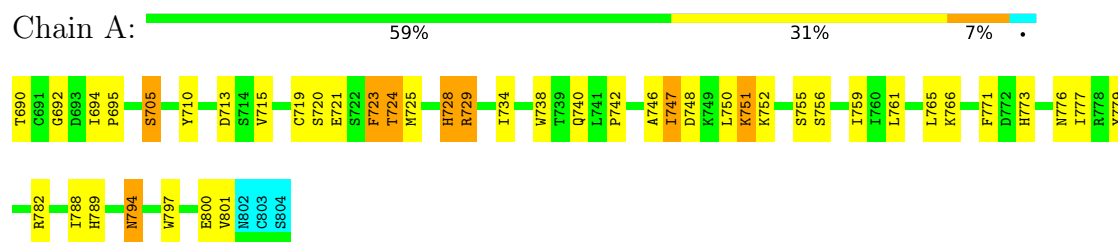
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Complement factor H



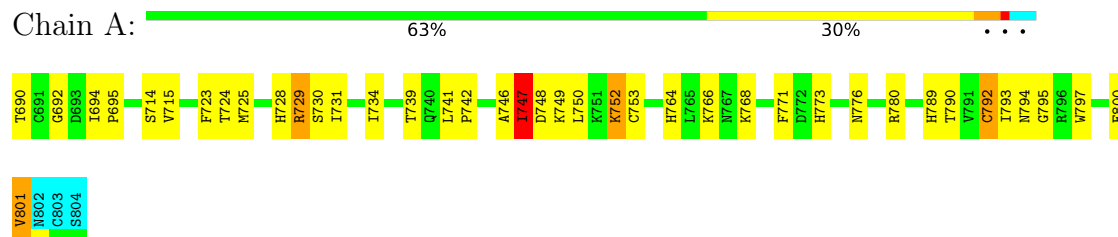
4.2.8 Score per residue for model 8

- Molecule 1: Complement factor H



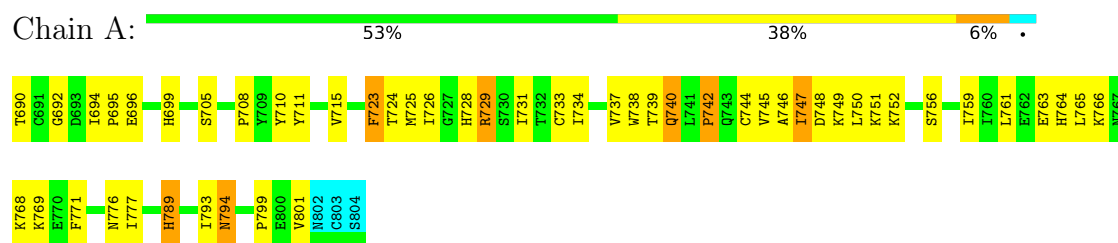
4.2.9 Score per residue for model 9

- Molecule 1: Complement factor H



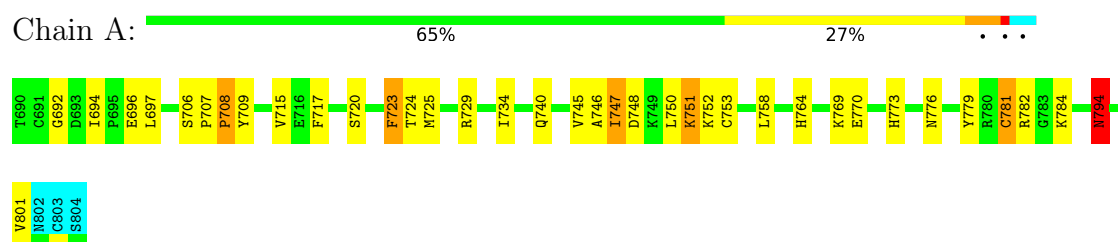
4.2.10 Score per residue for model 10

- Molecule 1: Complement factor H



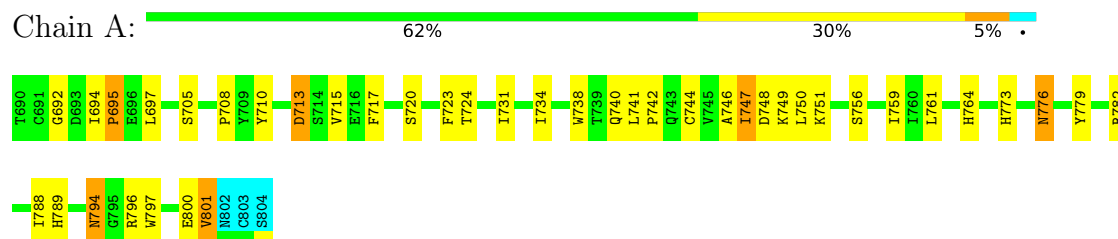
4.2.11 Score per residue for model 11

- Molecule 1: Complement factor H



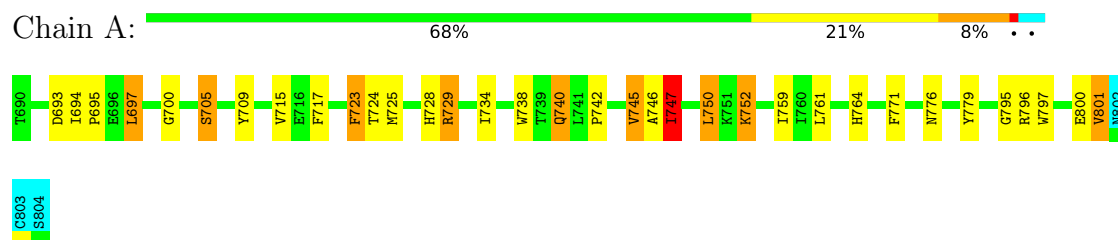
4.2.12 Score per residue for model 12

- Molecule 1: Complement factor H



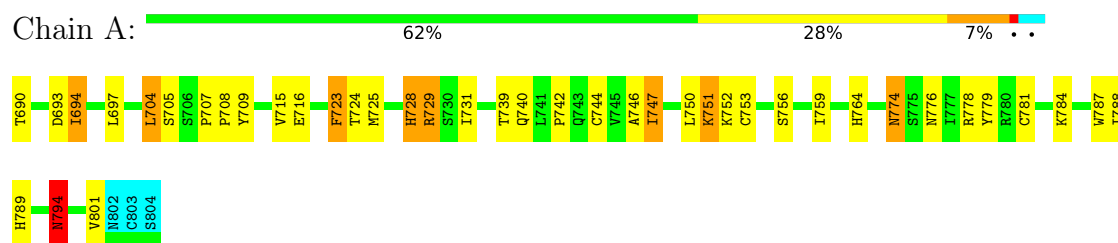
4.2.13 Score per residue for model 13

- Molecule 1: Complement factor H

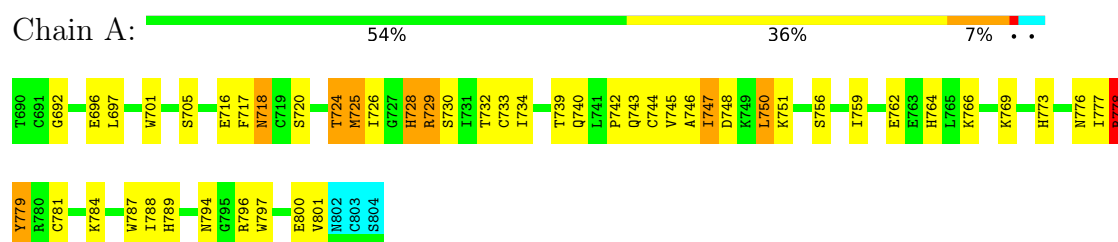


4.2.14 Score per residue for model 14

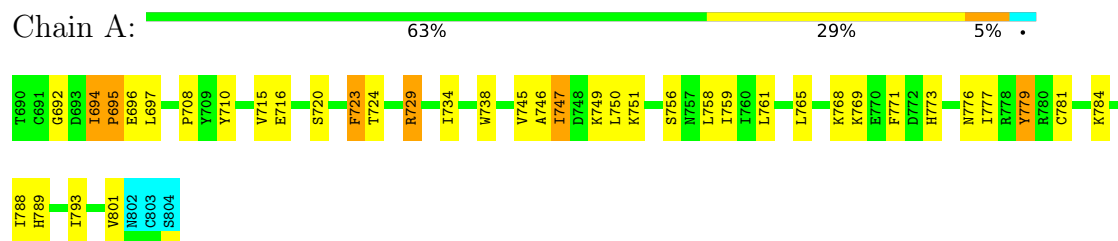
- Molecule 1: Complement factor H



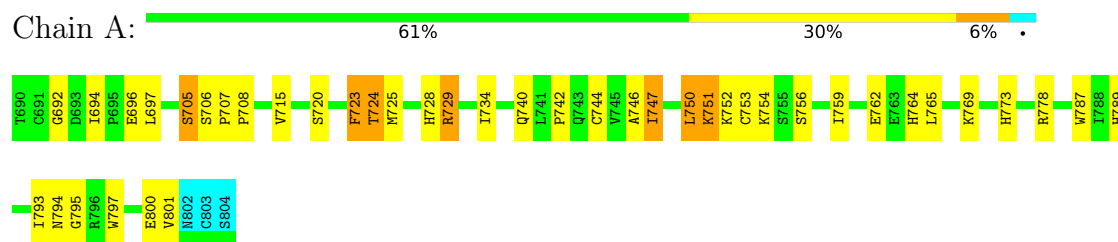
- Molecule 1: Complement factor H



- Molecule 1: Complement factor H

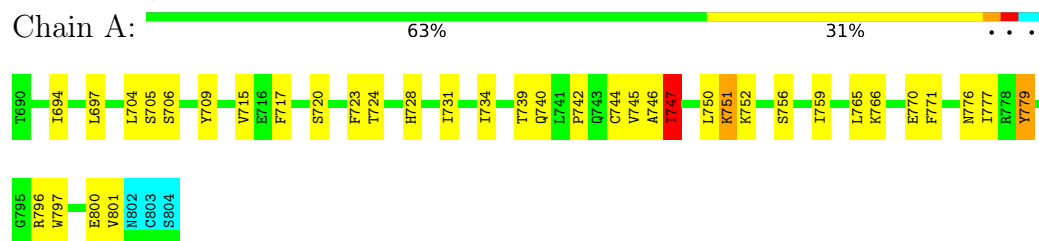


- Molecule 1: Complement factor H



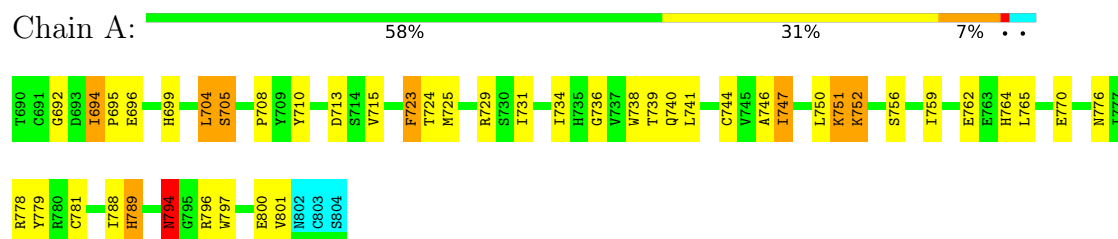
4.2.18 Score per residue for model 18

- Molecule 1: Complement factor H



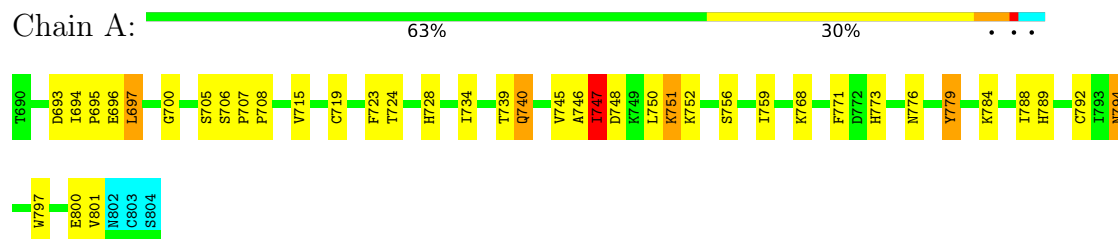
4.2.19 Score per residue for model 19

- 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: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	refinement	1.2
CYANA	refinement	2.1
CYANA	structure solution	2.1

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	1372
Number of shifts mapped to atoms	1347
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	1.47±0.05	7±2/933 (0.8± 0.2%)	0.96±0.03	1±1/1264 (0.0± 0.1%)
All	All	1.47	148/18660 (0.8%)	0.97	11/25280 (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	0.4±0.5
All	All	0	8

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	801	VAL	N-CA	-9.99	1.35	1.46	9	14
1	A	692	GLY	N-CA	-9.36	1.36	1.45	8	12
1	A	708	PRO	C-N	-7.85	1.23	1.33	11	1
1	A	751	LYS	C-N	-7.14	1.23	1.33	15	14
1	A	766	LYS	N-CA	-6.64	1.37	1.46	18	1
1	A	779	TYR	C-N	-6.58	1.25	1.33	11	7
1	A	705	SER	N-CA	-6.46	1.40	1.46	20	8
1	A	752	LYS	C-N	-6.45	1.24	1.33	18	16
1	A	705	SER	C-N	-6.24	1.25	1.33	1	1
1	A	718	ASN	N-CA	-6.21	1.38	1.46	15	1
1	A	723	PHE	C-N	-6.19	1.24	1.33	17	13
1	A	696	GLU	C-N	-6.16	1.24	1.33	17	11
1	A	716	GLU	N-CA	-6.13	1.38	1.46	14	1
1	A	796	ARG	C-N	-6.12	1.25	1.33	19	10
1	A	775	SER	N-CA	-6.08	1.39	1.46	1	1
1	A	751	LYS	N-CA	-5.95	1.38	1.45	15	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	747	ILE	C-N	-5.94	1.25	1.33	4	5
1	A	718	ASN	C-N	-5.91	1.25	1.33	15	1
1	A	723	PHE	N-CA	-5.85	1.38	1.46	13	1
1	A	690	THR	C-N	-5.63	1.25	1.33	8	1
1	A	770	GLU	C-N	-5.62	1.25	1.33	18	3
1	A	792	CYS	C-N	-5.62	1.26	1.33	20	3
1	A	778	ARG	N-CA	-5.60	1.39	1.46	1	3
1	A	696	GLU	N-CA	-5.58	1.38	1.45	11	1
1	A	737	VAL	N-CA	-5.53	1.39	1.46	3	1
1	A	745	VAL	N-CA	-5.38	1.39	1.46	11	2
1	A	745	VAL	C-N	-5.32	1.25	1.33	13	1
1	A	692	GLY	C-N	-5.32	1.26	1.33	10	1
1	A	733	CYS	N-CA	-5.27	1.39	1.46	15	1
1	A	770	GLU	N-CA	-5.22	1.39	1.46	1	1
1	A	728	HIS	N-CA	-5.10	1.39	1.46	20	1
1	A	777	ILE	C-N	-5.09	1.27	1.33	15	1
1	A	737	VAL	C-N	-5.04	1.26	1.33	10	1
1	A	781	CYS	N-CA	-5.00	1.40	1.45	11	1
1	A	793	ILE	N-CA	-5.00	1.40	1.46	9	1
1	A	692	GLY	CA-C	-5.00	1.47	1.51	8	1

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	794	ASN	CA-CB-CG	5.84	118.44	112.60	18	4
1	A	764	HIS	CA-CB-CG	5.83	119.63	113.80	19	3
1	A	764	HIS	N-CA-C	-5.78	106.57	113.97	17	2
1	A	774	ASN	CA-CB-CG	5.52	118.12	112.60	14	1
1	A	718	ASN	CA-CB-CG	5.32	117.92	112.60	15	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	729	ARG	Sidechain	2
1	A	778	ARG	Sidechain	2
1	A	782	ARG	Sidechain	2
1	A	796	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	780	ARG	Sidechain	1

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	907	872	865	22±3
All	All	18140	17440	17300	432

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:745:VAL:HG11	1:A:750:LEU:HD21	0.93	1.37	18	1
1:A:750:LEU:HG	1:A:794:ASN:HD22	0.88	1.29	5	3
1:A:747:ILE:HA	1:A:750:LEU:HD22	0.81	1.52	17	6
1:A:750:LEU:HG	1:A:794:ASN:ND2	0.73	1.98	8	5
1:A:747:ILE:HA	1:A:750:LEU:HG	0.72	1.61	19	12
1:A:693:ASP:HA	1:A:709:TYR:CE2	0.71	2.21	5	3
1:A:750:LEU:HD12	1:A:773:HIS:CD2	0.68	2.24	20	2
1:A:750:LEU:HD23	1:A:773:HIS:HB3	0.67	1.66	17	4
1:A:725:MET:SD	1:A:729:ARG:HB3	0.67	2.30	3	14
1:A:694:ILE:HG21	1:A:715:VAL:HG21	0.65	1.68	14	15
1:A:756:SER:HB3	1:A:759:ILE:HG13	0.64	1.67	19	4
1:A:697:LEU:HD13	1:A:744:CYS:SG	0.64	2.33	1	2
1:A:762:GLU:HB2	1:A:765:LEU:HD23	0.64	1.67	19	3
1:A:750:LEU:HG	1:A:794:ASN:HB2	0.64	1.70	4	1
1:A:769:LYS:HG3	1:A:770:GLU:HG2	0.63	1.70	1	1
1:A:750:LEU:HB2	1:A:773:HIS:CD2	0.62	2.30	9	1
1:A:723:PHE:CD1	1:A:746:ALA:HA	0.61	2.30	8	19
1:A:765:LEU:CD1	1:A:777:ILE:HB	0.61	2.25	16	6
1:A:699:HIS:HB2	1:A:744:CYS:HB2	0.61	1.71	19	3
1:A:791:VAL:HG22	1:A:798:ASP:HB3	0.60	1.73	4	1
1:A:771:PHE:CE2	1:A:777:ILE:HG21	0.59	2.32	2	3
1:A:747:ILE:HA	1:A:750:LEU:CG	0.59	2.27	7	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:768:LYS:HD2	1:A:771:PHE:CD2	0.59	2.33	9	3
1:A:761:LEU:HD13	1:A:771:PHE:HZ	0.59	1.58	7	4
1:A:745:VAL:HG11	1:A:750:LEU:CD1	0.59	2.26	13	1
1:A:779:TYR:CD2	1:A:801:VAL:HG13	0.58	2.32	20	6
1:A:705:SER:HB2	1:A:715:VAL:HG22	0.58	1.76	10	2
1:A:750:LEU:HD22	1:A:794:ASN:ND2	0.58	2.13	10	1
1:A:765:LEU:HD22	1:A:771:PHE:CE2	0.57	2.34	6	7
1:A:750:LEU:HD23	1:A:773:HIS:CG	0.57	2.34	8	2
1:A:781:CYS:HB3	1:A:784:LYS:HD3	0.57	1.76	15	3
1:A:745:VAL:HG11	1:A:750:LEU:HD13	0.57	1.76	13	1
1:A:765:LEU:HD11	1:A:777:ILE:HB	0.56	1.77	16	1
1:A:751:LYS:HB2	1:A:794:ASN:C	0.56	2.26	2	11
1:A:756:SER:HB2	1:A:759:ILE:CG1	0.56	2.31	18	4
1:A:756:SER:HB2	1:A:759:ILE:HG13	0.55	1.76	18	4
1:A:765:LEU:HD22	1:A:771:PHE:HE2	0.55	1.62	6	4
1:A:728:HIS:O	1:A:742:PRO:HB3	0.55	2.02	3	12
1:A:704:LEU:HD13	1:A:705:SER:N	0.54	2.17	19	2
1:A:708:PRO:HG2	1:A:710:TYR:CE2	0.54	2.37	1	5
1:A:723:PHE:HA	1:A:745:VAL:O	0.54	2.03	13	1
1:A:747:ILE:HA	1:A:750:LEU:CD1	0.53	2.33	3	8
1:A:756:SER:HB3	1:A:759:ILE:CG1	0.53	2.33	19	7
1:A:750:LEU:HD22	1:A:794:ASN:OD1	0.53	2.04	20	6
1:A:705:SER:CB	1:A:715:VAL:HG22	0.53	2.33	17	5
1:A:724:THR:O	1:A:744:CYS:HA	0.53	2.04	19	3
1:A:694:ILE:CG2	1:A:715:VAL:HG21	0.53	2.33	14	5
1:A:761:LEU:HD13	1:A:771:PHE:CZ	0.53	2.39	7	3
1:A:779:TYR:CE1	1:A:788:ILE:HB	0.52	2.39	5	10
1:A:781:CYS:HB3	1:A:784:LYS:HB2	0.52	1.80	14	2
1:A:745:VAL:CG1	1:A:749:LYS:HG3	0.52	2.34	16	1
1:A:697:LEU:HD21	1:A:744:CYS:SG	0.52	2.45	14	5
1:A:797:TRP:HB2	1:A:800:GLU:HA	0.52	1.82	4	13
1:A:745:VAL:HB	1:A:750:LEU:HD21	0.51	1.82	20	2
1:A:707:PRO:HB3	1:A:709:TYR:CE2	0.51	2.40	11	1
1:A:752:LYS:HE2	1:A:770:GLU:HB3	0.51	1.82	19	2
1:A:750:LEU:HD23	1:A:773:HIS:HB2	0.51	1.82	4	1
1:A:778:ARG:HB2	1:A:787:TRP:HB3	0.50	1.83	15	4
1:A:773:HIS:HD1	1:A:793:ILE:HA	0.50	1.66	7	3
1:A:720:SER:O	1:A:721:GLU:HG3	0.50	2.05	8	1
1:A:747:ILE:CA	1:A:750:LEU:HG	0.49	2.36	19	7
1:A:751:LYS:HB3	1:A:795:GLY:N	0.49	2.21	17	1
1:A:740:GLN:NE2	1:A:740:GLN:H	0.49	2.06	20	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:695:PRO:HD3	1:A:738:TRP:CD1	0.49	2.42	16	6
1:A:701:TRP:HE1	1:A:718:ASN:CG	0.49	2.15	15	1
1:A:708:PRO:HG2	1:A:710:TYR:CE1	0.49	2.43	10	1
1:A:750:LEU:HD23	1:A:773:HIS:CD2	0.48	2.43	8	2
1:A:714:SER:HA	1:A:731:ILE:O	0.48	2.08	9	2
1:A:746:ALA:O	1:A:747:ILE:HB	0.48	2.07	2	7
1:A:716:GLU:HG3	1:A:729:ARG:HG2	0.48	1.85	16	1
1:A:697:LEU:HD13	1:A:700:GLY:HA3	0.48	1.85	13	3
1:A:690:THR:HG21	1:A:708:PRO:HB2	0.47	1.85	10	1
1:A:726:ILE:HB	1:A:743:GLN:HB3	0.47	1.86	15	1
1:A:724:THR:HG21	1:A:750:LEU:HD21	0.47	1.86	2	5
1:A:740:GLN:O	1:A:741:LEU:HB2	0.47	2.09	4	1
1:A:707:PRO:HA	1:A:708:PRO:C	0.47	2.35	11	1
1:A:778:ARG:HA	1:A:789:HIS:HA	0.47	1.86	5	2
1:A:779:TYR:CD1	1:A:801:VAL:HG22	0.47	2.45	7	2
1:A:750:LEU:CG	1:A:794:ASN:HD22	0.46	2.15	15	2
1:A:741:LEU:HB3	1:A:742:PRO:HD2	0.46	1.86	12	1
1:A:751:LYS:HB3	1:A:795:GLY:CA	0.46	2.40	17	1
1:A:750:LEU:HA	1:A:794:ASN:ND2	0.46	2.25	9	1
1:A:762:GLU:CD	1:A:778:ARG:HE	0.46	2.19	1	1
1:A:750:LEU:HD12	1:A:773:HIS:HD2	0.46	1.70	9	1
1:A:697:LEU:HD22	1:A:717:PHE:HB3	0.46	1.88	12	7
1:A:790:THR:HG21	1:A:801:VAL:CG2	0.46	2.41	4	2
1:A:761:LEU:HB3	1:A:765:LEU:HB2	0.46	1.85	8	2
1:A:752:LYS:O	1:A:795:GLY:HA2	0.46	2.10	13	2
1:A:747:ILE:HG23	1:A:773:HIS:NE2	0.46	2.26	20	1
1:A:746:ALA:C	1:A:748:ASP:H	0.46	2.17	9	11
1:A:750:LEU:HD23	1:A:773:HIS:CB	0.46	2.41	5	4
1:A:697:LEU:HD12	1:A:717:PHE:HB3	0.46	1.87	13	1
1:A:750:LEU:HD22	1:A:794:ASN:CG	0.45	2.36	18	1
1:A:756:SER:HB2	1:A:759:ILE:HG12	0.45	1.86	17	2
1:A:750:LEU:HA	1:A:794:ASN:HD22	0.45	1.71	6	2
1:A:707:PRO:HA	1:A:709:TYR:N	0.45	2.27	14	2
1:A:726:ILE:HD12	1:A:793:ILE:HG23	0.45	1.86	10	1
1:A:764:HIS:CD2	1:A:765:LEU:HG	0.45	2.46	7	1
1:A:731:ILE:HG22	1:A:741:LEU:HA	0.45	1.87	12	1
1:A:745:VAL:CG1	1:A:750:LEU:HD21	0.45	2.28	18	1
1:A:710:TYR:O	1:A:713:ASP:HB2	0.45	2.12	12	2
1:A:715:VAL:O	1:A:730:SER:HA	0.45	2.12	9	2
1:A:759:ILE:HG12	1:A:801:VAL:HG11	0.45	1.89	4	3
1:A:724:THR:HG22	1:A:745:VAL:O	0.44	2.12	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:747:ILE:O	1:A:750:LEU:HB2	0.44	2.12	13	3
1:A:773:HIS:HA	1:A:792:CYS:SG	0.44	2.53	9	1
1:A:762:GLU:O	1:A:766:LYS:HG3	0.44	2.12	1	2
1:A:731:ILE:HA	1:A:739:THR:OG1	0.44	2.13	10	5
1:A:769:LYS:HG3	1:A:770:GLU:HG3	0.44	1.90	11	1
1:A:781:CYS:HB2	1:A:784:LYS:HB2	0.44	1.90	5	2
1:A:711:TYR:HA	1:A:733:CYS:SG	0.43	2.52	10	1
1:A:759:ILE:HD12	1:A:761:LEU:HD11	0.43	1.90	10	1
1:A:690:THR:CG2	1:A:708:PRO:HB2	0.43	2.43	14	1
1:A:709:TYR:HB3	1:A:738:TRP:CZ2	0.43	2.49	2	3
1:A:789:HIS:O	1:A:799:PRO:HD2	0.43	2.14	10	1
1:A:773:HIS:ND1	1:A:793:ILE:HA	0.43	2.28	17	1
1:A:719:CYS:HB3	1:A:723:PHE:HB2	0.43	1.89	8	4
1:A:790:THR:HG21	1:A:801:VAL:CG1	0.42	2.44	9	1
1:A:778:ARG:HB3	1:A:787:TRP:HB3	0.42	1.91	14	1
1:A:707:PRO:HB2	1:A:708:PRO:HA	0.41	1.92	17	2
1:A:771:PHE:CD2	1:A:777:ILE:HG21	0.41	2.50	8	1
1:A:779:TYR:CE1	1:A:801:VAL:HG12	0.41	2.50	13	1
1:A:768:LYS:HG2	1:A:771:PHE:CD2	0.41	2.51	20	1
1:A:705:SER:HB2	1:A:709:TYR:CE1	0.41	2.51	13	1
1:A:708:PRO:HG2	1:A:710:TYR:CZ	0.41	2.51	16	1
1:A:790:THR:OG1	1:A:797:TRP:HB3	0.41	2.15	5	1
1:A:760:ILE:HB	1:A:780:ARG:HG2	0.41	1.92	7	1
1:A:794:ASN:HD22	1:A:794:ASN:N	0.41	2.14	1	1
1:A:694:ILE:HG12	1:A:705:SER:CB	0.41	2.46	8	1
1:A:740:GLN:H	1:A:740:GLN:CD	0.41	2.24	13	1
1:A:716:GLU:HG2	1:A:730:SER:HB3	0.41	1.93	15	1
1:A:697:LEU:HG	1:A:717:PHE:HD2	0.41	1.76	18	1
1:A:776:ASN:HA	1:A:791:VAL:HG12	0.41	1.92	4	1
1:A:776:ASN:HD22	1:A:776:ASN:N	0.40	2.14	12	1
1:A:739:THR:HB	1:A:740:GLN:NE2	0.40	2.31	20	1
1:A:732:THR:O	1:A:739:THR:HG23	0.40	2.16	15	2
1:A:740:GLN:H	1:A:740:GLN:NE2	0.40	2.15	7	1
1:A:750:LEU:HG	1:A:794:ASN:CG	0.40	2.41	1	1
1:A:719:CYS:SG	1:A:725:MET:HA	0.40	2.56	2	1
1:A:759:ILE:HG12	1:A:801:VAL:CG1	0.40	2.46	7	1
1:A:754:LYS:HA	1:A:769:LYS:O	0.40	2.17	17	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	111/115 (97%)	91±2 (82±2%)	16±2 (14±2%)	4±1 (4±1%)	4	32
All	All	2220/2300 (97%)	1819 (82%)	318 (14%)	83 (4%)	4	32

All 17 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	747	ILE	20
1	A	789	HIS	16
1	A	720	SER	10
1	A	695	PRO	7
1	A	706	SER	7
1	A	693	ASP	4
1	A	736	GLY	3
1	A	741	LEU	3
1	A	724	THR	2
1	A	725	MET	2
1	A	709	TYR	2
1	A	705	SER	2
1	A	783	GLY	1
1	A	691	CYS	1
1	A	785	GLU	1
1	A	742	PRO	1
1	A	704	LEU	1

6.3.2 Protein sidechains [i](#)

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	102/105 (97%)	94±2 (92±2%)	8±2 (8±2%)	13	61
All	All	2040/2100 (97%)	1879 (92%)	161 (8%)	13	61

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	734	ILE	19
1	A	776	ASN	18
1	A	740	GLN	17
1	A	724	THR	16
1	A	794	ASN	10
1	A	729	ARG	10
1	A	764	HIS	8
1	A	694	ILE	8
1	A	750	LEU	7
1	A	728	HIS	5
1	A	749	LYS	5
1	A	713	ASP	4
1	A	766	LYS	4
1	A	697	LEU	4
1	A	769	LYS	4
1	A	753	CYS	4
1	A	690	THR	3
1	A	763	GLU	2
1	A	704	LEU	2
1	A	737	VAL	1
1	A	785	GLU	1
1	A	705	SER	1
1	A	755	SER	1
1	A	782	ARG	1
1	A	773	HIS	1
1	A	761	LEU	1
1	A	801	VAL	1
1	A	774	ASN	1
1	A	781	CYS	1
1	A	784	LYS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 86% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1372
Number of shifts mapped to atoms	1347
Number of unparsed shifts	0
Number of shifts with mapping errors	25
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

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

- No matching atom found in the structure. All 25 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	3	GLU	H	8.525	0.003	1
1	A	3	GLU	HA	4.164	0.008	1
1	A	3	GLU	HB2	1.935	0.011	2
1	A	3	GLU	HG2	2.234	0.003	2
1	A	3	GLU	C	175.758	0.001	1
1	A	3	GLU	CA	56.68	0.040	1
1	A	3	GLU	CB	30.19	0.037	1
1	A	3	GLU	CG	36.24	0.052	1
1	A	3	GLU	N	120.983	0.035	1
1	A	4	ALA	H	8.312	0.005	1
1	A	4	ALA	HA	4.218	0.011	1
1	A	4	ALA	HB1	1.315	0.003	1
1	A	4	ALA	HB2	1.315	0.003	1
1	A	4	ALA	HB3	1.315	0.003	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	ALA	C	174.782	0.002	1
1	A	4	ALA	CA	52.307	0.052	1
1	A	4	ALA	CB	19.258	0.045	1
1	A	4	ALA	N	125.434	0.029	1
1	A	6	GLY	H	7.778	0.010	1
1	A	6	GLY	HA2	3.309	0.004	2
1	A	6	GLY	HA3	3.608	0.008	2
1	A	6	GLY	C	178.709	0.003	1
1	A	6	GLY	CA	45.233	0.041	1
1	A	6	GLY	N	107.415	0.013	1
1	A	690	THR	H	7.721	0.004	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
$^{13}\text{C}_\alpha$	118	0.05 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	109	0.00 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	-1.66 ± 0.33	Should be applied
^{15}N	112	0.10 ± 0.44	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 86%, i.e. 1322 atoms were assigned a chemical shift out of a possible 1532. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	553/558 (99%)	226/227 (100%)	221/224 (99%)	106/107 (99%)
Sidechain	661/812 (81%)	436/524 (83%)	216/256 (84%)	9/32 (28%)
Aromatic	108/162 (67%)	54/79 (68%)	50/67 (75%)	4/16 (25%)
Overall	1322/1532 (86%)	716/830 (86%)	487/547 (89%)	119/155 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 86%, i.e. 1348 atoms were assigned a chemical shift out of a possible 1560. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	568/573 (99%)	232/233 (100%)	227/230 (99%)	109/110 (99%)
Sidechain	672/825 (81%)	443/532 (83%)	219/260 (84%)	10/33 (30%)
Aromatic	108/162 (67%)	54/79 (68%)	50/67 (75%)	4/16 (25%)
Overall	1348/1560 (86%)	729/844 (86%)	496/557 (89%)	123/159 (77%)

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
1	A	794	ASN	H	12.14	5.28 – 11.36	6.3
1	A	780	ARG	HD2	1.74	1.97 – 4.26	-6.0
1	A	718	ASN	HB2	0.99	1.27 – 4.34	-5.9

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:

