



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:24 PM BST

PDB ID : 1D7Q
Title : HUMAN TRANSLATION INITIATION FACTOR EIF1A
Authors : Battiste, J.L.; Pestova, T.V.; Hellen, C.U.T.; Wagner, G.
Deposited on : 1999-10-19

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
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

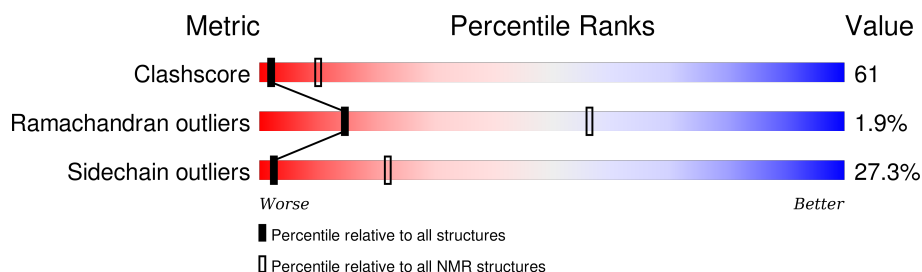
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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 ≥ 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	B	14	100%
2	A	143	27% 31% 6% 36%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 8 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:38-A:128 (91)	0.38	2

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 4 clusters and 2 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2496 atoms, of which 1230 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (N-TERMINAL HISTIDINE TAG).

Mol	Chain	Residues	Atoms						Trace
1	B	14	Total	C	H	N	O	S	0
			226	70	107	29	18	2	

- Molecule 2 is a protein called TRANSLATION INITIATION FACTOR 1A.

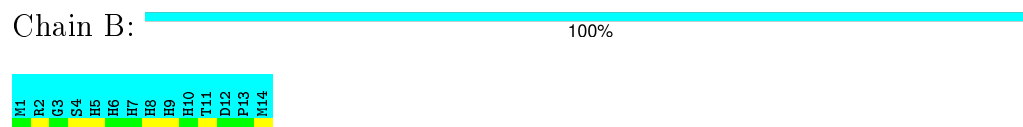
Mol	Chain	Residues	Atoms						Trace
2	A	143	Total	C	H	N	O	S	0
			2270	705	1123	207	231	4	

4 Residue-property plots

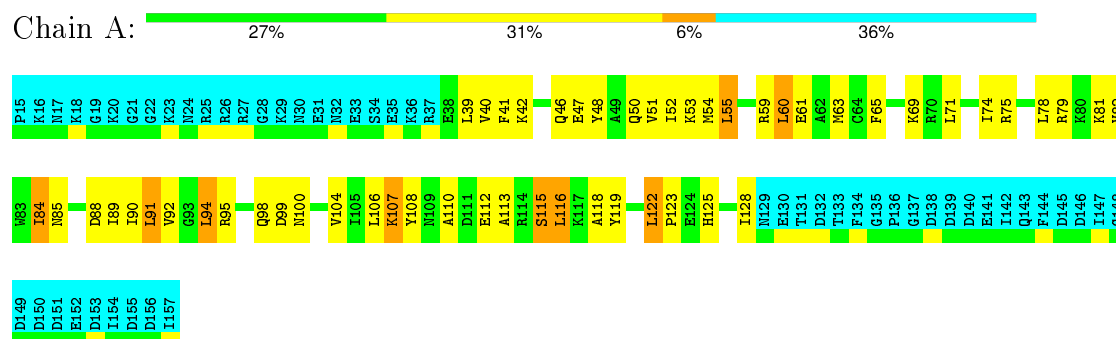
4.1 Average score per residue in the NMR ensemble

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: PROTEIN (N-TERMINAL HISTIDINE TAG)



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

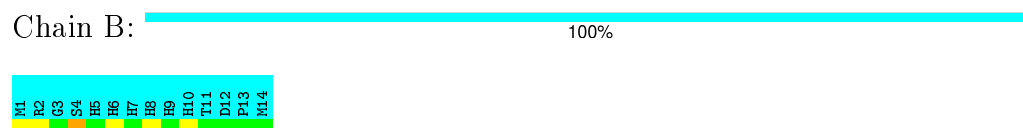


4.2 Scores per residue for each member of the ensemble

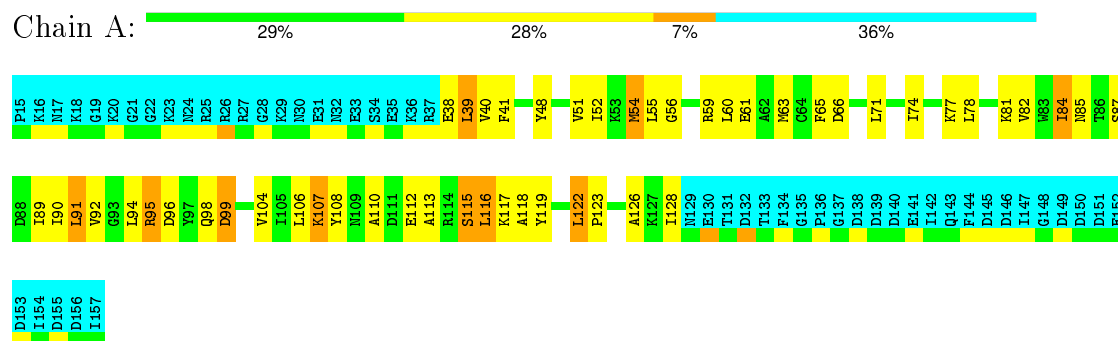
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

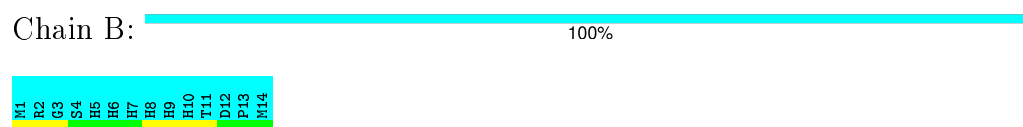


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

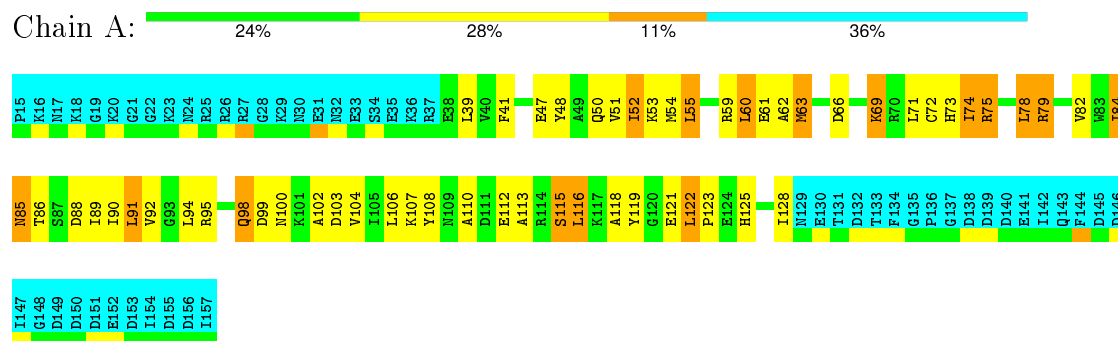


4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

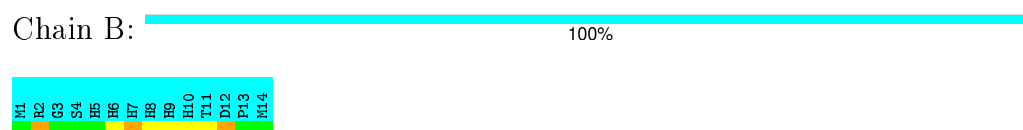


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

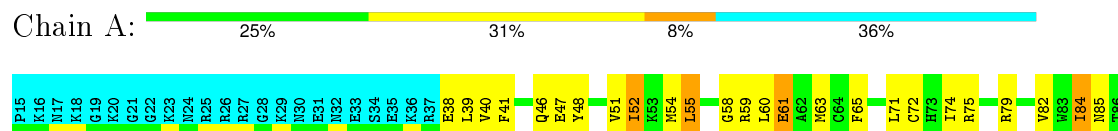


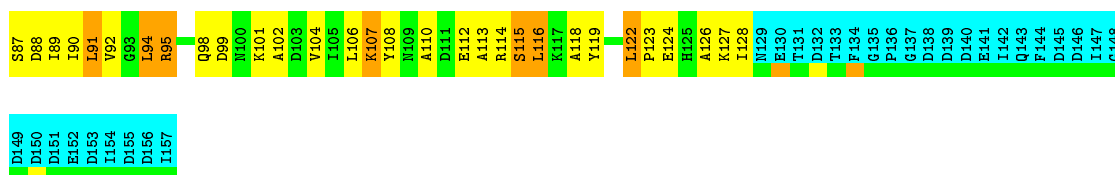
4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)



- Molecule 2: TRANSLATION INITIATION FACTOR 1A





4.2.4 Score per residue for model 4

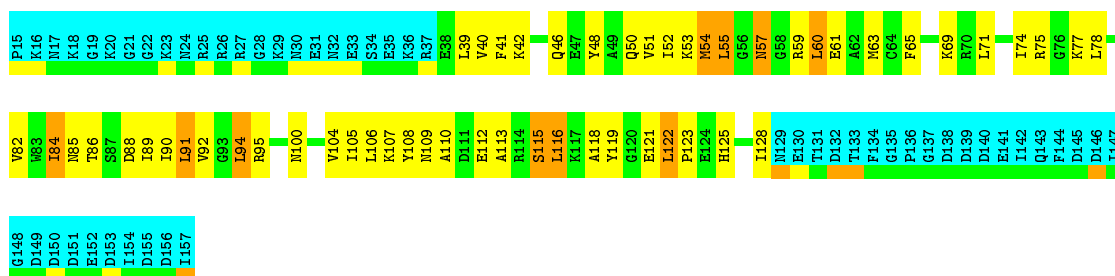
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B: 100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

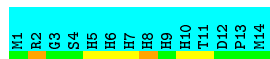
Chain A: 26% 31% 7% 36%



4.2.5 Score per residue for model 5

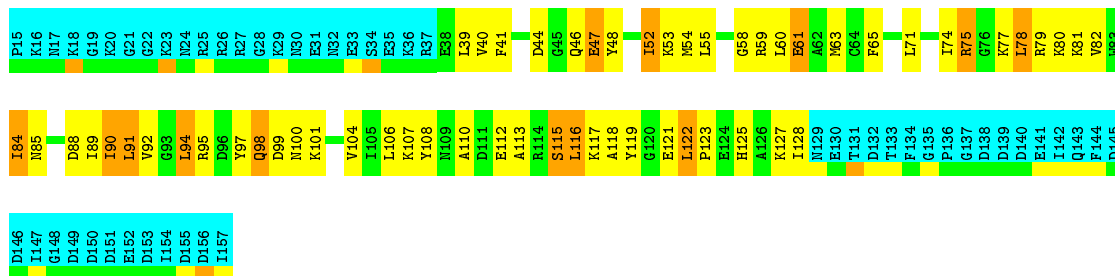
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B: 100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

Chain A: 23% 31% 9% 36%



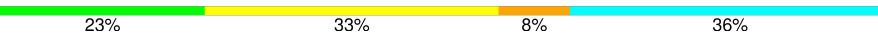
4.2.6 Score per residue for model 6

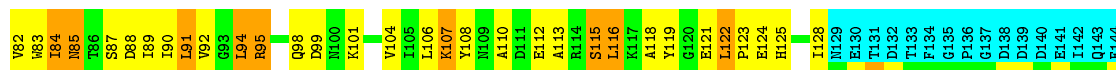
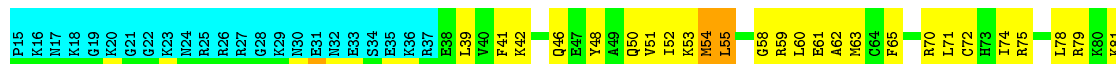
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

Chain A:  23% 33% 8% 36%



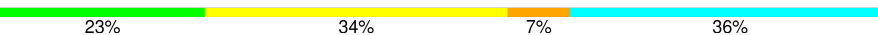
4.2.7 Score per residue for model 7

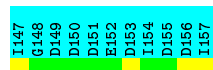
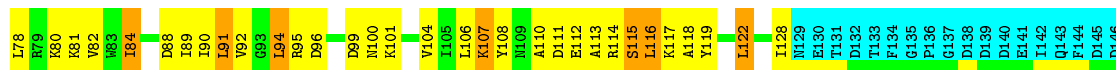
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

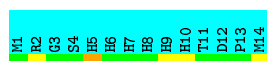
Chain A:  23% 34% 7% 36%



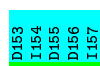
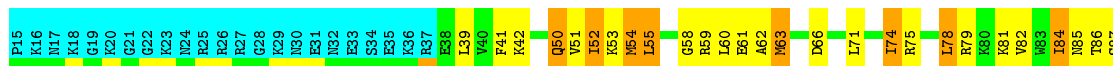
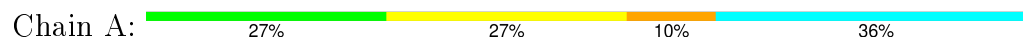
4.2.8 Score per residue for model 8

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%

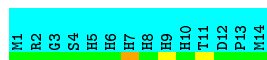


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

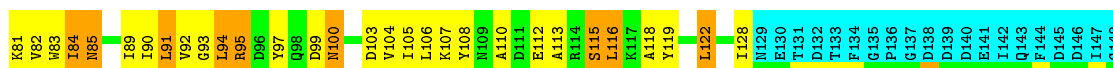
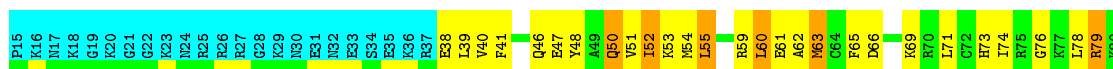
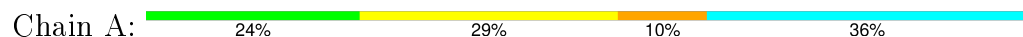


4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

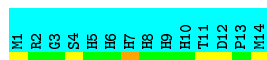


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

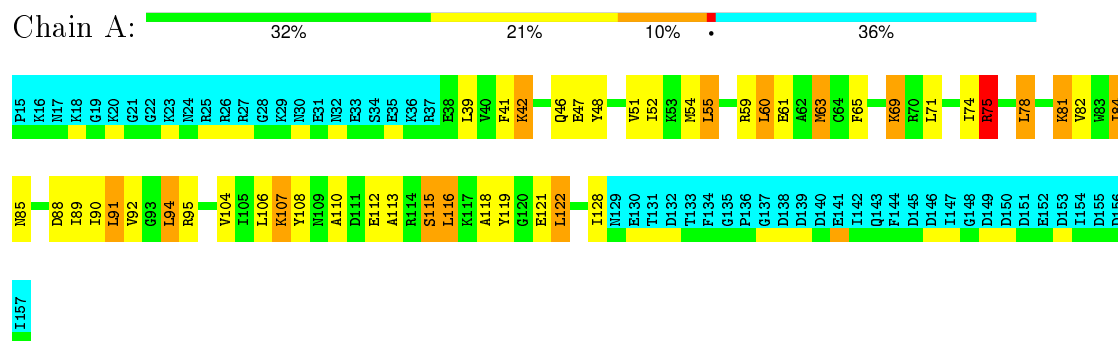


4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

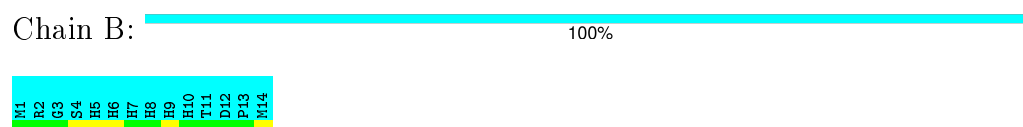


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

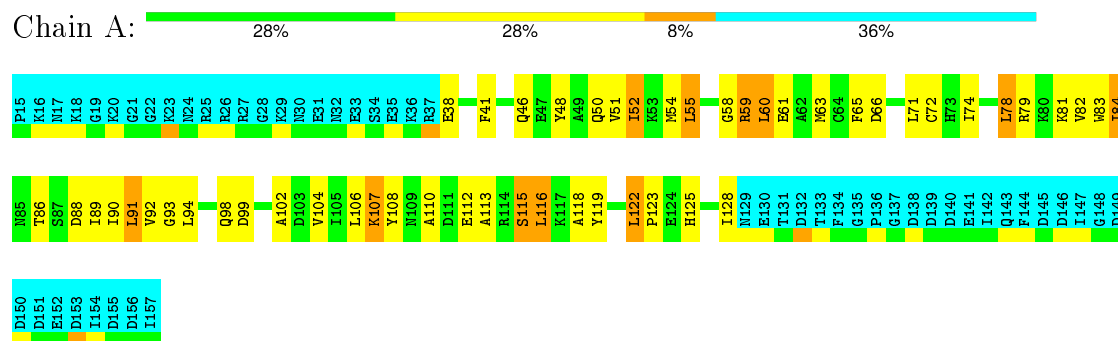


4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

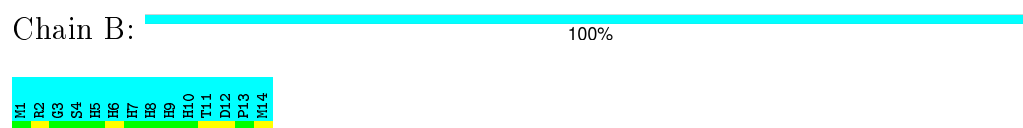


- Molecule 2: TRANSLATION INITIATION FACTOR 1A

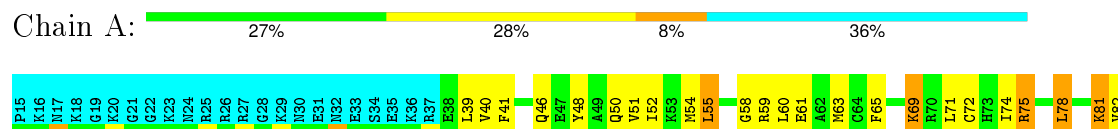


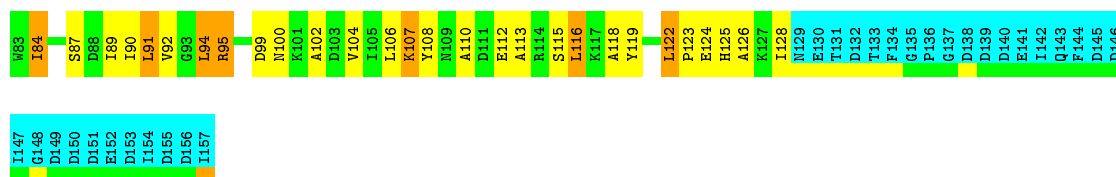
4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)



- Molecule 2: TRANSLATION INITIATION FACTOR 1A





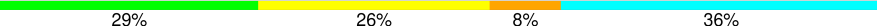
4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

Chain A:  29% 26% 8% 36%



4.2.14 Score per residue for model 14

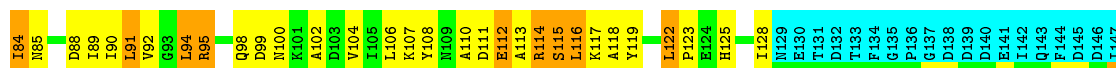
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

Chain A:  23% 31% 9% 36%




4.2.15 Score per residue for model 15

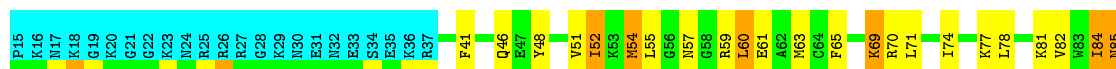
- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

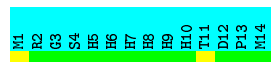
Chain A:  31% 24% 8% 36%



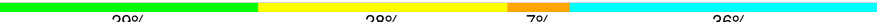
4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



- Molecule 2: TRANSLATION INITIATION FACTOR 1A

Chain A:  29% 28% 7% 36%



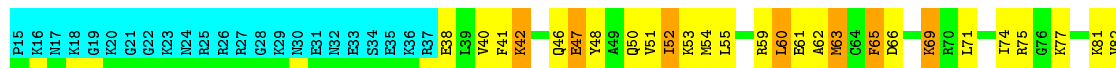
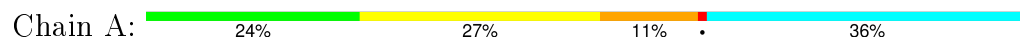
4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

Chain B:  100%



• Molecule 2: TRANSLATION INITIATION FACTOR 1A

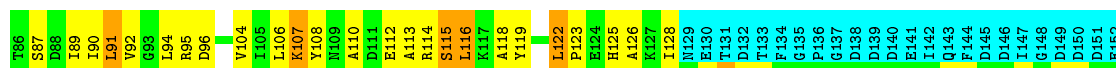
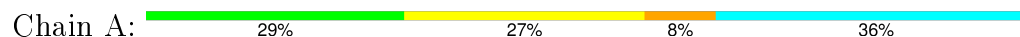


4.2.18 Score per residue for model 18

• Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

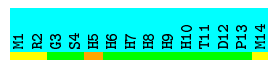


• Molecule 2: TRANSLATION INITIATION FACTOR 1A

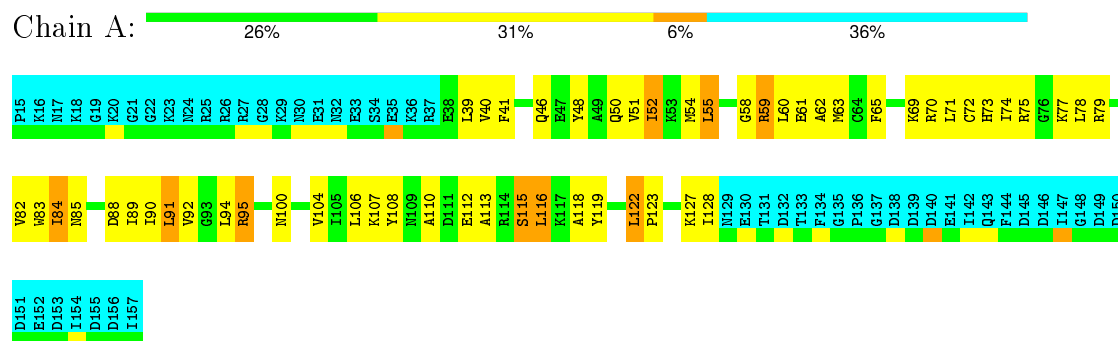


4.2.19 Score per residue for model 19

• Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)

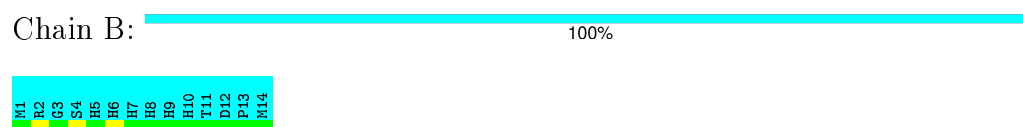


• Molecule 2: TRANSLATION INITIATION FACTOR 1A

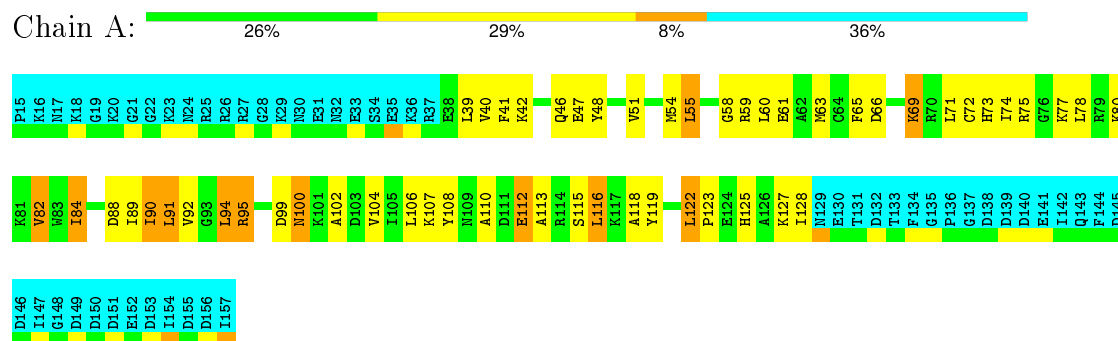


4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (N-TERMINAL HISTIDINE TAG)



- Molecule 2: TRANSLATION INITIATION FACTOR 1A



5 Refinement protocol and experimental data overview

The models were refined using the following method: *STRUCTURES WERE CALCULATED USING SIMULATED ANNEALING/MOLECULAR DYNAMICS FROM AN EXTENDED CONFORMATION WITH RANDOM PHI/PSI ANGLES..*

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS.*

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

Software name	Classification	Version
X-PLOR	structure solution	3.851
X-PLOR	refinement	3.851

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)	BMRB entry 4519
Number of chemical shift lists	1
Total number of shifts	1501
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	52
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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

6 Model quality ⓘ

6.1 Standard geometry ⓘ

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	0	0	0	0±0
2	A	733	755	753	90±5
All	All	14660	15100	15060	1809

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 61.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:55:LEU:HD11	2:A:71:LEU:HD12	0.99	1.30	3	19
2:A:106:LEU:HD11	2:A:108:TYR:CE1	0.97	1.95	4	20
2:A:113:ALA:HB1	2:A:128:ILE:HD12	0.96	1.29	12	5
2:A:60:LEU:HD22	2:A:84:ILE:HD13	0.94	1.40	18	12
2:A:113:ALA:HB1	2:A:128:ILE:HD13	0.91	1.42	20	14
2:A:74:ILE:HD11	2:A:84:ILE:HD11	0.88	1.45	4	3
2:A:89:ILE:HG21	2:A:116:LEU:CD1	0.85	2.01	14	20
2:A:106:LEU:HD11	2:A:108:TYR:CD1	0.84	2.07	8	20
2:A:52:ILE:HD11	2:A:63:MET:CB	0.83	2.03	12	6
2:A:60:LEU:HD22	2:A:84:ILE:HG21	0.82	1.51	11	7
2:A:52:ILE:HD11	2:A:63:MET:HB2	0.81	1.51	12	5
2:A:113:ALA:CB	2:A:128:ILE:HD13	0.80	2.06	20	13
2:A:52:ILE:HD13	2:A:63:MET:HB3	0.80	1.53	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:52:ILE:HD13	2:A:63:MET:CB	0.78	2.09	3	2
2:A:74:ILE:HD12	2:A:84:ILE:CD1	0.78	2.09	1	7
2:A:65:PHE:CZ	2:A:122:LEU:HD22	0.78	2.13	17	1
2:A:41:PHE:CE1	2:A:119:TYR:CD1	0.77	2.71	8	20
2:A:55:LEU:HD12	2:A:59:ARG:CD	0.77	2.09	4	15
2:A:52:ILE:HD11	2:A:63:MET:HB3	0.76	1.55	10	2
2:A:60:LEU:HD22	2:A:84:ILE:CD1	0.75	2.11	17	9
2:A:113:ALA:HA	2:A:116:LEU:HG	0.75	1.58	1	18
2:A:55:LEU:HD21	2:A:61:GLU:HB2	0.75	1.59	18	20
2:A:41:PHE:CD1	2:A:119:TYR:CD1	0.74	2.75	4	20
2:A:103:ASP:O	2:A:105:ILE:HD12	0.74	1.82	9	1
2:A:60:LEU:CD2	2:A:84:ILE:HD13	0.73	2.13	19	13
2:A:47:GLU:HB2	2:A:94:LEU:HD11	0.72	1.61	7	7
2:A:58:GLY:HA2	2:A:74:ILE:HG22	0.72	1.61	3	8
2:A:74:ILE:HD11	2:A:84:ILE:CD1	0.72	2.15	15	3
2:A:92:VAL:HG12	2:A:104:VAL:HA	0.71	1.60	12	20
2:A:84:ILE:HG22	2:A:90:ILE:HD13	0.71	1.61	12	13
2:A:113:ALA:CB	2:A:128:ILE:HG21	0.70	2.17	1	3
2:A:60:LEU:HD23	2:A:84:ILE:HD13	0.70	1.63	16	2
2:A:52:ILE:O	2:A:86:THR:HG23	0.69	1.87	8	4
2:A:113:ALA:HB1	2:A:128:ILE:CD1	0.67	2.18	17	15
2:A:55:LEU:HD12	2:A:59:ARG:HB3	0.66	1.65	3	2
2:A:55:LEU:HD11	2:A:71:LEU:CD1	0.66	2.19	14	4
2:A:89:ILE:HG21	2:A:116:LEU:HD11	0.66	1.67	1	20
2:A:116:LEU:HD22	2:A:119:TYR:CD2	0.65	2.26	17	20
2:A:55:LEU:HD12	2:A:59:ARG:HD2	0.65	1.66	17	12
2:A:50:GLN:O	2:A:62:ALA:HB1	0.65	1.92	8	3
2:A:94:LEU:HD23	2:A:102:ALA:HB2	0.65	1.69	20	1
2:A:84:ILE:HG22	2:A:90:ILE:CD1	0.65	2.22	17	15
2:A:92:VAL:HG12	2:A:104:VAL:CA	0.65	2.22	2	20
2:A:91:LEU:HD23	2:A:106:LEU:CD2	0.64	2.23	2	20
2:A:110:ALA:O	2:A:113:ALA:HB3	0.64	1.93	20	20
2:A:60:LEU:HD22	2:A:84:ILE:HG12	0.64	1.69	3	1
2:A:47:GLU:HB3	2:A:94:LEU:HD11	0.64	1.69	5	1
2:A:60:LEU:CD2	2:A:84:ILE:HG21	0.63	2.23	1	6
2:A:47:GLU:CB	2:A:94:LEU:HD11	0.63	2.23	7	8
2:A:112:GLU:O	2:A:116:LEU:HD23	0.62	1.94	17	16
2:A:116:LEU:HD22	2:A:119:TYR:CE2	0.62	2.29	18	20
2:A:116:LEU:HD22	2:A:119:TYR:CZ	0.62	2.30	18	20
2:A:116:LEU:HD13	2:A:119:TYR:CD2	0.62	2.29	9	8
2:A:116:LEU:HD22	2:A:119:TYR:CG	0.62	2.30	17	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:39:LEU:HD11	2:A:119:TYR:CE1	0.61	2.30	8	8
2:A:91:LEU:HD12	2:A:92:VAL:N	0.61	2.10	14	20
2:A:39:LEU:HD21	2:A:115:SER:CB	0.61	2.25	2	12
2:A:51:VAL:CG2	2:A:90:ILE:HD11	0.61	2.25	3	9
2:A:115:SER:O	2:A:118:ALA:N	0.61	2.33	20	20
2:A:55:LEU:N	2:A:55:LEU:HD23	0.61	2.09	17	12
2:A:60:LEU:HD21	2:A:104:VAL:HG21	0.61	1.72	3	2
2:A:82:VAL:HG23	2:A:107:LYS:HG2	0.61	1.71	17	2
2:A:52:ILE:HD12	2:A:63:MET:CB	0.60	2.26	13	1
2:A:74:ILE:HD12	2:A:84:ILE:HD11	0.60	1.71	1	5
2:A:116:LEU:HA	2:A:119:TYR:CG	0.60	2.32	18	20
2:A:108:TYR:CD1	2:A:119:TYR:HE2	0.60	2.15	19	20
2:A:79:ARG:HA	2:A:82:VAL:HG12	0.60	1.72	2	7
2:A:55:LEU:HD21	2:A:61:GLU:CB	0.60	2.27	18	10
2:A:39:LEU:HD11	2:A:119:TYR:HE1	0.60	1.57	8	7
2:A:72:CYS:HB3	2:A:92:VAL:HG11	0.60	1.74	13	8
2:A:48:TYR:CZ	2:A:108:TYR:CE2	0.60	2.90	17	1
2:A:55:LEU:HD12	2:A:59:ARG:HG3	0.59	1.73	5	14
2:A:55:LEU:HD12	2:A:59:ARG:CG	0.59	2.27	4	10
2:A:54:MET:SD	2:A:84:ILE:HD12	0.58	2.38	19	1
2:A:112:GLU:O	2:A:115:SER:N	0.58	2.36	1	16
2:A:106:LEU:C	2:A:106:LEU:HD12	0.58	2.18	8	13
2:A:90:ILE:CG2	2:A:104:VAL:HG13	0.58	2.29	10	20
2:A:54:MET:C	2:A:55:LEU:HD23	0.58	2.19	3	13
2:A:71:LEU:HD22	2:A:71:LEU:N	0.58	2.14	5	9
2:A:115:SER:O	2:A:118:ALA:HB3	0.58	1.98	17	20
2:A:108:TYR:CD1	2:A:119:TYR:CE2	0.58	2.92	19	20
2:A:82:VAL:HG13	2:A:82:VAL:O	0.58	1.99	2	10
2:A:39:LEU:HD23	2:A:41:PHE:CZ	0.57	2.34	12	5
2:A:106:LEU:HD12	2:A:106:LEU:C	0.57	2.19	10	7
2:A:106:LEU:HD12	2:A:107:LYS:N	0.57	2.14	6	20
2:A:91:LEU:HD23	2:A:106:LEU:HG	0.57	1.77	16	8
2:A:122:LEU:N	2:A:122:LEU:HD23	0.57	2.15	18	9
2:A:55:LEU:HD23	2:A:55:LEU:N	0.57	2.14	16	7
2:A:74:ILE:HD11	2:A:82:VAL:HG13	0.57	1.76	6	8
2:A:122:LEU:HD23	2:A:122:LEU:N	0.57	2.15	15	10
2:A:116:LEU:N	2:A:116:LEU:HD23	0.57	2.15	20	11
2:A:82:VAL:O	2:A:82:VAL:HG13	0.56	1.99	8	5
2:A:116:LEU:HD12	2:A:122:LEU:HD11	0.56	1.78	8	11
2:A:93:GLY:O	2:A:94:LEU:HD23	0.56	2.00	17	1
2:A:71:LEU:N	2:A:71:LEU:HD22	0.56	2.15	15	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:78:LEU:HD12	2:A:82:VAL:HB	0.56	1.77	11	5
2:A:60:LEU:HD21	2:A:104:VAL:CG2	0.56	2.30	3	1
2:A:116:LEU:CD2	2:A:119:TYR:CE2	0.56	2.89	17	20
2:A:113:ALA:HA	2:A:116:LEU:CD2	0.56	2.30	20	5
2:A:116:LEU:HD23	2:A:116:LEU:N	0.56	2.16	18	9
2:A:52:ILE:HD12	2:A:63:MET:HB3	0.55	1.78	13	1
2:A:39:LEU:HD21	2:A:115:SER:HB3	0.55	1.76	20	5
2:A:116:LEU:CD2	2:A:116:LEU:N	0.55	2.69	9	6
2:A:113:ALA:CB	2:A:128:ILE:HD12	0.55	2.30	9	3
2:A:51:VAL:HG22	2:A:60:LEU:CD1	0.55	2.31	17	4
2:A:94:LEU:N	2:A:94:LEU:HD23	0.55	2.17	6	1
2:A:113:ALA:CB	2:A:128:ILE:HG23	0.55	2.32	4	1
2:A:89:ILE:HG22	2:A:108:TYR:CD2	0.55	2.37	20	19
2:A:116:LEU:HD22	2:A:119:TYR:CE1	0.54	2.38	14	20
2:A:123:PRO:HD2	2:A:126:ALA:HB2	0.54	1.77	3	4
2:A:116:LEU:HD22	2:A:119:TYR:CD1	0.54	2.38	17	20
2:A:46:GLN:OE1	2:A:91:LEU:HD11	0.54	2.01	17	4
2:A:84:ILE:CG2	2:A:90:ILE:HD13	0.54	2.31	3	2
2:A:51:VAL:HG13	2:A:60:LEU:HD13	0.54	1.78	12	3
2:A:116:LEU:CD2	2:A:119:TYR:CZ	0.54	2.91	18	20
2:A:91:LEU:CB	2:A:108:TYR:CE2	0.54	2.91	17	20
2:A:39:LEU:HD12	2:A:112:GLU:HG2	0.54	1.79	5	3
2:A:89:ILE:HG22	2:A:108:TYR:HD2	0.54	1.63	20	20
2:A:116:LEU:N	2:A:116:LEU:CD2	0.54	2.71	20	14
2:A:89:ILE:HG21	2:A:116:LEU:HD12	0.54	1.79	9	5
2:A:39:LEU:CD1	2:A:112:GLU:CG	0.53	2.86	18	1
2:A:94:LEU:CD2	2:A:102:ALA:HB2	0.53	2.33	17	4
2:A:39:LEU:HD12	2:A:112:GLU:OE2	0.53	2.03	1	1
2:A:92:VAL:HG12	2:A:104:VAL:N	0.53	2.18	9	17
2:A:41:PHE:CD1	2:A:119:TYR:HA	0.53	2.38	17	10
2:A:92:VAL:HB	2:A:102:ALA:HB1	0.53	1.81	17	1
2:A:108:TYR:CG	2:A:119:TYR:HE2	0.52	2.22	2	19
2:A:48:TYR:CE2	2:A:108:TYR:CE2	0.52	2.97	17	1
2:A:82:VAL:HG21	2:A:107:LYS:CB	0.52	2.34	20	1
2:A:112:GLU:HB3	2:A:119:TYR:OH	0.52	2.04	10	3
2:A:94:LEU:HD23	2:A:94:LEU:N	0.52	2.19	4	1
2:A:90:ILE:HG23	2:A:107:LYS:HA	0.52	1.82	17	1
2:A:74:ILE:HD12	2:A:84:ILE:HG12	0.52	1.80	19	2
2:A:41:PHE:CE1	2:A:119:TYR:CE1	0.52	2.98	4	10
2:A:91:LEU:CB	2:A:108:TYR:CZ	0.51	2.93	4	20
2:A:113:ALA:HB1	2:A:128:ILE:HG23	0.51	1.82	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:78:LEU:N	2:A:78:LEU:CD2	0.51	2.73	10	1
2:A:39:LEU:HD11	2:A:119:TYR:OH	0.51	2.06	1	1
2:A:78:LEU:O	2:A:82:VAL:HG12	0.51	2.06	11	5
2:A:48:TYR:CE2	2:A:65:PHE:CG	0.50	3.00	16	2
2:A:89:ILE:HD12	2:A:89:ILE:N	0.50	2.21	15	1
2:A:90:ILE:HG22	2:A:91:LEU:H	0.50	1.66	8	20
2:A:48:TYR:OH	2:A:119:TYR:CD2	0.50	2.65	17	1
2:A:41:PHE:CG	2:A:119:TYR:HA	0.50	2.42	2	10
2:A:91:LEU:HD23	2:A:106:LEU:CG	0.50	2.37	16	6
2:A:48:TYR:CE2	2:A:65:PHE:CD1	0.50	2.99	3	11
2:A:39:LEU:HD12	2:A:112:GLU:CD	0.50	2.27	9	1
2:A:51:VAL:HG21	2:A:85:ASN:O	0.50	2.07	3	2
2:A:40:VAL:CG1	2:A:106:LEU:HD22	0.49	2.36	20	7
2:A:91:LEU:HB2	2:A:108:TYR:CE2	0.49	2.42	7	20
2:A:54:MET:HE2	2:A:84:ILE:HD12	0.49	1.84	4	1
2:A:40:VAL:HG11	2:A:106:LEU:CD2	0.49	2.37	17	1
2:A:78:LEU:O	2:A:82:VAL:N	0.49	2.45	18	5
2:A:54:MET:CE	2:A:84:ILE:HD12	0.49	2.38	4	1
2:A:46:GLN:HE21	2:A:91:LEU:HD11	0.48	1.67	5	2
2:A:90:ILE:HG22	2:A:104:VAL:HG13	0.48	1.86	4	12
2:A:72:CYS:SG	2:A:92:VAL:HG11	0.48	2.48	2	2
2:A:39:LEU:CD1	2:A:112:GLU:HG3	0.48	2.39	9	2
2:A:51:VAL:HG21	2:A:90:ILE:HD11	0.47	1.86	20	3
2:A:48:TYR:CE2	2:A:122:LEU:CD2	0.47	2.97	18	7
2:A:89:ILE:O	2:A:108:TYR:HB2	0.47	2.09	17	18
2:A:63:MET:HE3	2:A:69:LYS:HG3	0.47	1.87	16	1
2:A:78:LEU:CD2	2:A:78:LEU:N	0.47	2.77	5	4
2:A:91:LEU:C	2:A:91:LEU:HD12	0.47	2.29	14	10
2:A:50:GLN:OE1	2:A:89:ILE:HD13	0.47	2.09	2	2
2:A:82:VAL:HG21	2:A:107:LYS:HB2	0.46	1.88	20	1
2:A:63:MET:HE2	2:A:69:LYS:HA	0.46	1.87	15	3
2:A:82:VAL:HG23	2:A:107:LYS:HB3	0.46	1.87	8	1
2:A:93:GLY:C	2:A:94:LEU:HD23	0.46	2.30	8	2
2:A:90:ILE:HG21	2:A:104:VAL:HG13	0.46	1.87	3	5
2:A:48:TYR:OH	2:A:65:PHE:CB	0.46	2.63	16	11
2:A:74:ILE:HD12	2:A:84:ILE:HG13	0.46	1.88	12	1
2:A:110:ALA:O	2:A:113:ALA:CB	0.46	2.64	7	17
2:A:91:LEU:HB2	2:A:108:TYR:CZ	0.46	2.46	4	15
2:A:46:GLN:CB	2:A:91:LEU:HD11	0.46	2.41	10	11
2:A:93:GLY:O	2:A:102:ALA:HB1	0.46	2.10	11	1
2:A:39:LEU:CD2	2:A:41:PHE:CZ	0.46	2.99	1	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:116:LEU:H	2:A:116:LEU:HD23	0.46	1.70	9	1
2:A:111:ASP:O	2:A:114:ARG:CG	0.46	2.63	14	1
2:A:55:LEU:HD12	2:A:59:ARG:HB2	0.46	1.88	7	1
2:A:92:VAL:CG2	2:A:102:ALA:HB3	0.46	2.40	11	2
2:A:91:LEU:HD12	2:A:91:LEU:C	0.45	2.30	12	6
2:A:116:LEU:HD23	2:A:116:LEU:H	0.45	1.71	20	3
2:A:52:ILE:HD11	2:A:62:ALA:C	0.45	2.32	2	2
2:A:94:LEU:HD23	2:A:102:ALA:CB	0.45	2.39	20	1
2:A:82:VAL:CG1	2:A:82:VAL:O	0.45	2.65	16	5
2:A:63:MET:HE2	2:A:69:LYS:CA	0.45	2.42	12	1
2:A:39:LEU:HD21	2:A:119:TYR:HE1	0.45	1.72	1	1
2:A:61:GLU:OE2	2:A:71:LEU:HD11	0.45	2.11	3	1
2:A:123:PRO:CG	2:A:125:HIS:CE1	0.45	3.00	13	5
2:A:46:GLN:HB3	2:A:91:LEU:HD11	0.45	1.89	15	5
2:A:99:ASP:O	2:A:100:ASN:CB	0.45	2.64	20	3
2:A:57:ASN:OD1	2:A:57:ASN:N	0.45	2.50	4	1
2:A:51:VAL:CG2	2:A:90:ILE:CD1	0.44	2.95	3	6
2:A:75:ARG:NH2	2:A:105:ILE:HD12	0.44	2.27	4	1
2:A:123:PRO:CB	2:A:125:HIS:CE1	0.44	3.00	17	9
2:A:51:VAL:HB	2:A:85:ASN:O	0.44	2.12	17	8
2:A:113:ALA:O	2:A:116:LEU:CB	0.44	2.65	20	3
2:A:116:LEU:CB	2:A:122:LEU:HD11	0.44	2.42	14	1
2:A:91:LEU:HB2	2:A:108:TYR:OH	0.44	2.13	17	5
2:A:46:GLN:HB2	2:A:91:LEU:HD11	0.44	1.89	20	1
2:A:116:LEU:O	2:A:119:TYR:HB2	0.44	2.13	8	11
2:A:40:VAL:CG1	2:A:106:LEU:CD2	0.44	2.96	17	4
2:A:113:ALA:O	2:A:116:LEU:HB2	0.44	2.12	9	3
2:A:89:ILE:CD1	2:A:89:ILE:N	0.44	2.80	15	2
2:A:63:MET:HE1	2:A:69:LYS:HB2	0.44	1.88	13	2
2:A:93:GLY:N	2:A:105:ILE:CD1	0.44	2.80	9	1
2:A:98:GLN:O	2:A:99:ASP:CB	0.43	2.66	1	5
2:A:41:PHE:HD1	2:A:119:TYR:CD1	0.43	2.27	9	4
2:A:90:ILE:HG22	2:A:91:LEU:N	0.43	2.28	4	16
2:A:82:VAL:CG2	2:A:107:LYS:CB	0.43	2.96	20	2
2:A:55:LEU:N	2:A:55:LEU:CD2	0.43	2.80	17	1
2:A:97:TYR:O	2:A:98:GLN:HG2	0.43	2.13	5	1
2:A:39:LEU:HD13	2:A:112:GLU:OE2	0.43	2.13	8	1
2:A:63:MET:CE	2:A:69:LYS:CB	0.43	2.96	13	2
2:A:63:MET:HA	2:A:68:VAL:O	0.43	2.14	7	1
2:A:113:ALA:HB1	2:A:128:ILE:CG1	0.43	2.43	10	3
2:A:71:LEU:CD2	2:A:71:LEU:N	0.43	2.82	16	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:39:LEU:HD12	2:A:112:GLU:CG	0.43	2.44	18	1
2:A:123:PRO:HB2	2:A:125:HIS:CE1	0.43	2.49	17	6
2:A:74:ILE:O	2:A:75:ARG:CB	0.43	2.67	10	1
2:A:78:LEU:HG	2:A:106:LEU:HA	0.43	1.89	5	1
2:A:54:MET:HE3	2:A:84:ILE:HD12	0.43	1.89	8	1
2:A:119:TYR:HB3	2:A:121:GLU:HG3	0.42	1.91	10	2
2:A:48:TYR:OH	2:A:65:PHE:CG	0.42	2.72	9	3
2:A:60:LEU:HD22	2:A:84:ILE:HD12	0.42	1.90	10	1
2:A:39:LEU:HD21	2:A:119:TYR:CE1	0.42	2.49	1	1
2:A:51:VAL:CB	2:A:85:ASN:O	0.42	2.67	18	4
2:A:113:ALA:O	2:A:116:LEU:CG	0.42	2.66	14	2
2:A:58:GLY:CA	2:A:74:ILE:HG22	0.42	2.43	12	1
2:A:89:ILE:N	2:A:89:ILE:HD12	0.42	2.28	17	1
2:A:97:TYR:O	2:A:98:GLN:CG	0.42	2.67	5	1
2:A:122:LEU:CD2	2:A:122:LEU:N	0.42	2.82	16	4
2:A:112:GLU:CD	2:A:119:TYR:OH	0.42	2.58	14	1
2:A:73:HIS:CD2	2:A:97:TYR:OH	0.42	2.73	9	1
2:A:98:GLN:CG	2:A:98:GLN:O	0.42	2.66	5	1
2:A:91:LEU:HB3	2:A:108:TYR:CZ	0.42	2.49	13	8
2:A:71:LEU:N	2:A:71:LEU:CD2	0.42	2.82	5	6
2:A:113:ALA:HA	2:A:116:LEU:CG	0.42	2.45	8	5
2:A:116:LEU:O	2:A:119:TYR:N	0.42	2.52	16	11
2:A:92:VAL:CG2	2:A:102:ALA:CB	0.42	2.98	17	5
2:A:116:LEU:HB3	2:A:122:LEU:CD1	0.42	2.45	9	3
2:A:60:LEU:CD2	2:A:84:ILE:CD1	0.42	2.98	14	1
2:A:48:TYR:CZ	2:A:65:PHE:HB2	0.42	2.49	12	3
2:A:89:ILE:C	2:A:108:TYR:HB2	0.42	2.35	18	1
2:A:39:LEU:HD21	2:A:115:SER:HB2	0.42	1.92	19	1
2:A:70:ARG:NH1	2:A:94:LEU:HD22	0.42	2.30	13	1
2:A:73:HIS:CD2	2:A:97:TYR:CE2	0.42	3.08	16	1
2:A:74:ILE:HD12	2:A:84:ILE:HD13	0.42	1.88	1	1
2:A:50:GLN:O	2:A:63:MET:N	0.41	2.51	8	1
2:A:99:ASP:O	2:A:100:ASN:HB2	0.41	2.14	17	1
2:A:78:LEU:HD12	2:A:82:VAL:CB	0.41	2.45	16	1
2:A:75:ARG:CG	2:A:104:VAL:O	0.41	2.68	2	2
2:A:63:MET:CE	2:A:69:LYS:CA	0.41	2.97	10	3
2:A:48:TYR:CZ	2:A:121:GLU:HB3	0.41	2.50	16	1
2:A:51:VAL:CG1	2:A:60:LEU:HD13	0.41	2.46	12	1
2:A:54:MET:HE1	2:A:84:ILE:CD1	0.41	2.45	15	1
2:A:82:VAL:O	2:A:82:VAL:CG1	0.41	2.67	13	1
2:A:109:ASN:OD1	2:A:112:GLU:CG	0.41	2.69	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:52:ILE:HD13	2:A:63:MET:HB2	0.41	1.90	14	1
2:A:94:LEU:N	2:A:94:LEU:CD2	0.41	2.83	6	1
2:A:113:ALA:HB1	2:A:128:ILE:HG21	0.41	1.92	13	1
2:A:50:GLN:HG2	2:A:89:ILE:HD13	0.41	1.90	13	1
2:A:116:LEU:HA	2:A:119:TYR:CD1	0.41	2.51	14	5
2:A:40:VAL:HG11	2:A:106:LEU:HD22	0.41	1.91	20	2
2:A:48:TYR:CD1	2:A:121:GLU:OE1	0.41	2.74	6	4
2:A:48:TYR:CG	2:A:121:GLU:OE1	0.41	2.74	13	1
2:A:51:VAL:HA	2:A:62:ALA:CB	0.41	2.46	7	1
2:A:72:CYS:CB	2:A:92:VAL:HG11	0.41	2.45	20	1
2:A:74:ILE:CD1	2:A:84:ILE:HD11	0.41	2.45	1	1
2:A:94:LEU:CD2	2:A:102:ALA:CB	0.41	2.99	17	1
2:A:76:GLY:O	2:A:79:ARG:CG	0.41	2.69	9	1
2:A:89:ILE:CG2	2:A:116:LEU:HD11	0.40	2.46	20	1
2:A:115:SER:O	2:A:118:ALA:CB	0.40	2.69	1	2
2:A:111:ASP:O	2:A:114:ARG:HG2	0.40	2.16	14	1
2:A:94:LEU:O	2:A:95:ARG:CB	0.40	2.68	1	1
2:A:51:VAL:HG11	2:A:85:ASN:O	0.40	2.16	8	1
2:A:123:PRO:CG	2:A:125:HIS:NE2	0.40	2.85	18	1
2:A:112:GLU:HG3	2:A:119:TYR:OH	0.40	2.16	20	1
2:A:40:VAL:O	2:A:108:TYR:CE1	0.40	2.75	4	1
2:A:70:ARG:NH2	2:A:92:VAL:CG2	0.40	2.84	16	1
2:A:62:ALA:O	2:A:70:ARG:O	0.40	2.40	6	1
2:A:94:LEU:HD22	2:A:102:ALA:HB2	0.40	1.93	12	1
2:A:83:TRP:O	2:A:83:TRP:CD1	0.40	2.75	9	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	B	0	-	-	-	-	
2	A	91/143 (64%)	81±2 (88±3%)	9±2 (10±2%)	2±1 (2±2%)	14	56
All	All	1820/3140 (58%)	1610 (88%)	176 (10%)	34 (2%)	14	56

All 9 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	A	95	ARG	14
2	A	81	LYS	5
2	A	75	ARG	4
2	A	57	ASN	3
2	A	42	LYS	2
2	A	123	PRO	2
2	A	99	ASP	2
2	A	100	ASN	1
2	A	56	GLY	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	B	0	-	-	-	
2	A	77/122 (63%)	56±4 (73±5%)	21±4 (27±5%)	2	22
All	All	1540/2700 (57%)	1119 (73%)	421 (27%)	2	22

All 54 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)
2	A	91	LEU	20
2	A	84	ILE	20
2	A	116	LEU	20
2	A	122	LEU	20
2	A	115	SER	17
2	A	94	LEU	16
2	A	55	LEU	16
2	A	52	ILE	14
2	A	88	ASP	13
2	A	54	MET	13
2	A	75	ARG	12
2	A	81	LYS	12
2	A	53	LYS	11
2	A	100	ASN	11

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Mol	Chain	Res	Type	Models (Total)
2	A	107	LYS	11
2	A	63	MET	11
2	A	95	ARG	11
2	A	78	LEU	11
2	A	77	LYS	10
2	A	60	LEU	10
2	A	50	GLN	9
2	A	69	LYS	9
2	A	66	ASP	8
2	A	42	LYS	8
2	A	85	ASN	8
2	A	114	ARG	7
2	A	79	ARG	7
2	A	99	ASP	6
2	A	87	SER	6
2	A	117	LYS	6
2	A	73	HIS	6
2	A	38	GLU	6
2	A	127	LYS	5
2	A	98	GLN	5
2	A	101	LYS	5
2	A	74	ILE	4
2	A	80	LYS	4
2	A	70	ARG	3
2	A	82	VAL	3
2	A	96	ASP	3
2	A	83	TRP	3
2	A	124	GLU	3
2	A	112	GLU	2
2	A	47	GLU	2
2	A	61	GLU	2
2	A	46	GLN	2
2	A	59	ARG	2
2	A	90	ILE	2
2	A	43	GLU	1
2	A	103	ASP	1
2	A	39	LEU	1
2	A	111	ASP	1
2	A	65	PHE	1
2	A	44	ASP	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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 65% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 4519

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	1501
Number of shifts mapped to atoms	1449
Number of unparsed shifts	0
Number of shifts with mapping errors	52
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.

- Residue not found in structure. All 52 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	12	ASP	N	124.691	0.044	1
A	12	ASP	CA	52.614	0.068	1
A	10	HIS	CA	56.768	0.0	1
A	3	GLY	CA	45.122	0.189	1
A	3	GLY	HA2	4.01	0.0	1
A	3	GLY	N	110.762	0.034	1
A	13	PRO	HG3	2.032	0.0	1
A	4	SER	HB3	3.839	0.0	1
A	11	THR	HG22	1.171	0.019	1
A	11	THR	CA	61.479	0.139	1
A	14	MET	CA	53.026	0.0	1
A	11	THR	C	174.044	0.01	1
A	2	ARG	CB	31.086	0.0	1
A	13	PRO	CA	63.139	0.156	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	11	THR	H	8.033	0.004	1
A	4	SER	H	8.239	0.013	1
A	4	SER	C	174.546	0.0	1
A	11	THR	CB	69.957	0.136	1
A	3	GLY	C	174.247	0.0	1
A	4	SER	HA	4.428	0.015	1
A	3	GLY	H	8.613	0.007	1
A	12	ASP	H	8.376	0.015	1
A	11	THR	HB	4.18	0.018	1
A	11	THR	CG2	21.554	0.0	1
A	12	ASP	HB3	2.558	0.0	2
A	12	ASP	HA	4.872	0.019	1
A	14	MET	C	174.348	0.0	1
A	4	SER	HB2	3.839	0.0	1
A	11	THR	HG23	1.171	0.019	1
A	2	ARG	CA	56.809	0.0	1
A	10	HIS	HB3	3.133	0.0	1
A	11	THR	N	115.155	0.027	1
A	4	SER	N	115.132	0.052	1
A	4	SER	CA	58.44	0.274	1
A	13	PRO	HA	4.447	0.009	1
A	13	PRO	HD3	3.781	0.003	2
A	11	THR	HA	4.354	0.07	1
A	12	ASP	C	174.46	0.0	1
A	12	ASP	HB2	2.765	0.0	2
A	12	ASP	CB	41.256	0.0	1
A	13	PRO	CD	50.621	0.014	1
A	10	HIS	C	175.444	0.0	1
A	3	GLY	HA3	4.01	0.0	1
A	2	ARG	C	176.727	0.0	1
A	13	PRO	HG2	2.032	0.0	1
A	14	MET	N	121.594	0.202	1
A	10	HIS	HB2	3.133	0.0	1
A	14	MET	HA	4.759	0.004	1
A	11	THR	HG21	1.171	0.019	1
A	10	HIS	CB	30.816	0.189	1
A	13	PRO	HD2	3.858	0.004	2
A	14	MET	H	8.42	0.018	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
$^{13}\text{C}_\alpha$	137	-0.16 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	113	-0.12 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}'$	131	-0.15 ± 0.16	None needed (< 0.5 ppm)
^{15}N	125	-0.06 ± 0.47	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments ⓘ

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 973 atoms were assigned a chemical shift out of a possible 1175. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	442/453 (98%)	176/181 (97%)	180/182 (99%)	86/90 (96%)
Sidechain	494/644 (77%)	311/376 (83%)	178/233 (76%)	5/35 (14%)
Aromatic	37/78 (47%)	36/40 (90%)	0/33 (0%)	1/5 (20%)
Overall	973/1175 (83%)	523/597 (88%)	358/448 (80%)	92/130 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 1302 atoms were assigned a chemical shift out of a possible 1993. 16 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	615/777 (79%)	242/310 (78%)	253/314 (81%)	120/153 (78%)
Sidechain	642/1072 (60%)	399/629 (63%)	238/381 (62%)	5/62 (8%)
Aromatic	45/144 (31%)	44/74 (59%)	0/53 (0%)	1/17 (6%)
Overall	1302/1993 (65%)	685/1013 (68%)	491/748 (66%)	126/232 (54%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	98	GLN	CB	41.54	38.36 – 19.96	6.7
1	A	70	ARG	CG	34.60	33.23 – 21.23	6.1
1	A	46	GLN	CG	39.44	39.38 – 28.18	5.0

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:

