



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 03:32 PM BST

PDB ID : 1HUE  
Title : HISTONE-LIKE PROTEIN  
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Deposited on : 1995-05-26

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

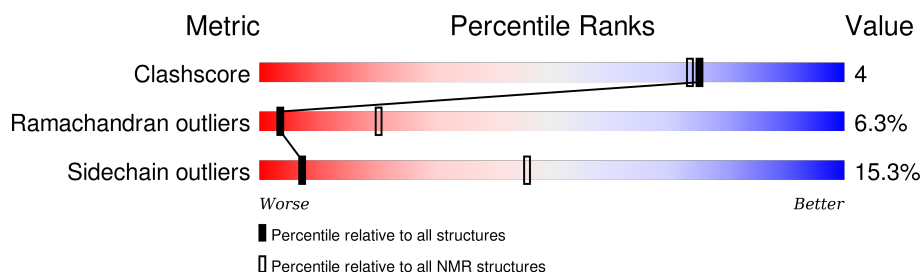
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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  $\geq 3$ , 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	90	
1	B	90	

## 2 Ensemble composition and analysis

This entry contains 25 models. Model 16 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:2-A:53, A:75-A:90, B:1-B:53, B:75-B:90 (137)	0.27	16

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, 5, 6, 7, 8, 10, 13, 14, 15, 16, 17, 18, 19, 21, 22, 23, 24, 25
2	9, 20
Single-model clusters	4; 11; 12

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2774 atoms, of which 1412 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called HU PROTEIN.

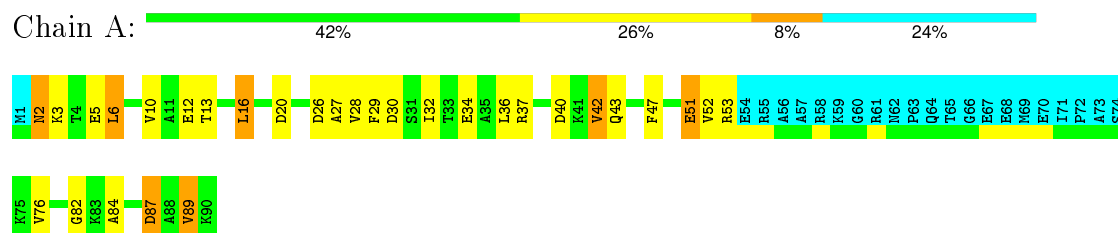
Mol	Chain	Residues	Atoms						Trace
1	A	90	Total	C	H	N	O	S	0
			1387	425	706	123	131	2	
1	B	90	Total	C	H	N	O	S	0
			1387	425	706	123	131	2	

## 4 Residue-property plots [i](#)

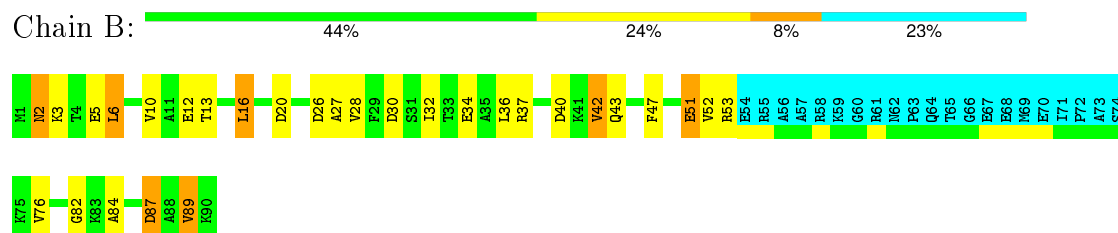
### 4.1 Average score per residue in the NMR ensemble

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: HU PROTEIN



#### • Molecule 1: HU PROTEIN

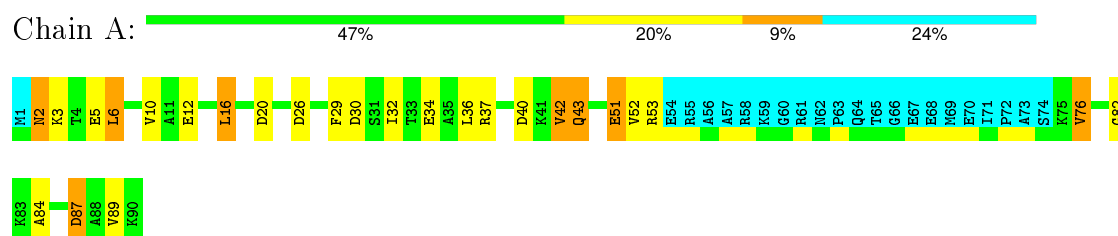


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

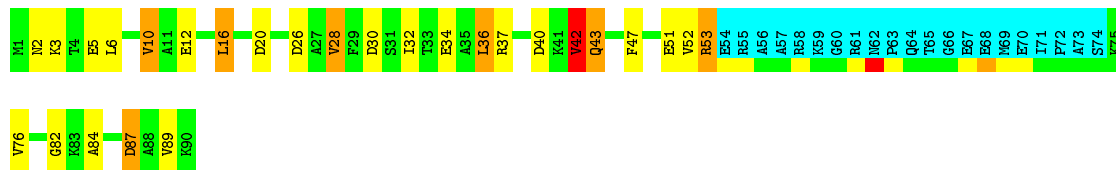
#### 4.2.1 Score per residue for model 1

#### • Molecule 1: HU PROTEIN



- Molecule 1: HU PROTEIN

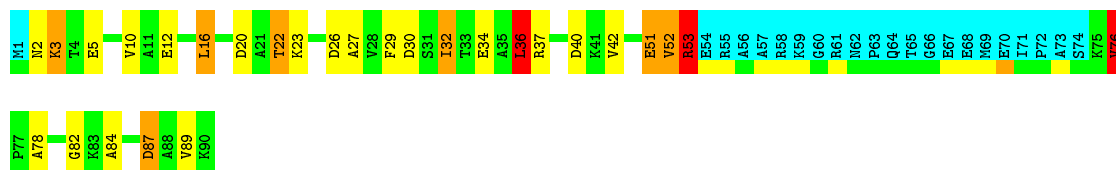
Chain B: 



#### 4.2.2 Score per residue for model 2

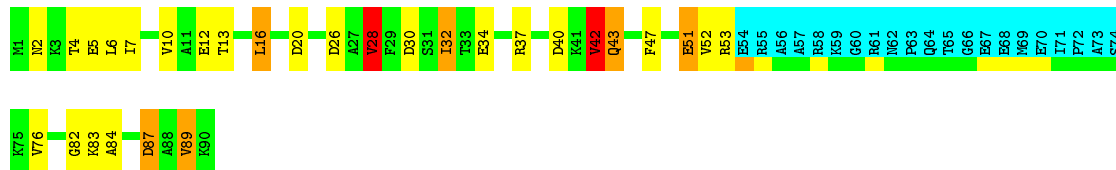
- Molecule 1: HU PROTEIN

Chain A: 



- Molecule 1: HU PROTEIN

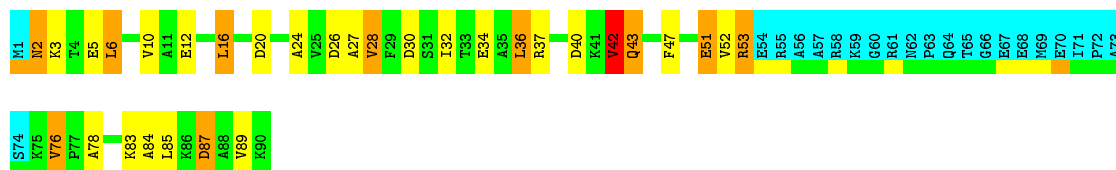
Chain B: 



#### 4.2.3 Score per residue for model 3

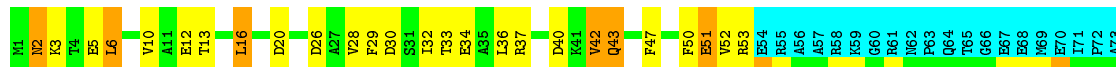
- Molecule 1: HU PROTEIN

Chain A: 



- Molecule 1: HU PROTEIN

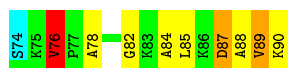
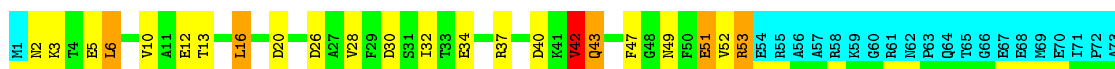
Chain B: 



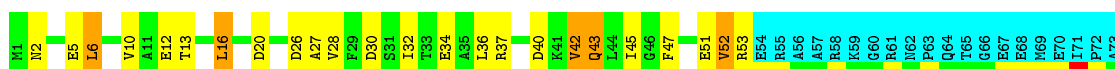


#### 4.2.4 Score per residue for model 4

- Molecule 1: HU PROTEIN

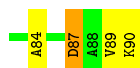
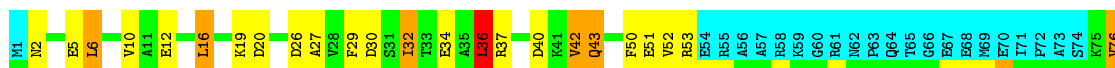


- Molecule 1: HU PROTEIN

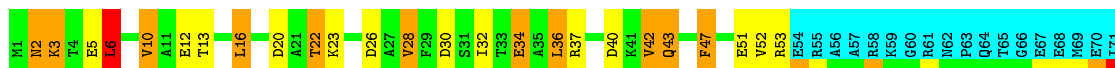


#### 4.2.5 Score per residue for model 5

- Molecule 1: HU PROTEIN

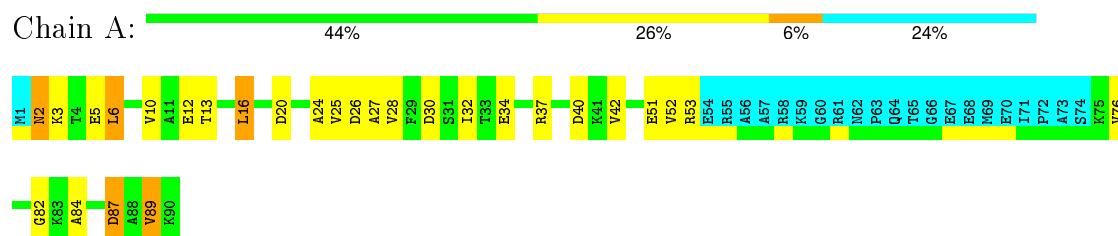


- Molecule 1: HU PROTEIN

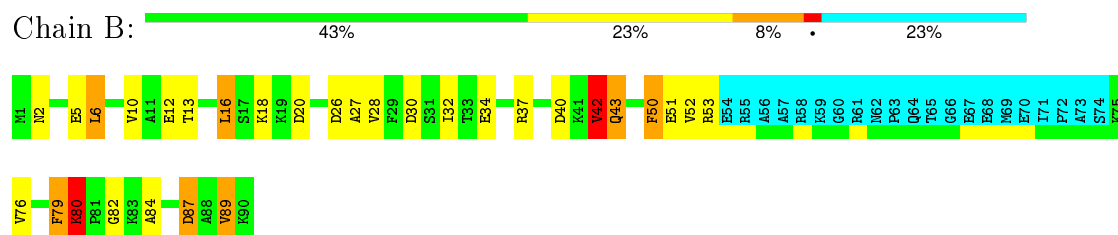


### 4.2.6 Score per residue for model 6

#### • Molecule 1: HU PROTEIN

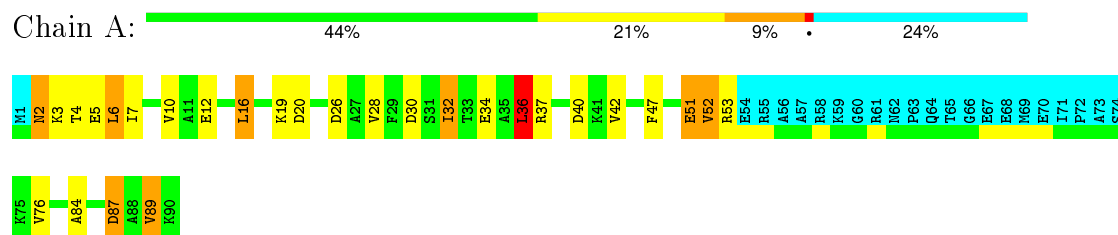


#### • Molecule 1: HU PROTEIN

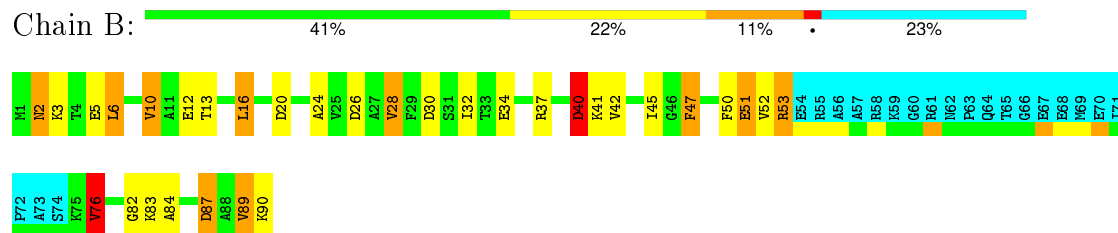


### 4.2.7 Score per residue for model 7

#### • Molecule 1: HU PROTEIN



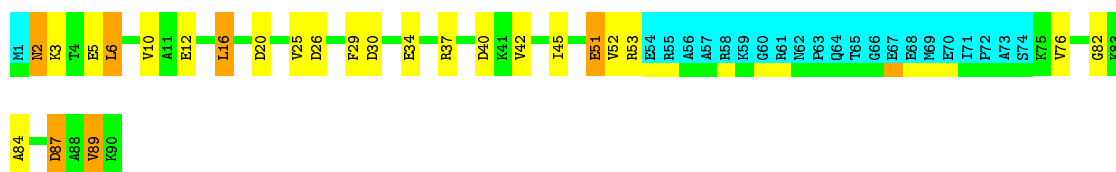
#### • Molecule 1: HU PROTEIN



### 4.2.8 Score per residue for model 8

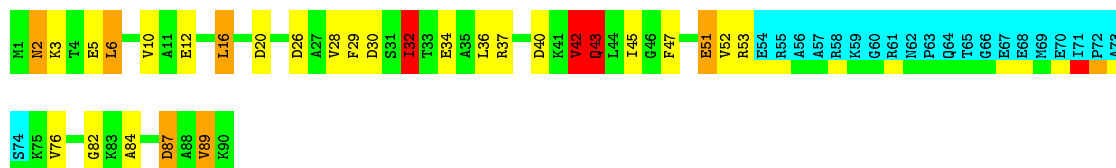
#### • Molecule 1: HU PROTEIN





• Molecule 1: HU PROTEIN

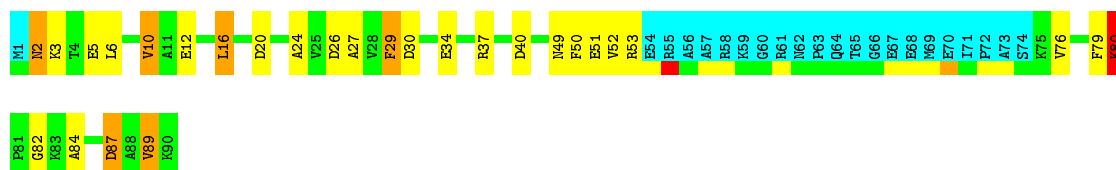
Chain B: 44% 22% 7% • 23%



#### 4.2.9 Score per residue for model 9

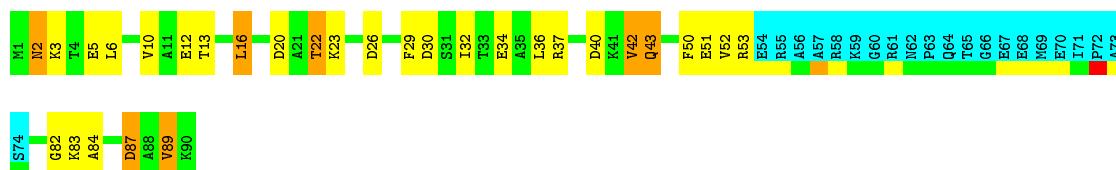
• Molecule 1: HU PROTEIN

Chain A: 44% 23% 7% • 24%



• Molecule 1: HU PROTEIN

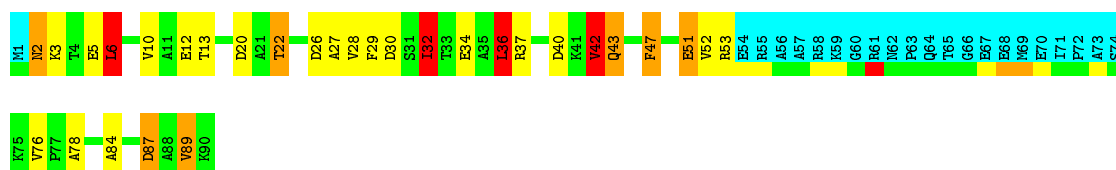
Chain B: 43% 26% 8% 23%



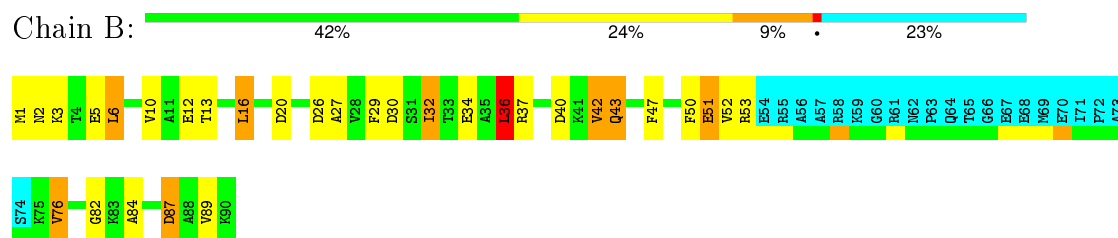
#### 4.2.10 Score per residue for model 10

• Molecule 1: HU PROTEIN

Chain A: 42% 21% 8% • 24%

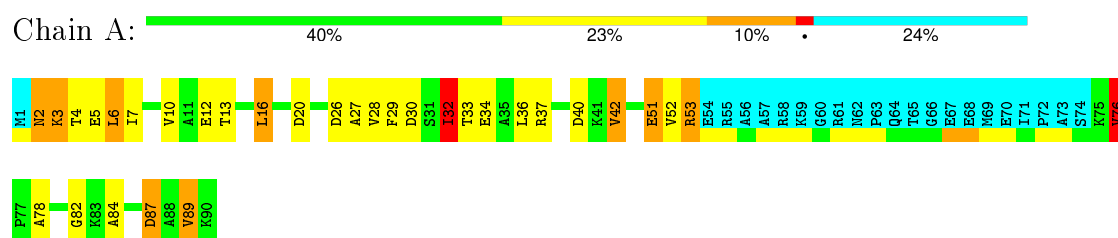


- Molecule 1: HU PROTEIN

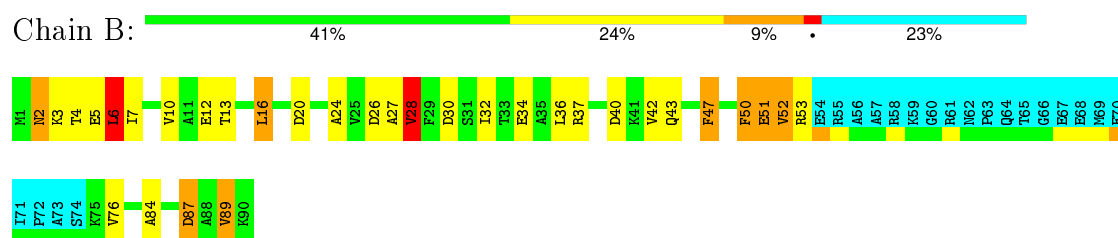


#### 4.2.11 Score per residue for model 11

- Molecule 1: HU PROTEIN

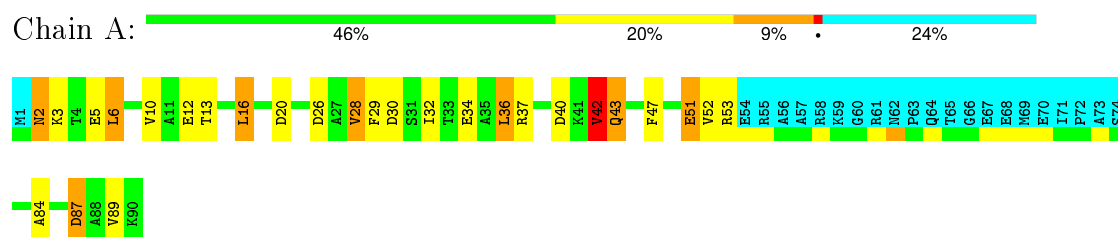


- Molecule 1: HU PROTEIN

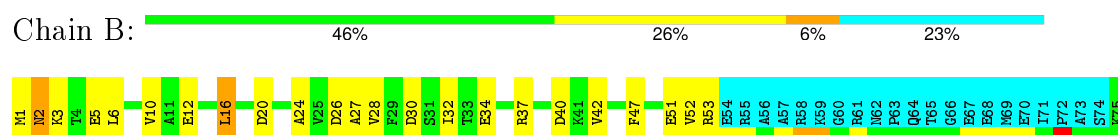


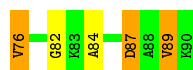
#### 4.2.12 Score per residue for model 12

- Molecule 1: HU PROTEIN



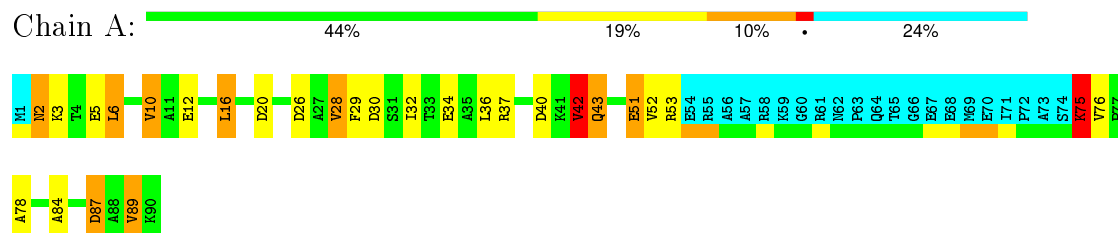
- Molecule 1: HU PROTEIN



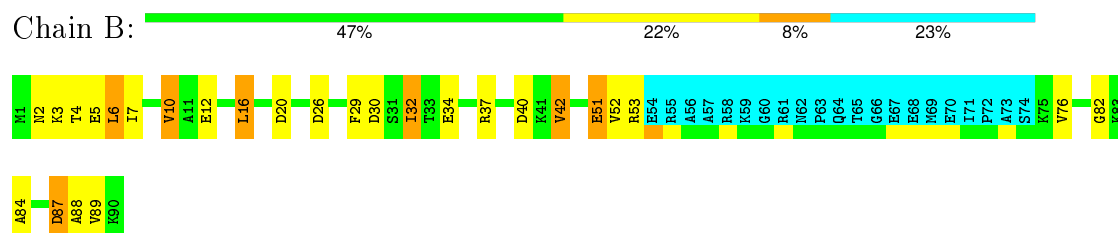


#### 4.2.13 Score per residue for model 13

- Molecule 1: HU PROTEIN

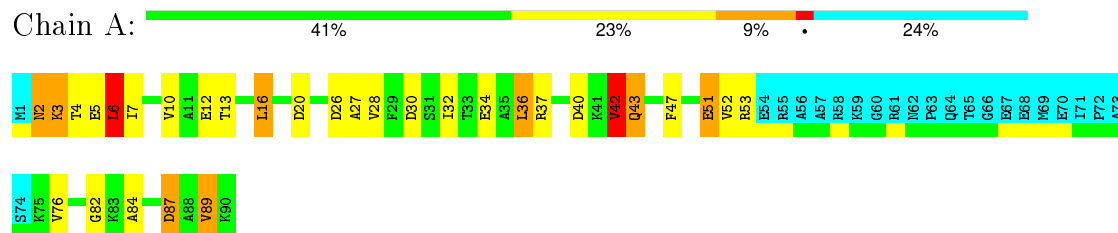


- Molecule 1: HU PROTEIN

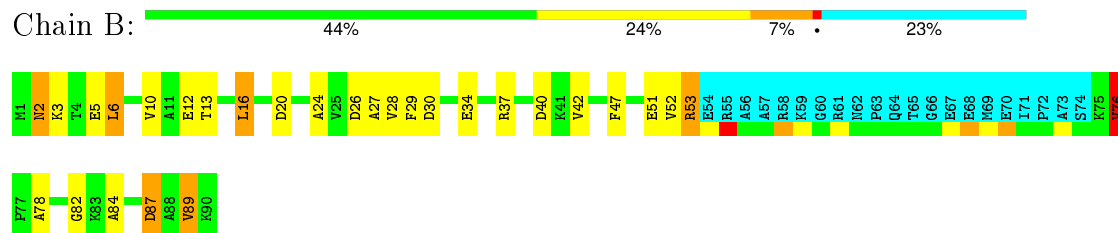


#### 4.2.14 Score per residue for model 14

- Molecule 1: HU PROTEIN

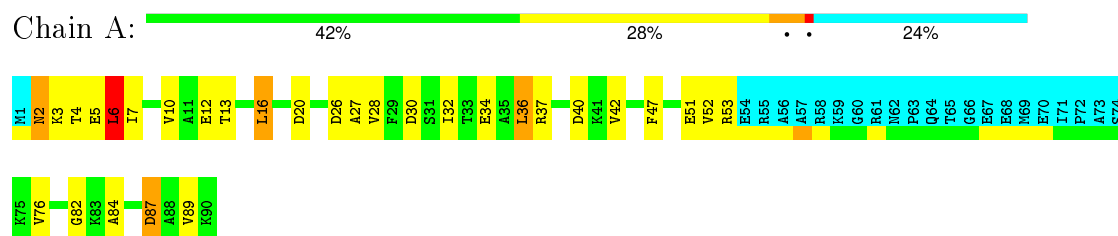


- Molecule 1: HU PROTEIN

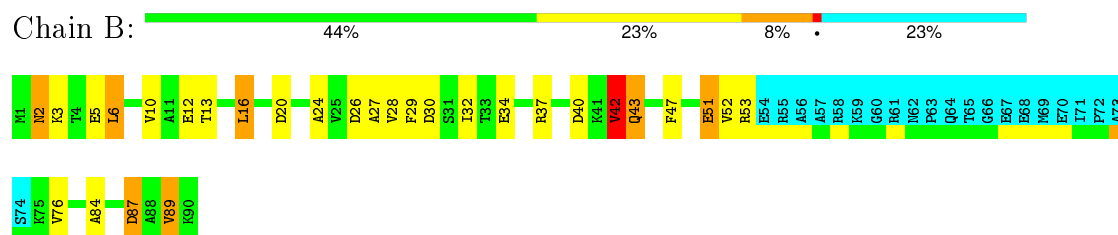


### 4.2.15 Score per residue for model 15

#### • Molecule 1: HU PROTEIN

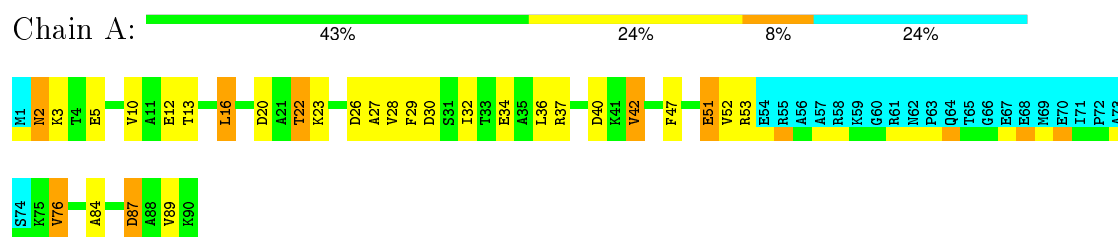


#### • Molecule 1: HU PROTEIN

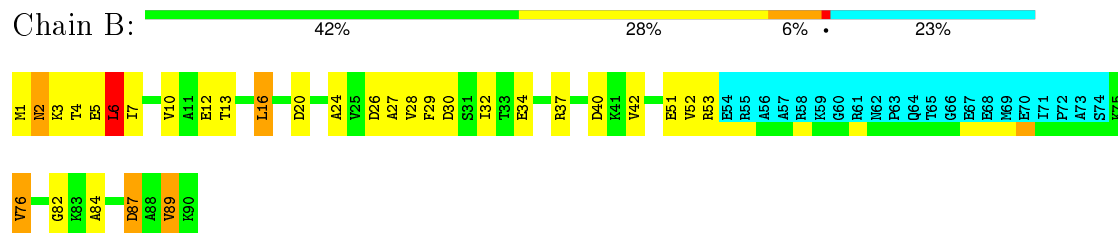


### 4.2.16 Score per residue for model 16 (medoid)

#### • Molecule 1: HU PROTEIN



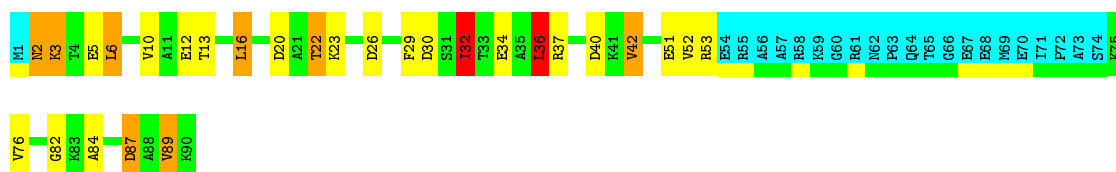
#### • Molecule 1: HU PROTEIN



### 4.2.17 Score per residue for model 17

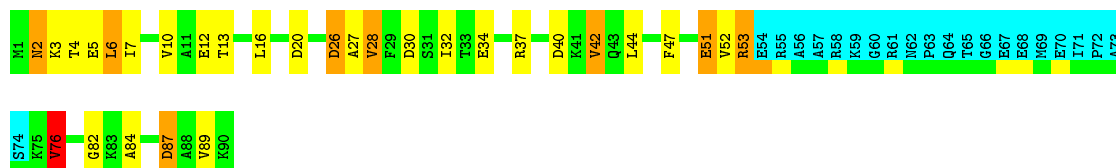
#### • Molecule 1: HU PROTEIN





• Molecule 1: HU PROTEIN

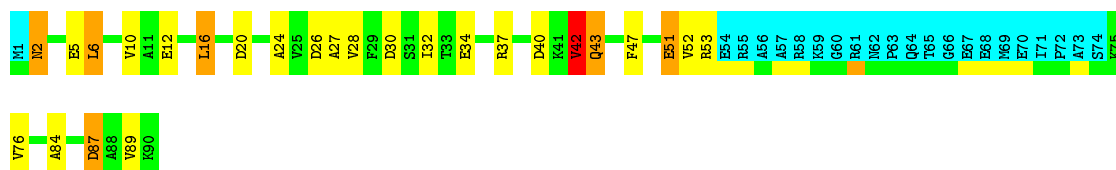
Chain B: 43% 23% 9% • 23%



#### 4.2.18 Score per residue for model 18

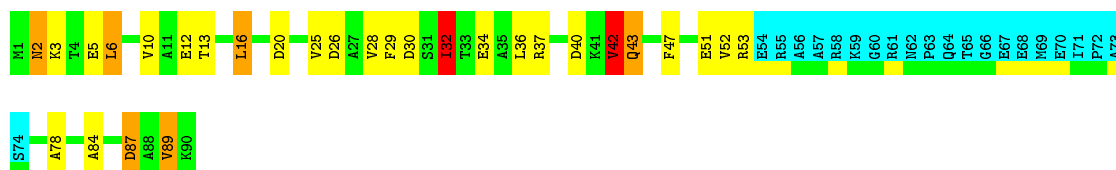
• Molecule 1: HU PROTEIN

Chain A: 47% 21% 7% • 24%



• Molecule 1: HU PROTEIN

Chain B: 44% 23% 7% • 23%



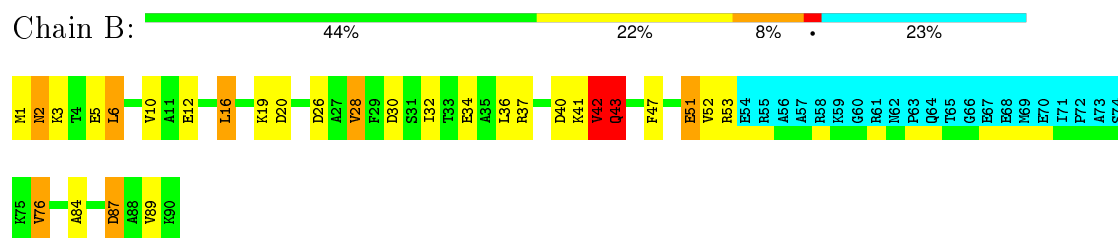
#### 4.2.19 Score per residue for model 19

• Molecule 1: HU PROTEIN

Chain A: 48% 20% 8% 24%

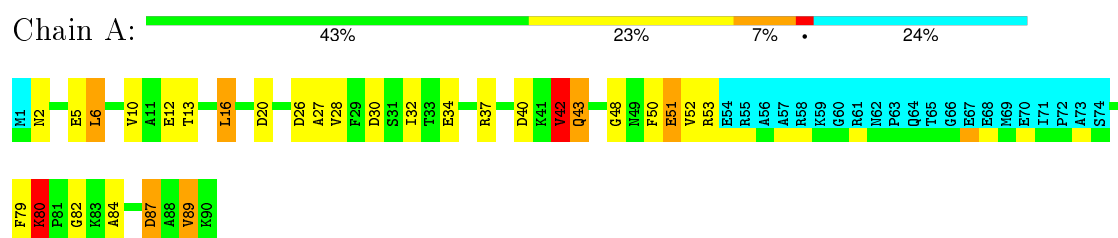


- Molecule 1: HU PROTEIN

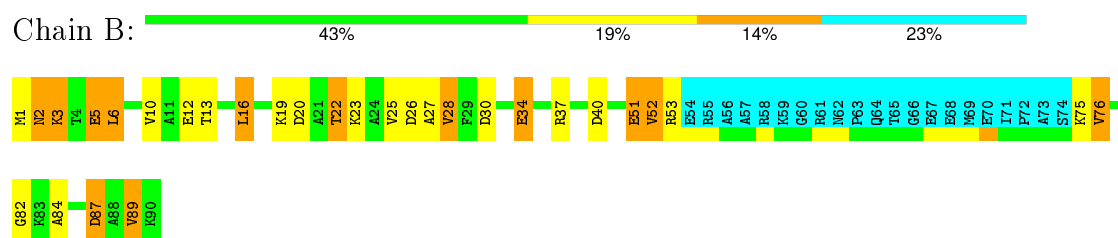


#### 4.2.20 Score per residue for model 20

- Molecule 1: HU PROTEIN

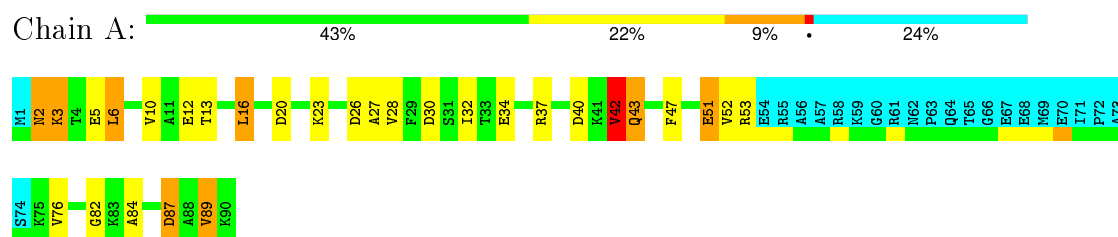


- Molecule 1: HU PROTEIN

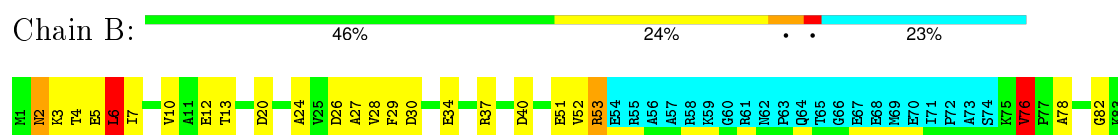


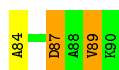
#### 4.2.21 Score per residue for model 21

- Molecule 1: HU PROTEIN



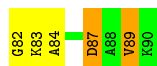
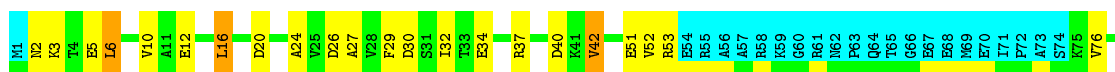
- Molecule 1: HU PROTEIN



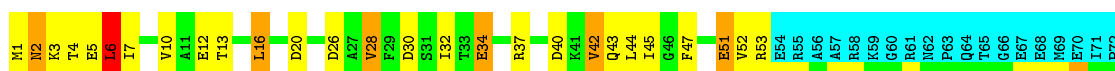


#### 4.2.22 Score per residue for model 22

- Molecule 1: HU PROTEIN

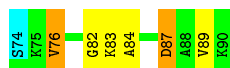
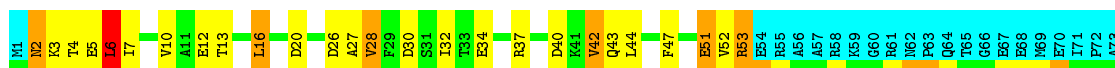


- Molecule 1: HU PROTEIN

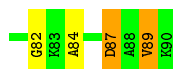
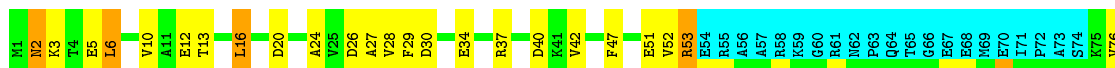


#### 4.2.23 Score per residue for model 23

- Molecule 1: HU PROTEIN

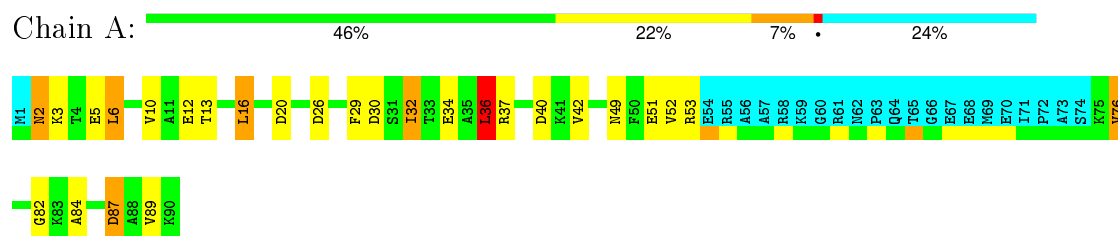


- Molecule 1: HU PROTEIN

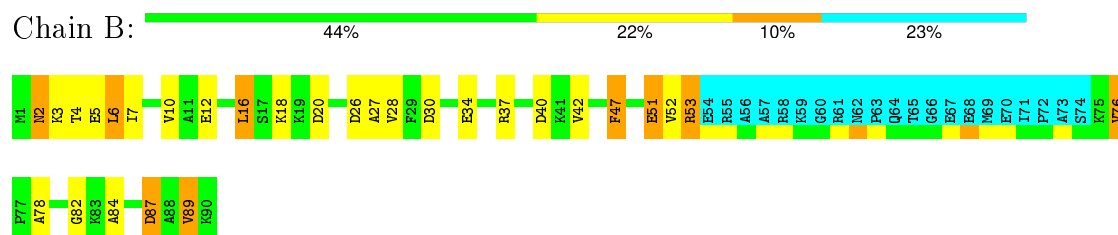


## 4.2.24 Score per residue for model 24

## • Molecule 1: HU PROTEIN

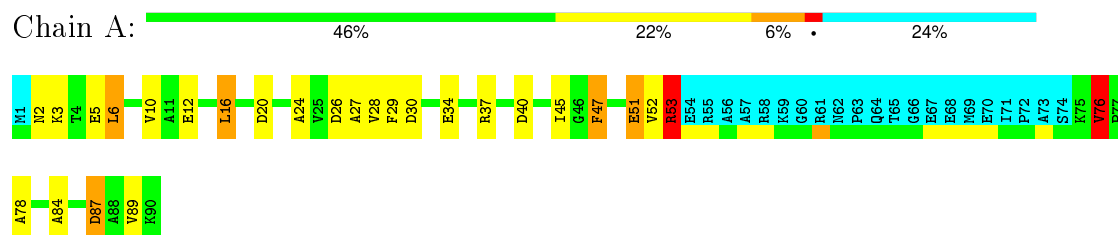


## • Molecule 1: HU PROTEIN

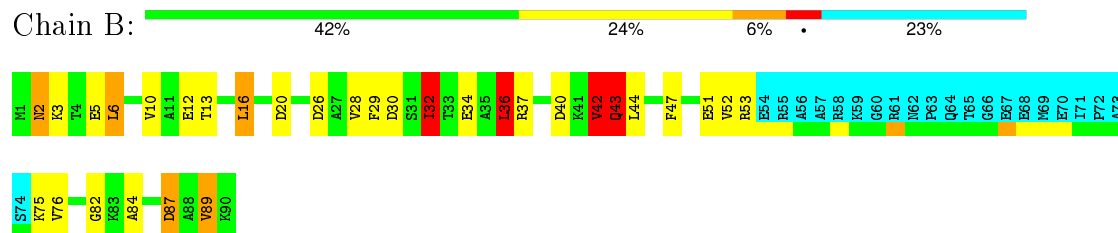


## 4.2.25 Score per residue for model 25

## • Molecule 1: HU PROTEIN



## • Molecule 1: HU PROTEIN



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 25 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
DGII	refinement	

No chemical shift data was provided. 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	1.49±0.01	9±0/517 (1.7±0.0%)	1.86±0.06	22±3/692 (3.2±0.4%)
1	B	1.49±0.01	9±0/525 (1.7±0.0%)	1.84±0.06	22±2/702 (3.1±0.3%)
All	All	1.49	450/26050 (1.7%)	1.85	1093/34850 (3.1%)

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	1.0±0.7
1	B	0.1±0.4	1.5±0.8
All	All	2	63

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	B	51	GLU	CD-OE2	11.01	1.37	1.25	21	25
1	A	5	GLU	CD-OE2	11.00	1.37	1.25	9	25
1	B	34	GLU	CD-OE2	10.98	1.37	1.25	2	25
1	B	12	GLU	CD-OE2	10.97	1.37	1.25	22	25
1	A	51	GLU	CD-OE2	10.97	1.37	1.25	2	25
1	A	12	GLU	CD-OE2	10.96	1.37	1.25	13	25
1	A	34	GLU	CD-OE2	10.96	1.37	1.25	23	25
1	B	5	GLU	CD-OE2	10.96	1.37	1.25	3	25
1	A	20	ASP	CG-OD2	5.41	1.37	1.25	6	25
1	B	20	ASP	CG-OD2	5.40	1.37	1.25	4	25
1	B	40	ASP	CG-OD2	5.40	1.37	1.25	9	25
1	A	30	ASP	CG-OD2	5.39	1.37	1.25	16	25
1	B	30	ASP	CG-OD2	5.37	1.37	1.25	1	25
1	B	87	ASP	CG-OD2	5.37	1.37	1.25	1	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	40	ASP	CG-OD2	5.37	1.37	1.25	1	25
1	A	87	ASP	CG-OD2	5.37	1.37	1.25	17	25
1	A	26	ASP	CG-OD2	5.37	1.37	1.25	5	25
1	B	26	ASP	CG-OD2	5.36	1.37	1.25	22	25

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	22	THR	CA-CB-CG2	13.73	131.62	112.40	10	4
1	B	22	THR	CA-CB-CG2	13.43	131.21	112.40	5	3
1	B	36	LEU	CB-CG-CD2	12.73	132.64	111.00	1	5
1	A	36	LEU	CB-CG-CD2	12.68	132.56	111.00	12	12
1	A	16	LEU	CB-CG-CD2	10.11	128.19	111.00	2	24
1	A	36	LEU	CB-CG-CD1	9.88	127.79	111.00	16	3
1	B	36	LEU	CB-CG-CD1	9.74	127.56	111.00	19	8
1	A	76	VAL	CA-CB-CG2	9.72	125.48	110.90	3	6
1	B	16	LEU	CB-CG-CD2	9.53	127.20	111.00	12	23
1	B	76	VAL	CA-CB-CG2	9.52	125.17	110.90	24	5
1	B	16	LEU	CB-CA-C	9.15	127.58	110.20	12	23
1	A	16	LEU	CB-CA-C	9.05	127.40	110.20	5	24
1	A	32	ILE	CA-CB-CG1	8.96	128.01	111.00	7	8
1	B	32	ILE	CA-CB-CG1	8.56	127.27	111.00	8	8
1	B	51	GLU	CB-CA-C	8.36	127.11	110.40	11	1
1	B	52	VAL	CB-CA-C	8.32	127.21	111.40	11	2
1	B	53	ARG	NE-CZ-NH1	8.13	124.36	120.30	23	25
1	B	37	ARG	NE-CZ-NH1	8.04	124.32	120.30	7	25
1	A	37	ARG	NE-CZ-NH1	8.00	124.30	120.30	19	25
1	A	53	ARG	NE-CZ-NH1	7.86	124.23	120.30	10	25
1	A	53	ARG	CB-CA-C	7.84	126.08	110.40	23	1
1	A	30	ASP	CB-CG-OD2	-7.68	111.39	118.30	6	25
1	A	40	ASP	CB-CG-OD2	-7.52	111.53	118.30	15	25
1	B	53	ARG	CB-CA-C	7.50	125.40	110.40	17	1
1	B	50	PHE	N-CA-CB	7.49	124.09	110.60	6	1
1	B	42	VAL	CB-CA-C	7.45	125.56	111.40	5	5
1	A	50	PHE	N-CA-CB	7.42	123.96	110.60	20	1
1	A	42	VAL	CG1-CB-CG2	-7.39	99.08	110.90	1	23
1	A	80	LYS	N-CA-C	7.32	130.76	111.00	9	2
1	A	89	VAL	N-CA-CB	-7.31	95.41	111.50	1	25
1	A	2	ASN	N-CA-CB	7.30	123.74	110.60	6	17
1	B	89	VAL	N-CA-CB	-7.29	95.46	111.50	19	24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	2	ASN	N-CA-CB	7.22	123.60	110.60	12	19
1	B	20	ASP	CB-CG-OD2	-7.22	111.80	118.30	17	25
1	A	80	LYS	CA-CB-CG	7.15	129.13	113.40	9	2
1	A	76	VAL	N-CA-CB	-7.13	95.80	111.50	13	8
1	A	43	GLN	N-CA-CB	7.06	123.31	110.60	13	11
1	A	30	ASP	CB-CG-OD1	7.03	124.63	118.30	6	25
1	B	80	LYS	N-CA-C	7.03	129.98	111.00	6	1
1	B	42	VAL	CG1-CB-CG2	-7.01	99.68	110.90	9	22
1	A	87	ASP	CB-CG-OD2	-6.94	112.05	118.30	23	25
1	B	87	ASP	CB-CG-OD2	-6.93	112.06	118.30	10	25
1	B	26	ASP	CB-CG-OD2	-6.92	112.08	118.30	11	25
1	B	40	ASP	CB-CG-OD2	-6.90	112.09	118.30	19	25
1	B	30	ASP	CB-CG-OD2	-6.89	112.10	118.30	23	25
1	B	43	GLN	N-CA-CB	6.89	123.00	110.60	4	13
1	A	20	ASP	CB-CG-OD2	-6.87	112.12	118.30	25	25
1	A	84	ALA	N-CA-CB	-6.82	100.55	110.10	21	25
1	A	26	ASP	CB-CG-OD2	-6.80	112.18	118.30	17	25
1	A	40	ASP	CB-CG-OD1	6.79	124.41	118.30	15	25
1	B	84	ALA	N-CA-CB	-6.76	100.64	110.10	25	25
1	A	50	PHE	CB-CG-CD2	-6.62	116.16	120.80	20	1
1	B	28	VAL	CA-CB-CG2	6.57	120.76	110.90	2	5
1	A	42	VAL	CB-CA-C	6.54	123.83	111.40	4	5
1	B	89	VAL	CA-CB-CG1	6.52	120.68	110.90	12	1
1	B	20	ASP	CB-CG-OD1	6.48	124.13	118.30	17	25
1	B	80	LYS	CA-CB-CG	6.43	127.56	113.40	6	1
1	B	32	ILE	CB-CG1-CD1	6.42	131.89	113.90	18	4
1	A	80	LYS	N-CA-CB	-6.38	99.11	110.60	9	2
1	A	6	LEU	CB-CG-CD1	6.37	121.82	111.00	10	5
1	A	32	ILE	CB-CG1-CD1	6.26	131.42	113.90	17	6
1	A	76	VAL	CB-CA-C	6.25	123.28	111.40	13	1
1	B	80	LYS	N-CA-CB	-6.24	99.38	110.60	6	1
1	B	89	VAL	CB-CA-C	6.19	123.17	111.40	13	1
1	B	6	LEU	CB-CG-CD1	6.19	121.53	111.00	5	8
1	A	78	ALA	N-CA-CB	-6.14	101.51	110.10	13	7
1	A	89	VAL	CG1-CB-CG2	-6.07	101.19	110.90	4	1
1	B	50	PHE	CB-CG-CD2	-6.04	116.58	120.80	6	1
1	B	40	ASP	CB-CG-OD1	6.03	123.72	118.30	19	25
1	B	76	VAL	N-CA-CB	-5.87	98.58	111.50	22	9
1	A	87	ASP	CB-CG-OD1	5.86	123.57	118.30	18	25
1	A	33	THR	CA-CB-CG2	5.84	120.58	112.40	11	1
1	A	20	ASP	CB-CG-OD1	5.84	123.55	118.30	20	25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	75	LYS	N-CA-CB	5.83	121.10	110.60	22	1
1	B	26	ASP	CB-CG-OD1	5.80	123.52	118.30	22	25
1	B	87	ASP	CB-CG-OD1	5.79	123.51	118.30	10	25
1	A	26	ASP	CB-CG-OD1	5.76	123.49	118.30	24	25
1	B	30	ASP	CB-CG-OD1	5.74	123.46	118.30	1	25
1	B	78	ALA	N-CA-CB	-5.69	102.14	110.10	24	4
1	A	75	LYS	CG-CD-CE	5.62	128.75	111.90	13	1
1	A	23	LYS	N-CA-CB	-5.60	100.52	110.60	17	3
1	B	23	LYS	N-CA-CB	-5.52	100.66	110.60	5	3
1	B	1	MET	CB-CA-C	5.51	121.42	110.40	20	2
1	A	88	ALA	CB-CA-C	-5.44	101.94	110.10	4	1
1	B	89	VAL	CG1-CB-CG2	-5.41	102.24	110.90	12	1
1	A	89	VAL	CA-CB-CG1	5.37	118.96	110.90	4	1
1	B	5	GLU	N-CA-CB	-5.32	101.03	110.60	10	4
1	B	53	ARG	NE-CZ-NH2	-5.31	117.64	120.30	23	1
1	A	3	LYS	N-CA-CB	5.29	120.12	110.60	14	5
1	B	3	LYS	N-CA-CB	5.28	120.11	110.60	5	2
1	A	52	VAL	N-CA-CB	-5.24	99.97	111.50	13	3
1	B	42	VAL	N-CA-CB	-5.22	100.03	111.50	2	2
1	A	33	THR	N-CA-CB	5.20	120.18	110.30	11	1
1	A	42	VAL	N-CA-CB	-5.20	100.06	111.50	13	2
1	A	52	VAL	CB-CA-C	5.18	121.23	111.40	19	2
1	A	5	GLU	N-CA-CB	-5.14	101.34	110.60	14	2
1	A	28	VAL	CA-CB-CG2	5.10	118.55	110.90	13	1
1	A	2	ASN	N-CA-C	5.10	124.76	111.00	18	1
1	B	79	PHE	CA-C-N	-5.08	106.03	117.20	6	1
1	B	52	VAL	N-CA-CB	-5.07	100.35	111.50	4	1
1	A	48	GLY	N-CA-C	5.06	125.75	113.10	20	1
1	B	88	ALA	CB-CA-C	-5.04	102.54	110.10	13	1
1	B	43	GLN	CB-CA-C	5.03	120.46	110.40	11	1

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

Mol	Chain	Res	Type	Atoms	Models (Total)
1	B	51	GLU	CA	1
1	B	52	VAL	CA	1

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	B	47	PHE	Sidechain	18
1	A	29	PHE	Sidechain	13
1	B	29	PHE	Sidechain	12
1	A	47	PHE	Sidechain	11
1	B	50	PHE	Sidechain,Peptide	6
1	A	50	PHE	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	512	539	543	5±2
1	B	520	549	554	5±2
All	All	25800	27200	27425	210

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:6:LEU:HD21	1:B:28:VAL:HG13	0.82	1.52	6	14
1:B:53:ARG:HB3	1:B:76:VAL:HG22	0.81	1.52	14	5
1:A:53:ARG:HB3	1:A:76:VAL:HG22	0.80	1.52	11	6
1:B:32:ILE:HG23	1:B:42:VAL:HG21	0.76	1.55	11	12
1:A:32:ILE:HG23	1:A:42:VAL:HG21	0.75	1.58	17	14
1:B:28:VAL:HG12	1:B:32:ILE:HD11	0.73	1.61	6	12
1:A:28:VAL:HG12	1:A:32:ILE:HD11	0.72	1.62	21	12
1:A:28:VAL:HG13	1:B:6:LEU:HD21	0.70	1.63	3	11
1:B:53:ARG:CB	1:B:76:VAL:HG22	0.65	2.22	17	5
1:A:53:ARG:CB	1:A:76:VAL:HG22	0.63	2.22	23	6
1:A:10:VAL:HA	1:B:27:ALA:HB1	0.58	1.75	10	13
1:A:27:ALA:HB1	1:B:10:VAL:HA	0.56	1.76	3	16
1:A:32:ILE:CG2	1:A:36:LEU:HD22	0.56	2.31	7	4
1:A:32:ILE:HG22	1:A:36:LEU:HD22	0.53	1.80	10	2
1:A:32:ILE:O	1:A:36:LEU:HG	0.51	2.05	15	2
1:B:4:THR:HA	1:B:7:ILE:HD12	0.49	1.84	16	8
1:B:6:LEU:O	1:B:10:VAL:HG23	0.48	2.08	21	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:THR:HA	1:A:7:ILE:HD12	0.47	1.85	14	5
1:B:32:ILE:HG22	1:B:36:LEU:HD22	0.47	1.86	25	1
1:B:6:LEU:HD22	1:B:25:VAL:CG2	0.47	2.40	20	2
1:A:85:LEU:O	1:A:89:VAL:HG12	0.46	2.09	4	1
1:A:6:LEU:O	1:A:10:VAL:HG23	0.45	2.11	10	13
1:B:32:ILE:O	1:B:36:LEU:HG	0.45	2.10	5	1
1:B:32:ILE:CG2	1:B:36:LEU:HD22	0.45	2.42	10	1
1:A:75:LYS:CD	1:A:75:LYS:N	0.44	2.80	13	1
1:B:24:ALA:O	1:B:28:VAL:HG23	0.44	2.11	7	1
1:A:24:ALA:HA	1:A:27:ALA:HB3	0.44	1.89	22	6
1:B:6:LEU:HD22	1:B:25:VAL:HG22	0.44	1.90	18	1
1:A:6:LEU:HD12	1:B:44:LEU:HD22	0.44	1.89	22	1
1:A:2:ASN:HA	1:B:43:GLN:O	0.44	2.13	19	1
1:B:24:ALA:HA	1:B:27:ALA:HB3	0.43	1.91	15	7
1:A:75:LYS:HD3	1:A:75:LYS:N	0.43	2.28	13	1
1:B:43:GLN:O	1:B:44:LEU:HD23	0.42	2.15	22	1
1:A:49:ASN:H	1:A:80:LYS:CA	0.42	2.28	9	1
1:A:6:LEU:HD22	1:A:25:VAL:HG22	0.41	1.92	6	2
1:A:85:LEU:HD13	1:B:33:THR:HG22	0.41	1.92	3	1
1:B:32:ILE:HG21	1:B:50:PHE:HE2	0.41	1.74	11	1
1:A:44:LEU:HD22	1:B:6:LEU:CD1	0.41	2.46	23	1
1:B:42:VAL:HG12	1:B:43:GLN:H	0.40	1.77	25	2
1:A:43:GLN:O	1:A:44:LEU:HD23	0.40	2.17	23	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	67/90 (74%)	55±1 (82±2%)	8±1 (12±2%)	4±1 (6±2%)	4	22
1	B	67/90 (74%)	55±1 (82±2%)	8±1 (12±2%)	5±1 (7±1%)	3	19
All	All	3350/4500 (74%)	2750 (82%)	388 (12%)	212 (6%)	3	20

All 25 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	2	ASN	25
1	A	2	ASN	25
1	B	3	LYS	22
1	A	3	LYS	21
1	B	82	GLY	18
1	A	82	GLY	16
1	B	43	GLN	13
1	B	42	VAL	13
1	A	43	GLN	11
1	A	42	VAL	11
1	B	28	VAL	10
1	A	28	VAL	6
1	A	47	PHE	4
1	B	47	PHE	4
1	A	29	PHE	2
1	A	80	LYS	2
1	A	75	LYS	1
1	B	80	LYS	1
1	B	40	ASP	1
1	B	52	VAL	1
1	B	51	GLU	1
1	B	83	LYS	1
1	B	26	ASP	1
1	B	41	LYS	1
1	B	16	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	54/71 (76%)	46±1 (85±2%)	8±1 (15±2%)	7	46
1	B	55/71 (77%)	46±2 (84±3%)	9±2 (16±3%)	7	45
All	All	2725/3550 (77%)	2307 (85%)	418 (15%)	7	46

All 51 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	87	ASP	25
1	B	87	ASP	25
1	B	6	LEU	24
1	A	16	LEU	24
1	B	52	VAL	24
1	A	52	VAL	24
1	B	16	LEU	23
1	A	6	LEU	22
1	B	13	THR	19
1	B	76	VAL	18
1	B	89	VAL	17
1	A	51	GLU	17
1	A	76	VAL	17
1	A	13	THR	13
1	B	51	GLU	12
1	A	89	VAL	12
1	A	10	VAL	12
1	A	36	LEU	10
1	B	10	VAL	9
1	B	32	ILE	5
1	B	45	ILE	4
1	B	83	LYS	4
1	B	1	MET	4
1	A	22	THR	4
1	B	34	GLU	3
1	B	36	LEU	3
1	B	75	LYS	3
1	A	32	ILE	3
1	B	22	THR	3
1	A	83	LYS	3
1	B	80	LYS	2
1	B	19	LYS	2
1	A	19	LYS	2
1	A	79	PHE	2
1	A	90	LYS	2
1	B	53	ARG	2
1	A	45	ILE	2
1	A	53	ARG	2
1	A	49	ASN	2
1	B	18	LYS	2
1	B	44	LEU	2
1	A	75	LYS	1
1	B	40	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	B	5	GLU	1
1	B	47	PHE	1
1	B	28	VAL	1
1	A	23	LYS	1
1	B	41	LYS	1
1	B	79	PHE	1
1	A	80	LYS	1
1	B	90	LYS	1

### 6.3.3 RNA [i](#)

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 carbohydrates 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

No chemical shift data were provided