



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:19 PM BST

PDB ID : 2JSC  
Title : NMR structure of the cadmium metal-sensor CMTR from Mycobacterium tuberculosis  
Authors : Banci, L.; Bertini, I.; Cantini, F.; Ciofi-Baffoni, S.; Cavet, J.S.; Dennison, C.; Graham, A.I.; Harvie, D.R.; Robinson, N.J.; Structural Proteomics in Europe (SPINE)  
Deposited on : 2007-07-02

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

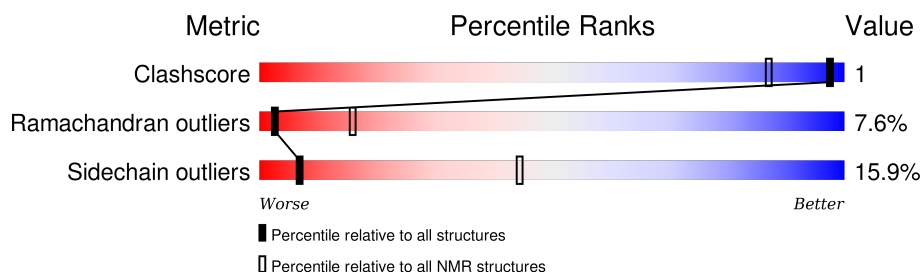
# 1 Overall quality at a glance

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	118	 63% 15% • 19%
1	B	118	 55% 17% 10% 18%

## 2 Ensemble composition and analysis ⓘ

This entry contains 30 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:102, B:11-B:95 (177)	0.90	3

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

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

There are 2 unique types of molecules in this entry. The entry contains 2920 atoms, of which 1481 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator Rv1994c/MT2050.

Mol	Chain	Residues	Atoms						Trace
1	A	96	Total	C	H	N	O	S	0
			1454	444	738	138	129	5	
1	B	97	Total	C	H	N	O	S	0
			1464	447	743	139	130	5	

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

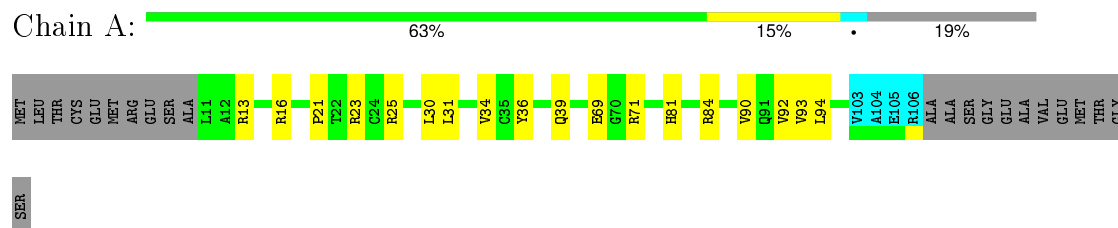
Mol	Chain	Residues	Atoms	
2	B	1	Total	Cd
			1	1
2	A	1	Total	Cd
			1	1

## 4 Residue-property plots

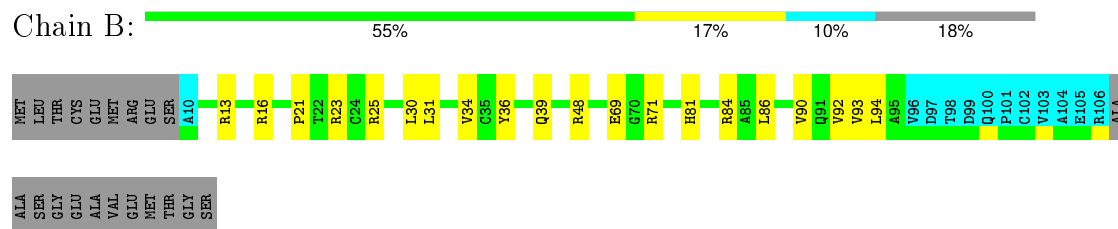
### 4.1 Average score per residue in the NMR ensemble

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: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

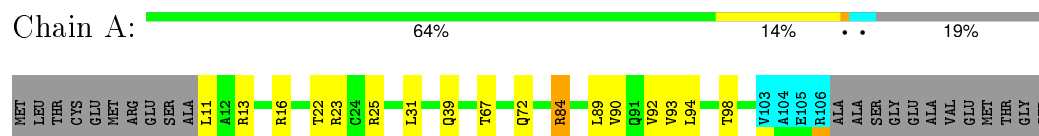


### 4.2 Scores per residue for each member of the ensemble

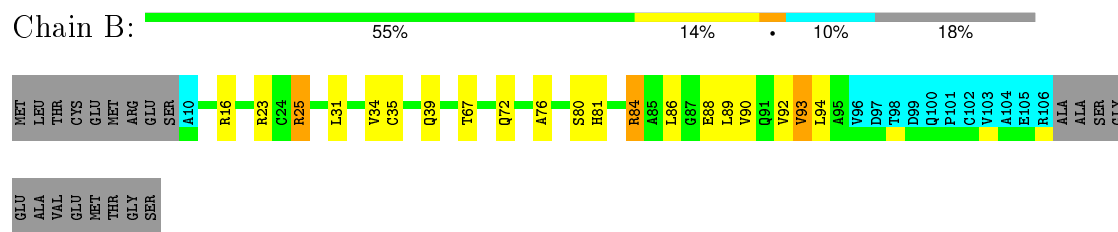
Colouring as in section 4.1 above.

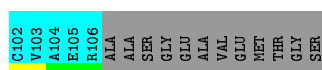
#### 4.2.1 Score per residue for model 1

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



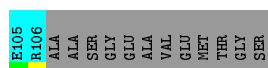
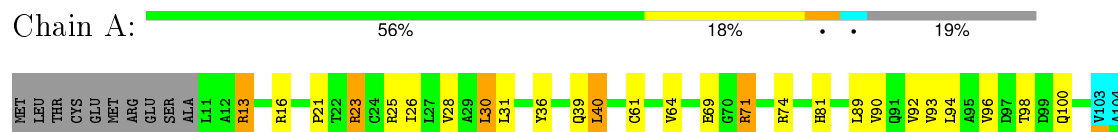
- Molecule 1: Transcriptional regulator Rv1994c/MT2050



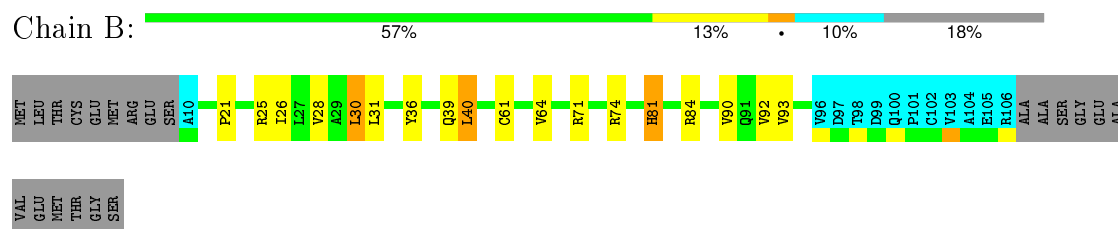


#### 4.2.4 Score per residue for model 4

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

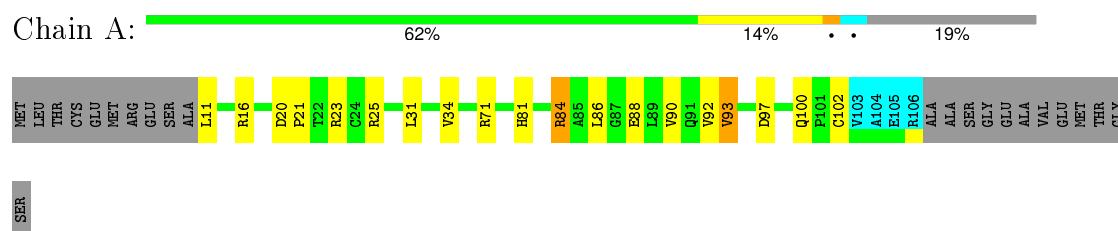


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

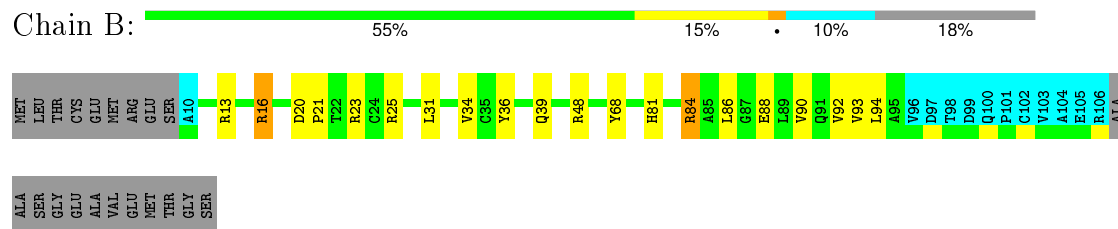


#### 4.2.5 Score per residue for model 5

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

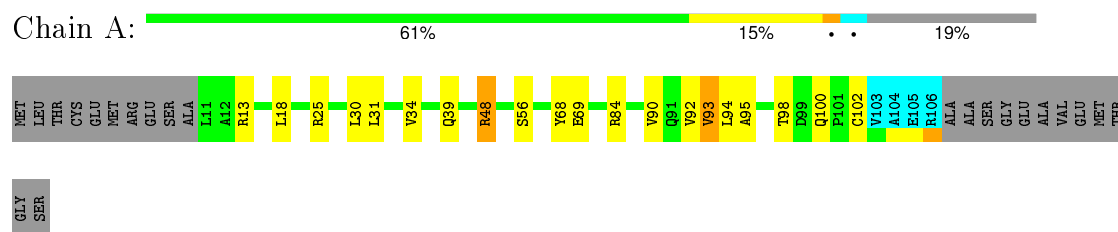


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

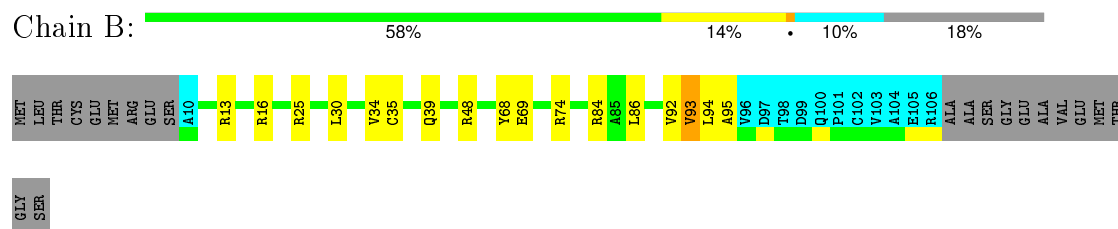


### 4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

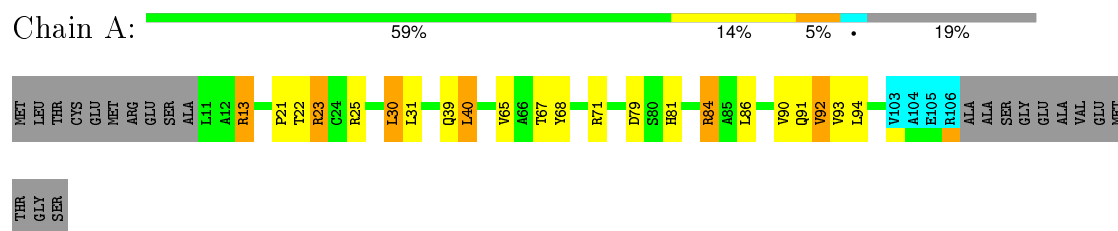


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

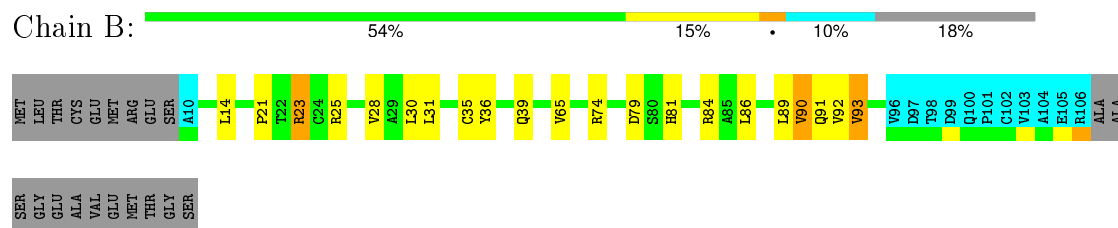


### 4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

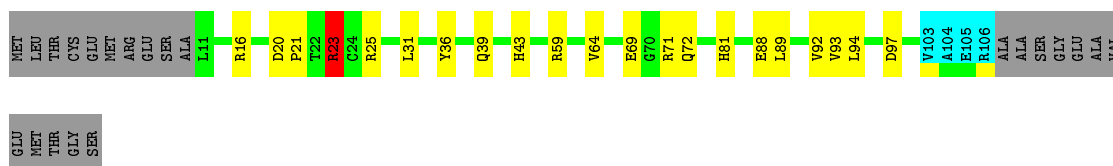


### 4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

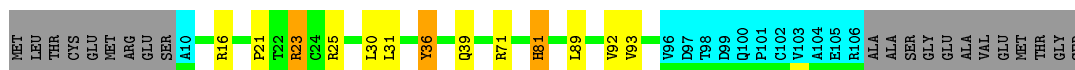






- Molecule 1: Transcriptional regulator Rv1994c/MT2050

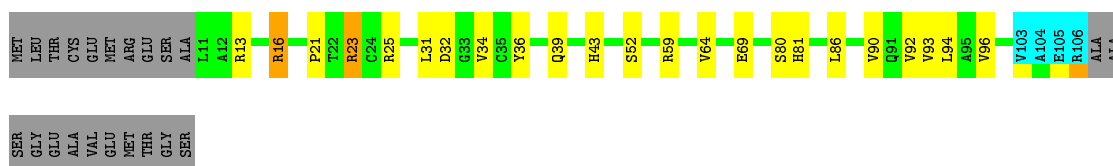
Chain B: 61% 8% 10% 18%



#### 4.2.9 Score per residue for model 9

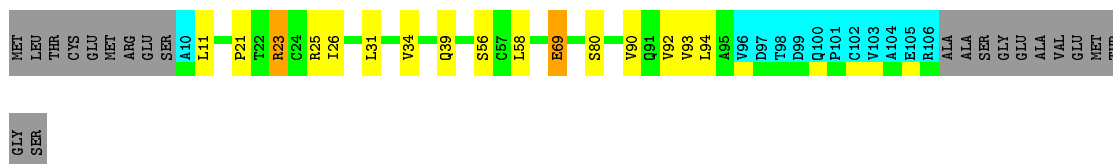
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 58% 18% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

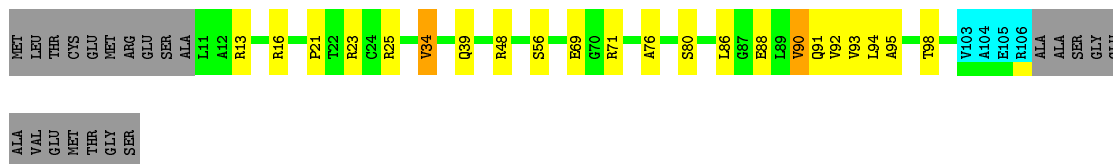
Chain B: 58% 12% 10% 18%



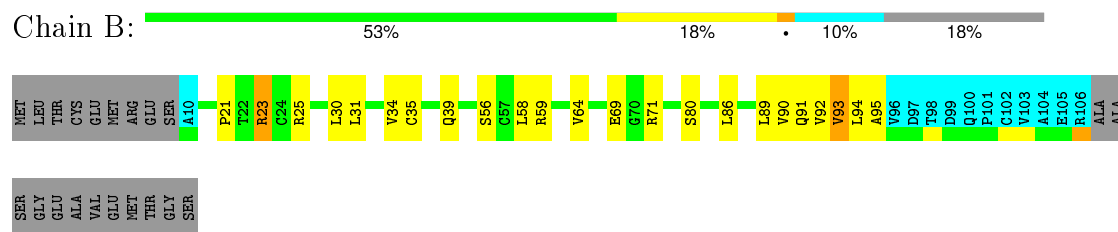
#### 4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 59% 17% 19%

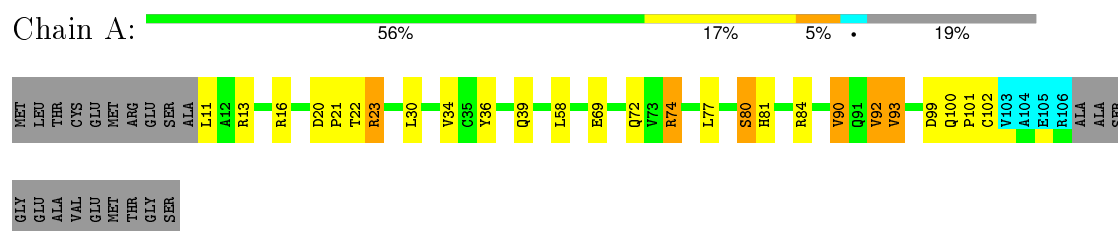


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

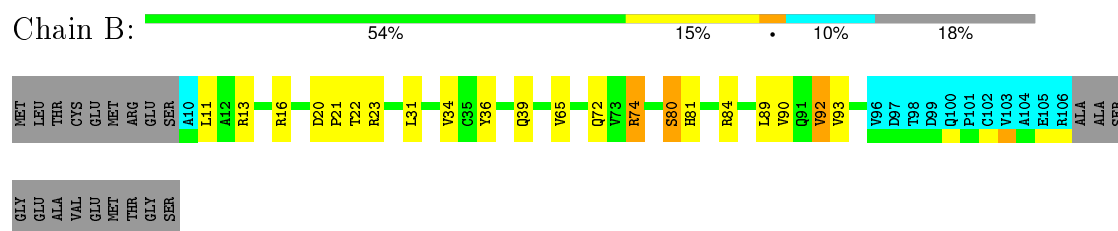


#### 4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

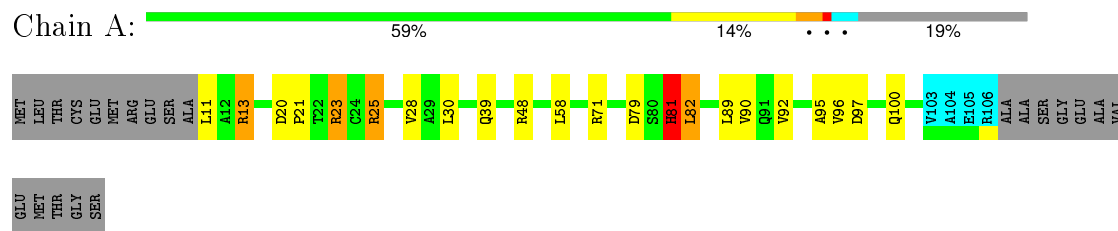


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

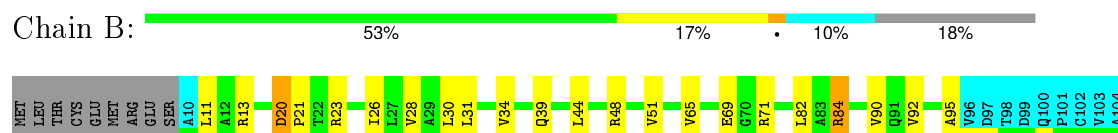


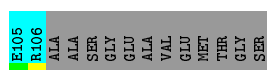
#### 4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

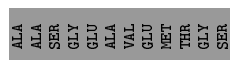
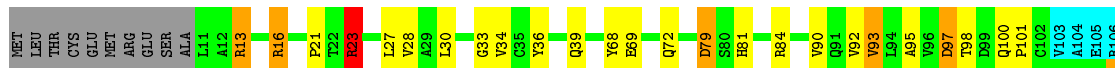




#### 4.2.13 Score per residue for model 13

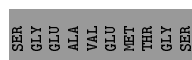
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 57% 16% 19%



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

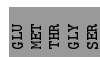
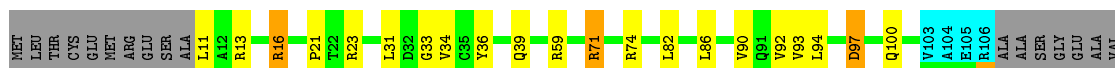
Chain B: 52% 19% 10% 18%



#### 4.2.14 Score per residue for model 14

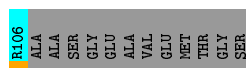
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 60% 15% 19%



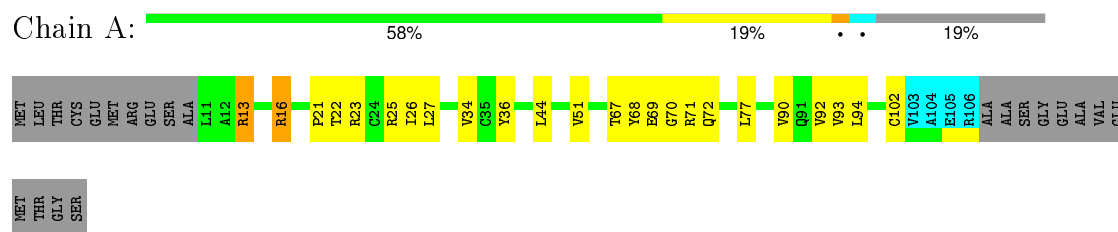
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 53% 17% 10% 18%

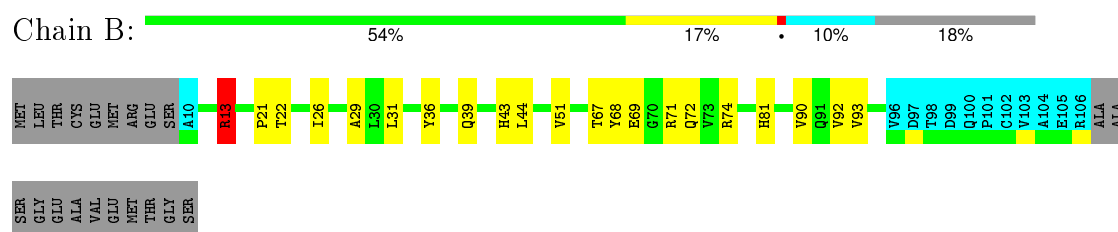


### 4.2.15 Score per residue for model 15

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

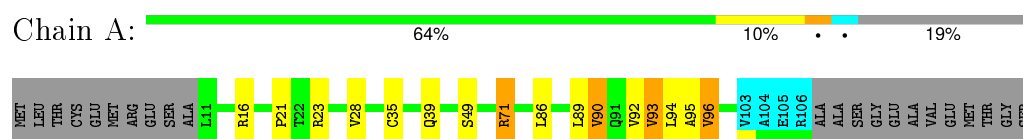


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

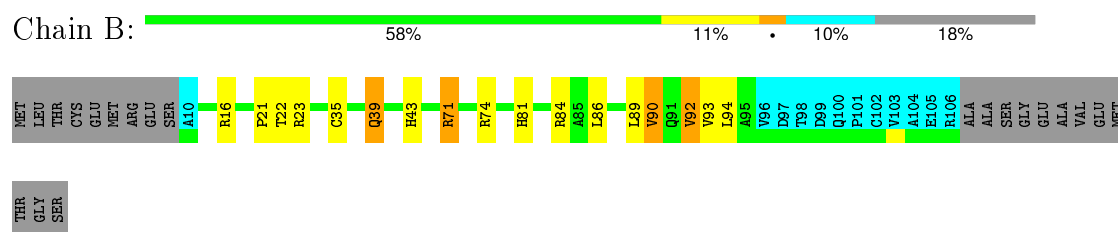


### 4.2.16 Score per residue for model 16

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



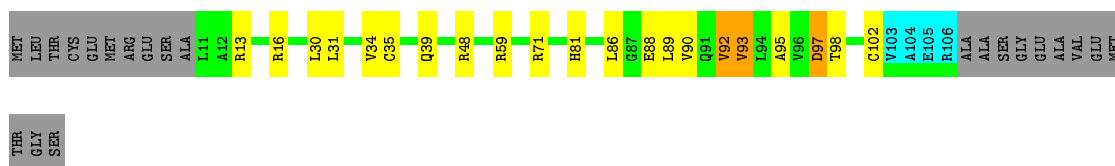
- Molecule 1: Transcriptional regulator Rv1994c/MT2050



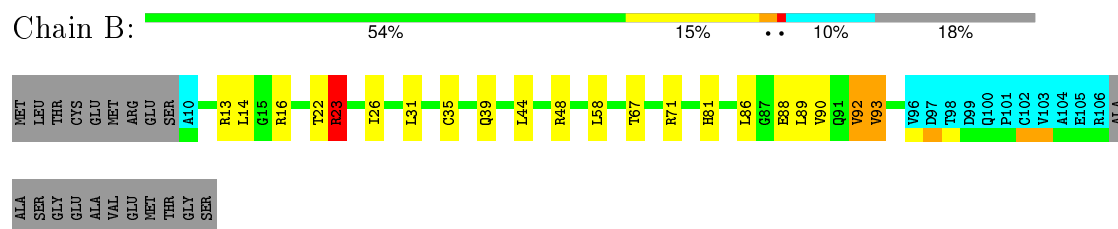
### 4.2.17 Score per residue for model 17

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



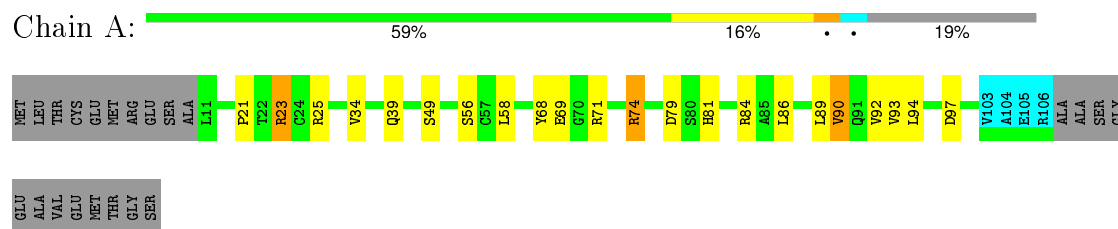


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

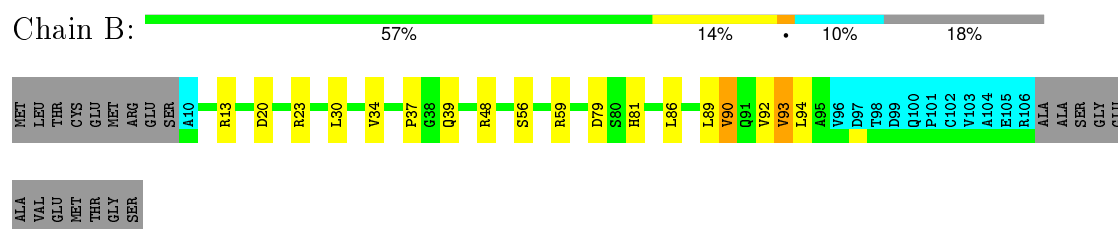


#### 4.2.18 Score per residue for model 18

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

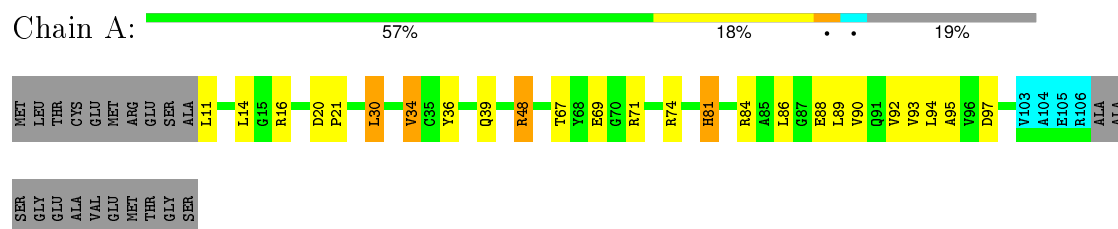


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

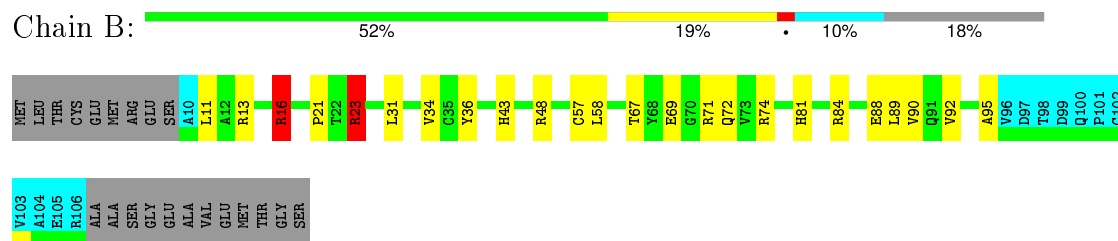


#### 4.2.19 Score per residue for model 19

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

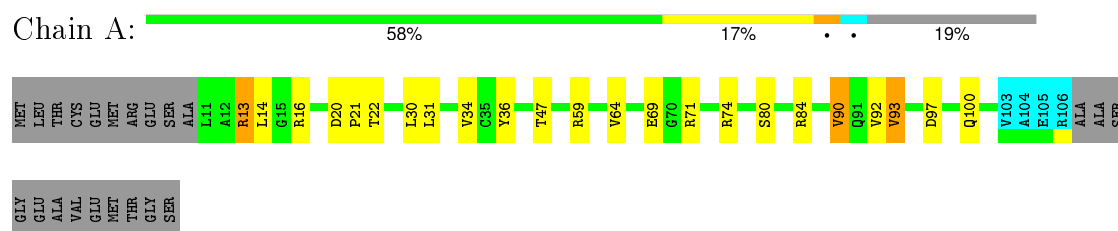


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

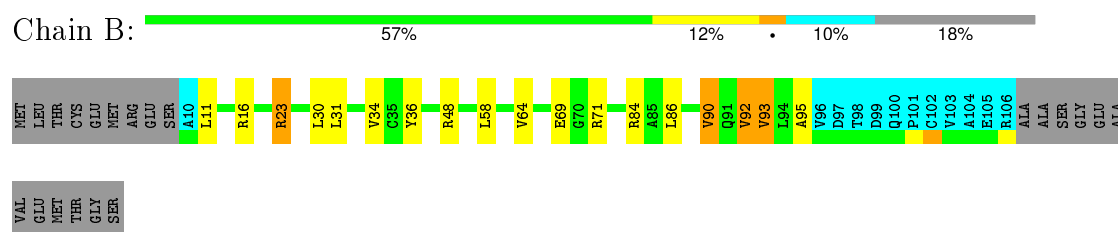


#### 4.2.20 Score per residue for model 20

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

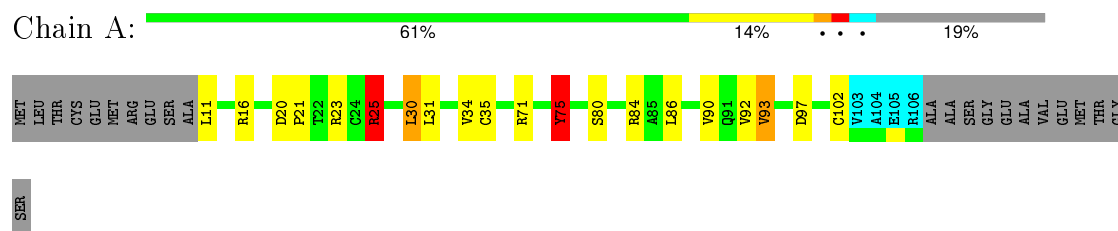


- Molecule 1: Transcriptional regulator Rv1994c/MT2050



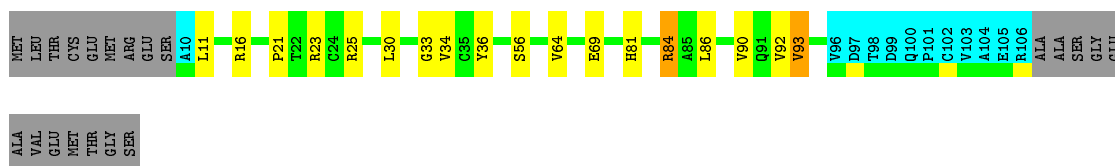
#### 4.2.21 Score per residue for model 21

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

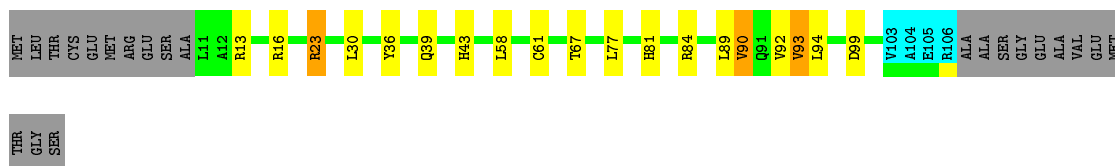




#### 4.2.22 Score per residue for model 22

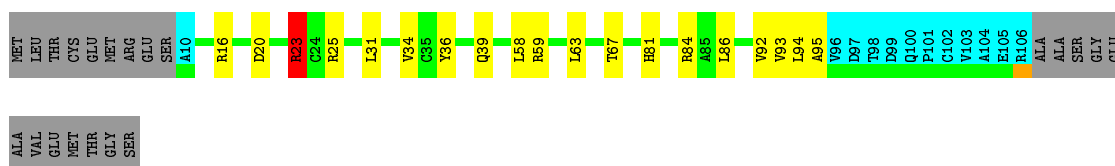
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

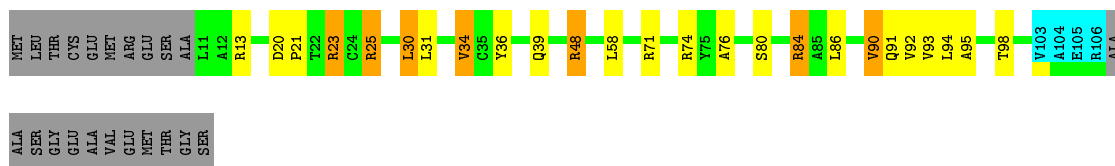
Chain B:



#### 4.2.23 Score per residue for model 23

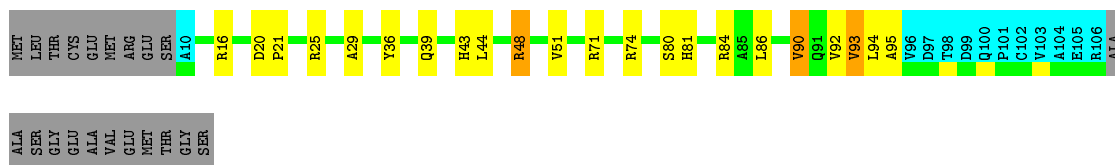
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



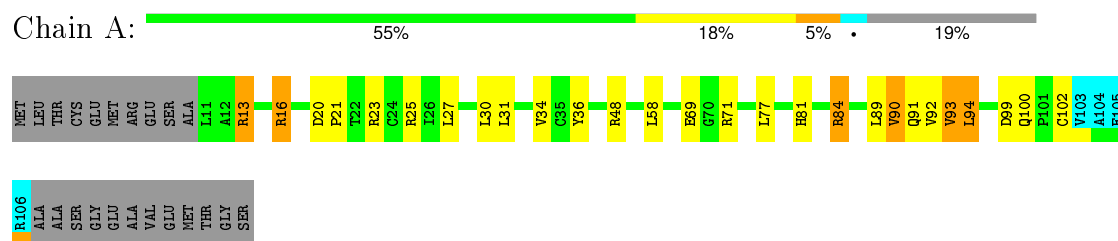
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

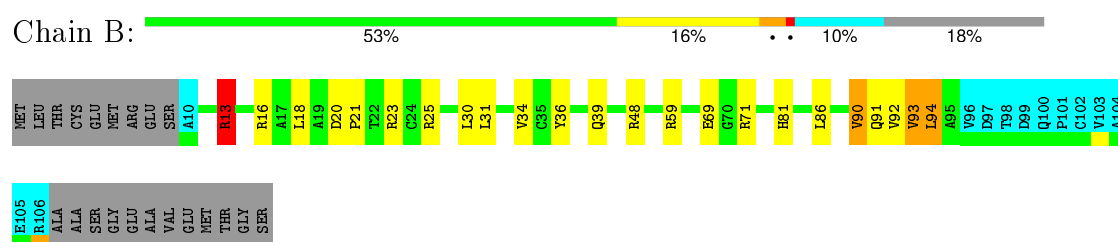


### 4.2.24 Score per residue for model 24

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

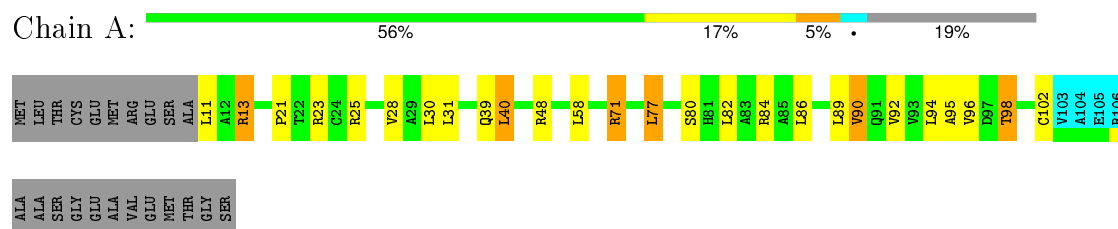


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

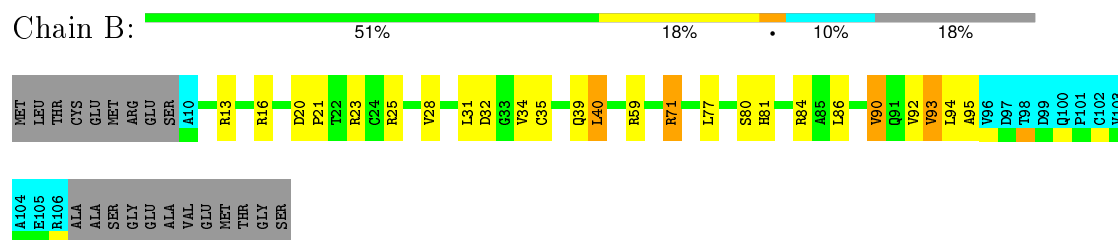


### 4.2.25 Score per residue for model 25

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



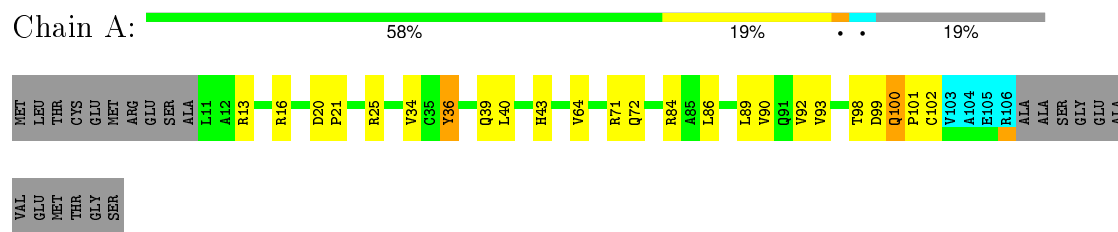
- Molecule 1: Transcriptional regulator Rv1994c/MT2050



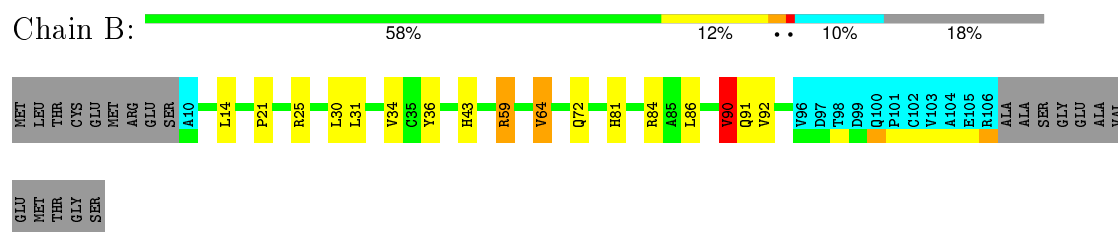
### 4.2.26 Score per residue for model 26

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



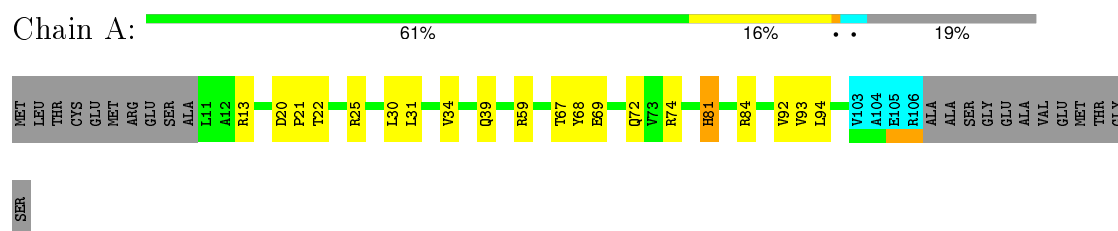


- Molecule 1: Transcriptional regulator Rv1994c/MT2050

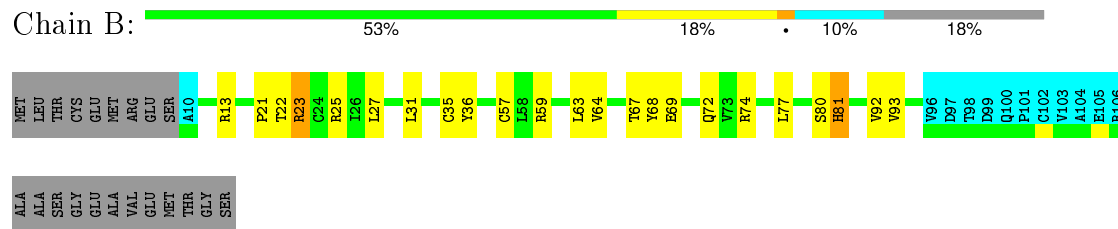


#### 4.2.27 Score per residue for model 27

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

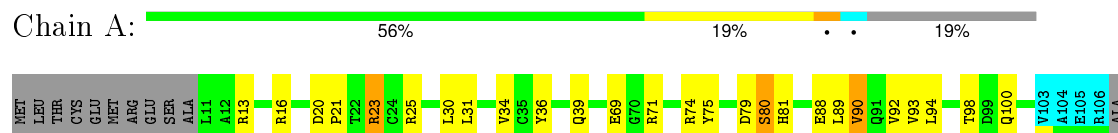


- Molecule 1: Transcriptional regulator Rv1994c/MT2050



#### 4.2.28 Score per residue for model 28

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



ALA  
SER  
GLY  
GLU  
ALA  
VAL  
GLU  
MET  
THR  
GLY  
SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 50% 19% 10% 18%

MET LEU THR CYS MET ARG GLU SER A10 R13 R16 P21 T22 R23 C24 R25 L30 L31 Q39 H43 R48 S56 R59 E69 G70 R71 R74 D79 S80 H81 L86 G87 E88 L89 V90 Q91 V92 V93 A95 V96 D97 T98 Q100 P101  
G102 V103 A104 E105 A106 ALA ALA VAL MET THR GLY SER

#### 4.2.29 Score per residue for model 29

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 61% 14% 19%

MET LEU THR CYS MET ARG GLU SER L11 A12 R13 R16 P21 T22 R23 C24 R25 L30 L31 V34 G35 Y36 H43 R48 E69 S80 H81 L82 V90 Q91 V92 V93 L94 C102 V103 A104 E105 R106 ALA ALA SER GLY ALA VAL GLU MET THR  
GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 57% 13% 10% 18%

MET LEU THR CYS MET ARG GLU SER A10 R16 P21 T22 R23 C24 R25 L30 L31 V34 C35 R48 E69 G70 Y75 S80 H81 L82 V90 Q91 V92 V93 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY ALA VAL GLU  
MET THR GLY SER

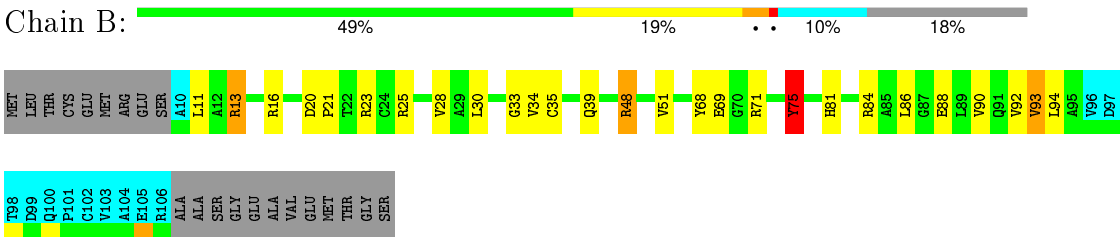
#### 4.2.30 Score per residue for model 30

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 53% 21% 19%

MET LEU THR CYS MET ARG GLU SER L11 A12 R13 R16 A19 D20 P21 T22 R23 V28 A29 L30 G33 Y36 Q39 R48 T67 Y68 E69 G70 R71 V72 V73 Y75 H81 R84 E88 L89 V90 Q91 V92 V93 L94 A95 Q100 V103  
A104 E105 R106 ALA ALA VAL GLU MET THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS COUPLED WITH SIMULATED ANNEALING FOLLOWED BY RESTRAINED ENERGY MINIMIZATION*.

Of the 300 calculated structures, 30 were deposited, based on the following criterion: *TARGET FUNCTION*.

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

Software name	Classification	Version
AMBER	refinement	8.0
CYANA	structure solution	1.1

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 i

### 6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.63±0.01	0±0/693 (0.0±0.0%)	1.28±0.05	5±2/944 (0.5±0.2%)
1	B	0.63±0.01	0±0/640 (0.0±0.0%)	1.28±0.05	5±2/870 (0.6±0.2%)
All	All	0.63	0/39990 (0.0%)	1.28	288/54420 (0.5%)

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	1.6±1.1
1	B	0.0±0.0	1.4±1.1
All	All	0	92

There are no bond-length outliers.

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	B	23	ARG	NE-CZ-NH1	13.22	126.91	120.30	25	13
1	B	25	ARG	NE-CZ-NH1	10.17	125.38	120.30	30	17
1	A	13	ARG	NE-CZ-NH1	10.15	125.37	120.30	12	17
1	A	23	ARG	NE-CZ-NH1	10.04	125.32	120.30	25	12
1	A	16	ARG	NE-CZ-NH1	9.87	125.23	120.30	22	14
1	A	13	ARG	NE-CZ-NH2	-9.79	115.41	120.30	28	4
1	B	84	ARG	NE-CZ-NH1	9.26	124.93	120.30	22	18
1	B	71	ARG	NE-CZ-NH1	8.92	124.76	120.30	10	8
1	A	71	ARG	NE-CZ-NH1	8.88	124.74	120.30	10	8
1	A	84	ARG	NE-CZ-NH1	8.76	124.68	120.30	22	16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	B	74	ARG	NE-CZ-NH1	8.66	124.63	120.30	28	7
1	B	48	ARG	NE-CZ-NH2	-8.09	116.25	120.30	28	2
1	A	25	ARG	NE-CZ-NH1	8.03	124.31	120.30	28	15
1	A	84	ARG	NE-CZ-NH2	-8.02	116.29	120.30	19	4
1	B	13	ARG	NE-CZ-NH2	-7.93	116.33	120.30	28	2
1	B	13	ARG	NE-CZ-NH1	7.72	124.16	120.30	11	14
1	B	16	ARG	NE-CZ-NH1	7.70	124.15	120.30	19	10
1	A	48	ARG	NE-CZ-NH1	7.70	124.15	120.30	23	9
1	B	48	ARG	NE-CZ-NH1	7.66	124.13	120.30	17	10
1	A	71	ARG	NE-CZ-NH2	-7.63	116.48	120.30	30	2
1	B	59	ARG	NE-CZ-NH1	7.46	124.03	120.30	13	9
1	A	59	ARG	NE-CZ-NH2	7.20	123.90	120.30	9	1
1	A	25	ARG	NE-CZ-NH2	-7.16	116.72	120.30	9	3
1	B	75	TYR	CB-CG-CD2	-7.11	116.73	121.00	30	2
1	A	75	TYR	CB-CG-CD2	-7.00	116.80	121.00	21	3
1	A	16	ARG	NE-CZ-NH2	-6.86	116.87	120.30	15	2
1	B	23	ARG	CD-NE-CZ	6.83	133.16	123.60	17	2
1	B	92	VAL	CA-CB-CG1	-6.83	100.66	110.90	17	2
1	B	74	ARG	NE-CZ-NH2	-6.71	116.94	120.30	7	3
1	B	84	ARG	NE-CZ-NH2	-6.63	116.98	120.30	19	6
1	A	23	ARG	NE-CZ-NH2	-6.49	117.05	120.30	9	3
1	A	74	ARG	NE-CZ-NH1	6.45	123.53	120.30	23	5
1	A	13	ARG	CD-NE-CZ	6.33	132.46	123.60	7	1
1	B	84	ARG	CD-NE-CZ	6.19	132.27	123.60	19	1
1	A	92	VAL	CA-CB-CG1	-6.18	101.62	110.90	17	1
1	A	59	ARG	NE-CZ-NH1	6.09	123.34	120.30	14	3
1	A	30	LEU	CB-CG-CD2	-6.04	100.74	111.00	28	7
1	B	25	ARG	NE-CZ-NH2	-6.01	117.30	120.30	9	2
1	A	84	ARG	CD-NE-CZ	6.00	132.00	123.60	19	2
1	B	30	LEU	CB-CG-CD2	-5.92	100.94	111.00	6	6
1	B	16	ARG	NE-CZ-NH2	-5.88	117.36	120.30	29	1
1	B	23	ARG	NE-CZ-NH2	-5.75	117.43	120.30	9	2
1	B	48	ARG	CD-NE-CZ	5.73	131.62	123.60	28	1
1	B	79	ASP	CB-CG-OD2	-5.68	113.19	118.30	13	1
1	B	16	ARG	CD-NE-CZ	5.49	131.28	123.60	17	1
1	B	91	GLN	CA-CB-CG	5.48	125.45	113.40	26	1
1	A	36	TYR	CB-CG-CD1	-5.47	117.72	121.00	26	1
1	B	36	TYR	CB-CG-CD1	-5.40	117.76	121.00	26	1
1	B	91	GLN	N-CA-CB	-5.32	101.02	110.60	10	1
1	A	89	LEU	C-N-CA	5.29	134.94	121.70	26	2
1	A	30	LEU	CB-CG-CD1	5.29	120.00	111.00	4	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	16	ARG	CD-NE-CZ	5.24	130.94	123.60	17	1
1	B	91	GLN	C-N-CA	5.20	134.70	121.70	13	1
1	B	20	ASP	CB-CG-OD2	-5.18	113.64	118.30	25	1
1	A	79	ASP	CB-CG-OD2	-5.17	113.64	118.30	13	1
1	B	30	LEU	CB-CG-CD1	5.15	119.76	111.00	4	1
1	B	86	LEU	CB-CG-CD1	5.08	119.64	111.00	30	1
1	B	69	GLU	CA-CB-CG	5.05	124.51	113.40	9	1
1	B	90	VAL	CA-CB-CG1	5.00	118.40	110.90	13	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	B	81	HIS	Sidechain	14
1	A	81	HIS	Sidechain	13
1	B	90	VAL	Peptide	9
1	A	90	VAL	Peptide	8
1	A	23	ARG	Sidechain	6
1	B	23	ARG	Sidechain	6
1	A	43	HIS	Sidechain	4
1	A	13	ARG	Sidechain	3
1	A	25	ARG	Sidechain	3
1	A	74	ARG	Sidechain	3
1	A	59	ARG	Sidechain	2
1	B	59	ARG	Sidechain	2
1	B	75	TYR	Sidechain	2
1	A	16	ARG	Sidechain	2
1	B	13	ARG	Sidechain	2
1	A	75	TYR	Sidechain	2
1	B	74	ARG	Sidechain	2
1	B	71	ARG	Sidechain	1
1	B	43	HIS	Sidechain	1
1	A	36	TYR	Sidechain	1
1	B	36	TYR	Sidechain	1
1	B	48	ARG	Sidechain	1
1	A	48	ARG	Sidechain	1
1	B	16	ARG	Sidechain	1
1	B	84	ARG	Sidechain	1
1	A	84	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	B	632	662	661	1±1
1	A	684	705	704	1±1
All	All	39540	41010	40949	68

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:LEU:CD1	1:B:92:VAL:HG21	0.57	2.29	20	1
1:B:23:ARG:CD	1:B:58:LEU:HD13	0.56	2.29	22	1
1:B:27:LEU:HD22	1:B:77:LEU:HD21	0.55	1.79	27	1
1:B:90:VAL:HG23	1:B:92:VAL:HG12	0.54	1.79	11	1
1:A:90:VAL:HG23	1:A:92:VAL:HG12	0.52	1.78	11	1
1:B:23:ARG:HH21	1:B:57:CYS:CB	0.52	2.18	27	1
1:A:40:LEU:H	1:A:40:LEU:HD12	0.51	1.64	7	3
1:B:44:LEU:HD12	1:B:51:VAL:HG22	0.50	1.82	23	3
1:A:27:LEU:HD22	1:A:77:LEU:HD21	0.49	1.84	15	2
1:B:23:ARG:HG2	1:B:58:LEU:HD13	0.49	1.85	20	3
1:B:26:ILE:HG12	1:B:44:LEU:HD11	0.49	1.85	17	2
1:B:28:VAL:HG22	1:B:86:LEU:HD21	0.48	1.85	7	1
1:A:30:LEU:O	1:A:34:VAL:HG13	0.47	2.09	23	3
1:A:58:LEU:H	1:A:58:LEU:HD12	0.46	1.68	23	1
1:B:40:LEU:H	1:B:40:LEU:HD12	0.46	1.69	25	3
1:A:40:LEU:HD12	1:A:40:LEU:H	0.46	1.69	25	1
1:A:34:VAL:HG12	1:A:76:ALA:HA	0.46	1.88	10	2
1:A:82:LEU:HD22	1:A:82:LEU:H	0.46	1.71	12	1
1:B:89:LEU:O	1:B:90:VAL:HG13	0.46	2.11	16	1
1:A:11:LEU:HD12	1:A:11:LEU:H	0.45	1.70	5	1
1:B:30:LEU:HD11	1:B:64:VAL:CG1	0.45	2.41	26	1
1:B:29:ALA:HB1	1:B:43:HIS:CD2	0.45	2.45	23	2
1:B:23:ARG:CG	1:B:58:LEU:HD13	0.45	2.42	20	2
1:A:23:ARG:CD	1:A:58:LEU:HD13	0.45	2.42	18	3
1:A:30:LEU:HD21	1:A:75:TYR:CE2	0.45	2.47	30	1
1:B:30:LEU:HD21	1:B:75:TYR:CD2	0.44	2.46	30	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:THR:HG22	1:A:68:TYR:H	0.44	1.71	7	1
1:A:23:ARG:CG	1:A:58:LEU:HD11	0.44	2.43	23	1
1:A:89:LEU:O	1:A:90:VAL:HG13	0.44	2.12	24	1
1:B:92:VAL:O	1:B:92:VAL:HG13	0.44	2.13	16	1
1:B:58:LEU:HD12	1:B:63:LEU:HD12	0.44	1.88	22	1
1:B:23:ARG:HD2	1:B:58:LEU:HD13	0.43	1.88	22	1
1:A:23:ARG:HH21	1:A:27:LEU:HD12	0.43	1.73	13	1
1:B:39:GLN:HE22	1:B:43:HIS:CD2	0.43	2.31	16	2
1:A:77:LEU:HB3	1:A:82:LEU:CD1	0.43	2.44	25	1
1:B:30:LEU:HD21	1:B:75:TYR:CE2	0.43	2.48	30	1
1:A:58:LEU:HD12	1:A:58:LEU:N	0.43	2.28	23	1
1:A:14:LEU:HD12	1:B:92:VAL:HG21	0.42	1.89	20	1
1:A:44:LEU:HD12	1:A:51:VAL:HG22	0.42	1.91	15	1
1:B:23:ARG:HH12	1:B:57:CYS:CB	0.42	2.27	2	1
1:B:34:VAL:HG12	1:B:76:ALA:HA	0.42	1.90	1	1
1:A:23:ARG:HG2	1:A:58:LEU:HD13	0.42	1.91	12	1
1:A:30:LEU:HD22	1:A:75:TYR:CE2	0.41	2.50	21	1
1:B:23:ARG:HH12	1:B:57:CYS:HB3	0.41	1.75	2	1
1:B:20:ASP:CG	1:B:23:ARG:HE	0.41	2.19	2	1
1:A:97:ASP:HA	1:B:12:ALA:HB3	0.41	1.92	13	1
1:B:20:ASP:CB	1:B:23:ARG:HB3	0.41	2.46	12	1
1:B:63:LEU:O	1:B:77:LEU:HD23	0.41	2.16	27	1
1:A:92:VAL:HG21	1:B:14:LEU:CD2	0.40	2.46	7	1
1:B:14:LEU:CD2	1:B:63:LEU:HD22	0.40	2.46	3	1

## 6.3 Torsion angles ⓘ

### 6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	92/118 (78%)	74±3 (81±3%)	10±3 (11±3%)	7±1 (8±2%)	2	14
1	B	85/118 (72%)	69±2 (81±3%)	10±3 (12±3%)	6±1 (7±2%)	3	18
All	All	5309/7080 (75%)	4293 (81%)	615 (12%)	401 (8%)	2	16

All 46 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	92	VAL	29
1	A	92	VAL	29
1	A	93	VAL	28
1	A	90	VAL	27
1	A	21	PRO	26
1	B	93	VAL	25
1	B	21	PRO	24
1	B	90	VAL	22
1	A	94	LEU	22
1	A	34	VAL	19
1	B	94	LEU	15
1	B	34	VAL	14
1	A	89	LEU	12
1	A	95	ALA	11
1	B	95	ALA	11
1	B	89	LEU	11
1	A	97	ASP	7
1	A	71	ARG	5
1	B	80	SER	4
1	A	102	CYS	4
1	A	80	SER	4
1	A	98	THR	4
1	B	71	ARG	4
1	A	101	PRO	3
1	B	35	CYS	3
1	B	79	ASP	3
1	A	99	ASP	3
1	A	33	GLY	3
1	B	11	LEU	3
1	B	33	GLY	3
1	A	91	GLN	2
1	B	91	GLN	2
1	A	79	ASP	2
1	A	61	CYS	2
1	B	70	GLY	2
1	A	69	GLU	2
1	A	96	VAL	2
1	A	81	HIS	1
1	B	37	PRO	1
1	B	61	CYS	1
1	B	69	GLU	1
1	A	100	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	19	ALA	1
1	A	11	LEU	1
1	A	70	GLY	1
1	A	35	CYS	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	72/91 (79%)	60±3 (84±4%)	12±3 (16±4%)	7	44
1	B	65/91 (71%)	55±2 (84±4%)	10±2 (16±4%)	7	45
All	All	4110/5460 (75%)	3457 (84%)	653 (16%)	7	44

All 100 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	B	39	GLN	24
1	A	39	GLN	24
1	B	31	LEU	23
1	A	31	LEU	19
1	B	86	LEU	18
1	A	69	GLU	16
1	B	81	HIS	15
1	B	36	TYR	15
1	A	86	LEU	15
1	A	36	TYR	15
1	B	69	GLU	15
1	A	20	ASP	14
1	A	100	GLN	14
1	B	93	VAL	14
1	A	71	ARG	13
1	B	16	ARG	13
1	A	16	ARG	13
1	A	93	VAL	12
1	B	23	ARG	11
1	B	20	ASP	11

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Mol	Chain	Res	Type	Models (Total)
1	A	23	ARG	11
1	A	30	LEU	9
1	A	81	HIS	8
1	A	84	ARG	8
1	A	67	THR	8
1	B	88	GLU	8
1	B	71	ARG	8
1	A	72	GLN	8
1	B	35	CYS	8
1	B	30	LEU	8
1	A	98	THR	7
1	B	64	VAL	7
1	A	97	ASP	7
1	A	22	THR	7
1	A	88	GLU	7
1	A	102	CYS	7
1	B	80	SER	7
1	A	80	SER	7
1	A	13	ARG	7
1	B	56	SER	6
1	B	25	ARG	6
1	A	28	VAL	6
1	B	68	TYR	6
1	B	22	THR	6
1	A	25	ARG	6
1	A	68	TYR	6
1	A	11	LEU	6
1	B	72	GLN	6
1	B	67	THR	6
1	B	48	ARG	5
1	A	64	VAL	5
1	A	48	ARG	5
1	A	40	LEU	5
1	B	11	LEU	5
1	B	13	ARG	5
1	A	96	VAL	4
1	A	58	LEU	4
1	B	28	VAL	4
1	B	84	ARG	4
1	A	79	ASP	3
1	A	91	GLN	3
1	A	74	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	B	82	LEU	3
1	A	77	LEU	3
1	B	94	LEU	3
1	B	26	ILE	3
1	B	65	VAL	3
1	B	34	VAL	3
1	B	40	LEU	3
1	B	14	LEU	3
1	A	35	CYS	3
1	A	82	LEU	3
1	B	43	HIS	3
1	A	56	SER	3
1	B	57	CYS	2
1	A	26	ILE	2
1	A	92	VAL	2
1	A	94	LEU	2
1	B	58	LEU	2
1	B	91	GLN	2
1	B	79	ASP	2
1	B	18	LEU	2
1	B	32	ASP	2
1	B	90	VAL	2
1	A	43	HIS	2
1	A	49	SER	2
1	A	14	LEU	2
1	A	90	VAL	2
1	B	74	ARG	2
1	A	52	SER	1
1	A	47	THR	1
1	A	99	ASP	1
1	A	65	VAL	1
1	A	73	VAL	1
1	A	75	TYR	1
1	B	77	LEU	1
1	A	18	LEU	1
1	B	51	VAL	1
1	B	75	TYR	1
1	A	32	ASP	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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 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