Full wwPDB NMR Structure Validation Report (i)

Dec 13, 2023 – 09:47 PM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

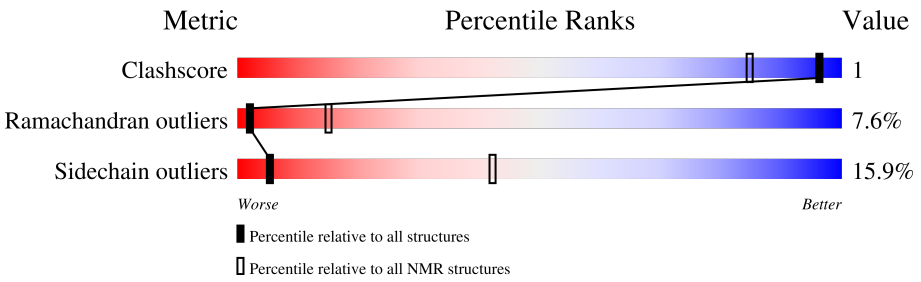
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=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 (i)

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)	1.56	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
			Total	C	H	N	O	S	
1	A	96	1454	444	738	138	129	5	0
1	B	97	1464	447	743	139	130	5	0

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

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

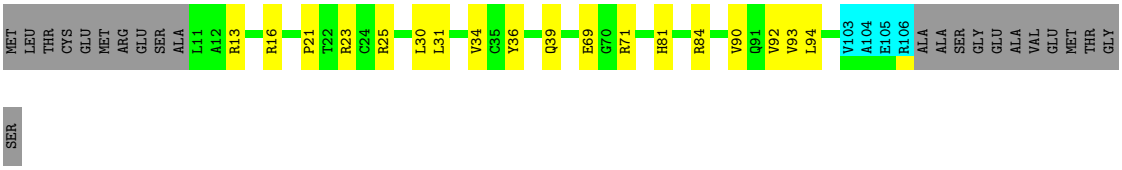
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

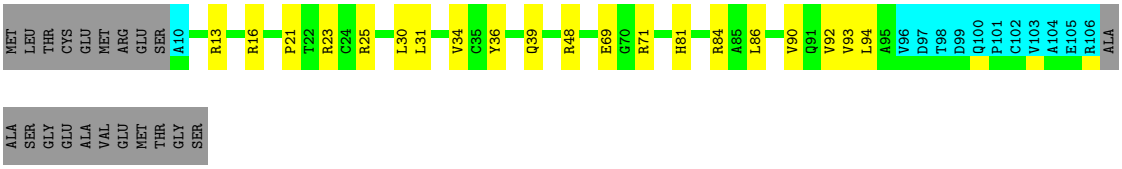
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 63% 15% • 19%



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 55% 17% 10% 18%



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

Chain A: 64% 14% • • 19%

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 55% 14% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 R16 R23 C24 R25 L31 V34 C35 Q39 T67 Q72 A76 S80 H81 R84 A85 L86 G87 E88 L89 V90 Q91 V92 V93 L94 A95 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY

GLU ALA VAL GLU MET THR GLY SER

4.2.2 Score per residue for model 2

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 55% 19% • • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 L14 G15 R16 D20 P21 T22 R25 L31 V34 Q39 L40 R48 L58 T67 Y68 E69 G70 R71 H81 R84 A85 L86 L89 V90 Q91 V92 V93 L94 D97 Q100 P101 C102 V103 A104

E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 53% 15% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 L14 L18 A19 D20 P21 T22 R23 C24 R25 G33 Q39 L40 H43 R48 C57 E69 G70 R71 H81 R84 A85 L86 L89 V92 V93 L94 A95 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106

ALA ALA SER GLY GLU ALA VAL GLU MET THR GLY SER

4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 60% 17% • • 19%

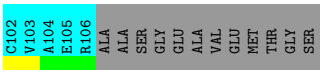
MET LEU THR CYS GLU MET ARG GLU SER ALA L11 R16 P21 T22 R23 C24 R25 L31 C35 Q39 H43 R48 L58 T67 Y68 E69 H81 R84 A85 L86 V90 Q91 V92 V93 L94 A95 Q100 V103 A104 E105 R106 ALA ALA SER GLY GLU

ALA VAL GLU MET THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 51% 19% • 10% 18%

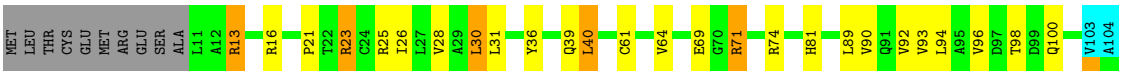
MET LEU THR CYS GLU MET ARG GLU SER A10 R13 L14 G15 R16 P21 T22 R23 C24 R25 L31 C35 Q39 R48 S56 C57 L58 L63 E69 D79 S80 H81 R84 A85 L86 G87 E88 L89 V90 Q91 V92 V93 L94 A95 V96 D97 T98 D99 Q100 P101

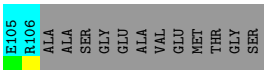


4.2.4 Score per residue for model 4

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:





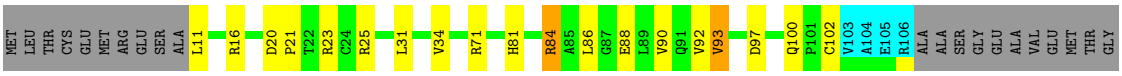
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

4.2.5 Score per residue for model 5

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 61% 15% • • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 L18 R25 L30 L31 V34 Q39 R48 S56 Y68 E69 R84 V90 Q91 V92 V93 L94 A95 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET THR

GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 58% 14% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 R13 R16 R25 L30 V34 C35 Q39 R48 Y68 E69 R74 R84 A85 L86 V92 V93 L94 A95 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET THR

GLY SER

4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 59% 14% 5% • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 P21 T22 R23 C24 R25 L30 L31 Q39 L40 V65 A66 T67 Y68 R71 D79 S80 H81 R84 A85 L86 V90 Q91 V92 V93 L94 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET

THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 54% 15% • 10% 18%

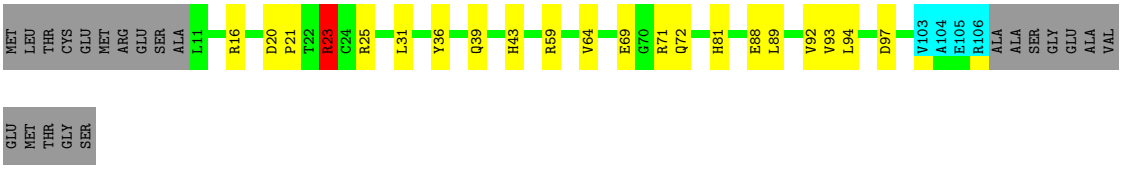
MET LEU THR CYS GLU MET ARG GLU SER A10 L14 P21 T22 R23 C24 R25 V28 A29 L30 L31 C35 Y36 Q39 V65 R74 D79 S80 H81 R84 A85 L86 L89 V90 Q91 V92 V93 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA

SER GLY GLU ALA VAL GLU MET THR GLY SER

4.2.8 Score per residue for model 8

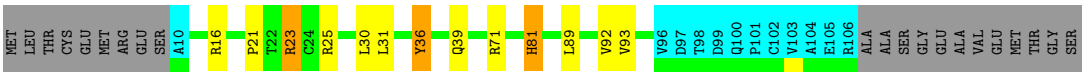
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 60% 17% • • 19%



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

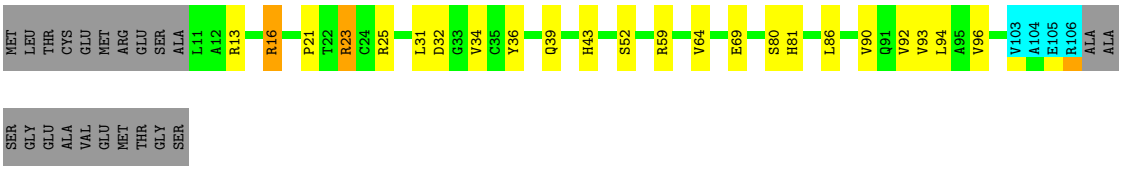
Chain B:



4.2.9 Score per residue for model 9

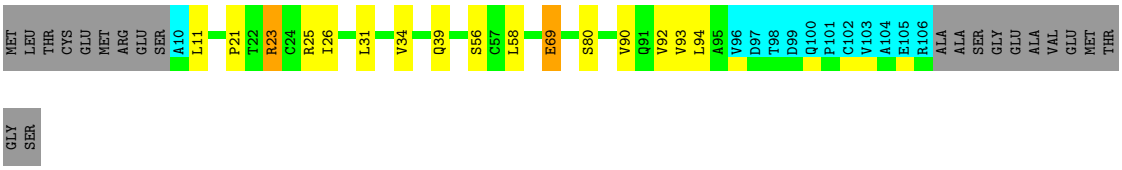
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

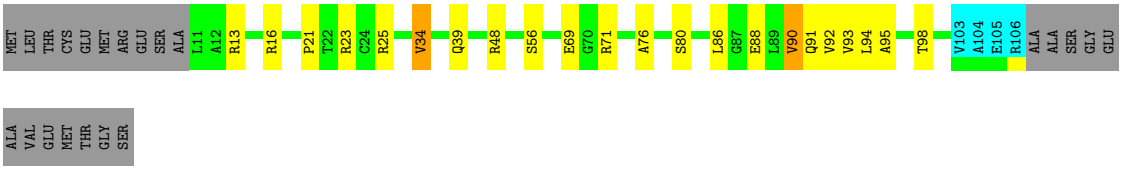
Chain B:



4.2.10 Score per residue for model 10

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 53% 18% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 P21 T22 R23 C24 R25 L30 L31 V34 C35 Q39 S56 C57 L58 R59 V64 E69 G70 R71 S80 L86 L89 V90 Q91 V92 V93 L94 A95 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA

SER GLY GLU ALA VAL GLU MET THR GLY SER

4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 56% 17% 5% • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 R16 D20 P21 T22 R23 L30 V34 C35 Y36 Q39 L58 E69 Q72 V73 R74 L77 S80 H81 R84 V90 Q91 V92 V93 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER

GLY GLU ALA VAL GLU MET THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 54% 15% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 L11 A12 R13 R16 D20 P21 T22 R23 L31 V34 C35 Y36 Q39 V65 Q72 V73 R74 S80 H81 R84 L89 V90 Q91 V92 V93 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER

GLY GLU ALA VAL GLU MET THR GLY SER

4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 59% 14% • • • 19%

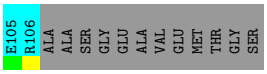
MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 D20 P21 T22 R23 C24 R25 V28 A29 L30 Q39 R48 L58 R71 D79 S80 H81 L82 L89 V90 Q91 V92 A95 V96 D97 Q100 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL

GLU MET THR GLY SER

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 53% 17% • 10% 18%

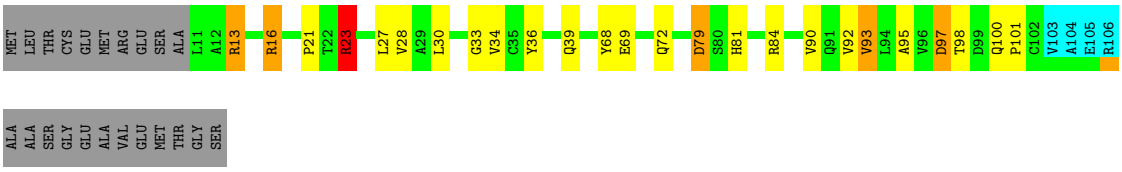
MET LEU THR CYS GLU MET ARG GLU SER A10 L11 A12 R13 D20 P21 T22 R23 I26 L27 V28 A29 L30 L31 V34 Q39 L44 R48 V51 V65 E69 G70 R71 L82 A83 R84 V90 Q91 V92 A95 V96 D97 T98 D99 Q100 P101 C102 V103 A104



4.2.13 Score per residue for model 13

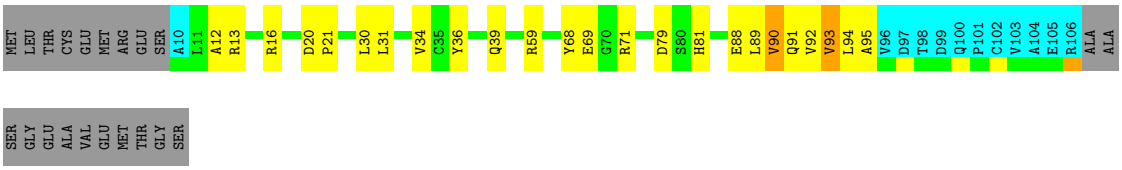
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

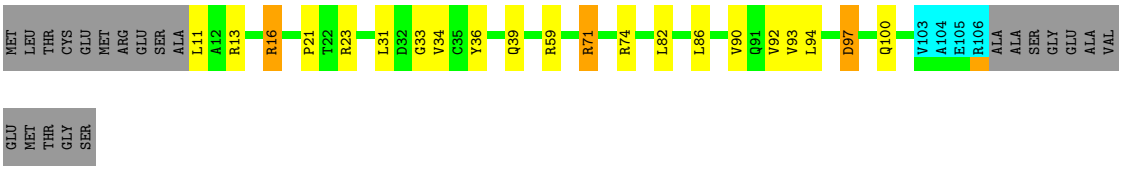
Chain B:



4.2.14 Score per residue for model 14

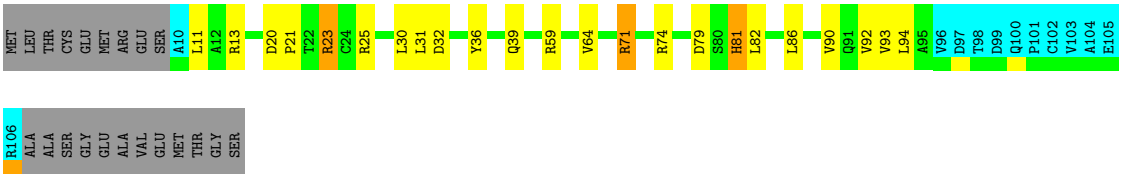
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

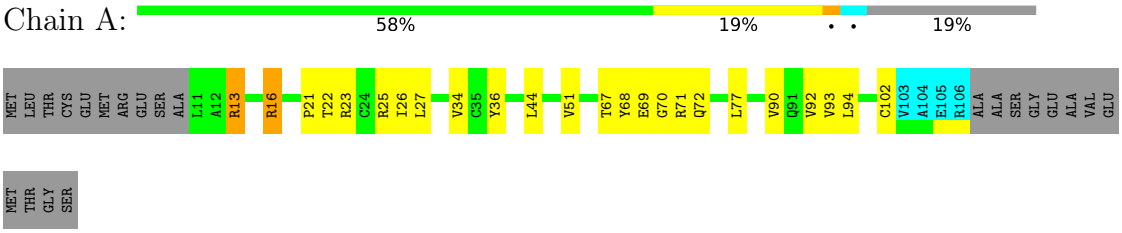
Chain B:



4.2.15 Score per residue for model 15

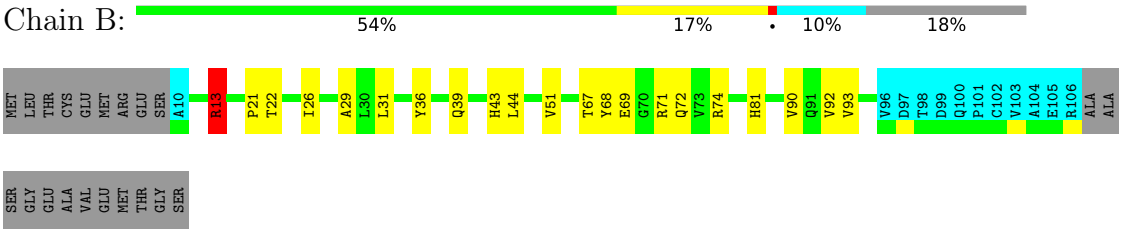
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

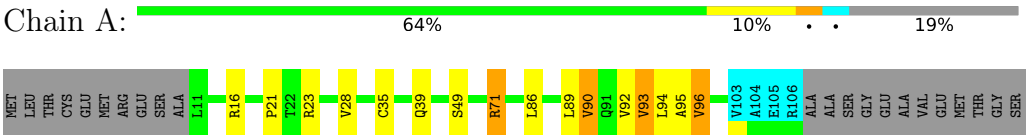
Chain B:



4.2.16 Score per residue for model 16

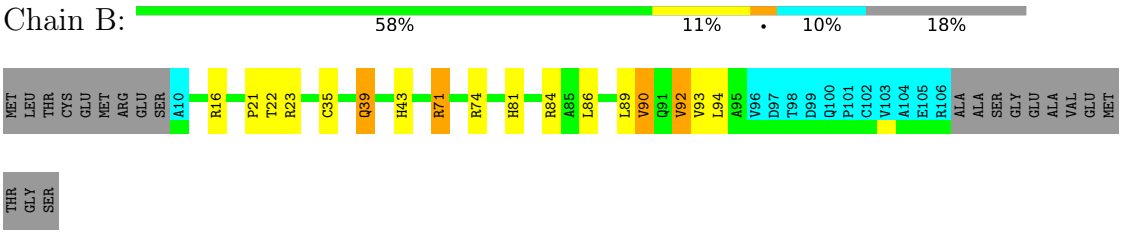
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

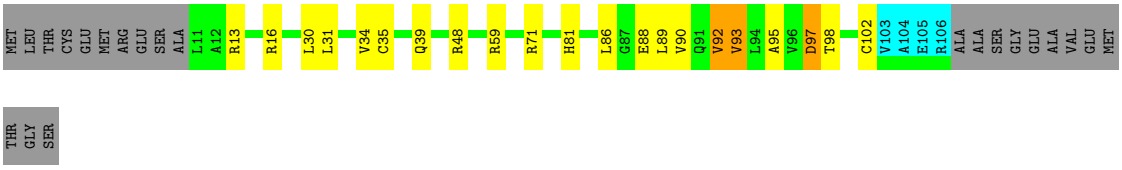
Chain B:



4.2.17 Score per residue for model 17

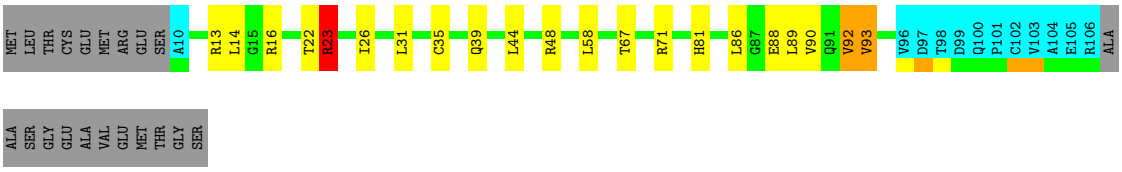
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

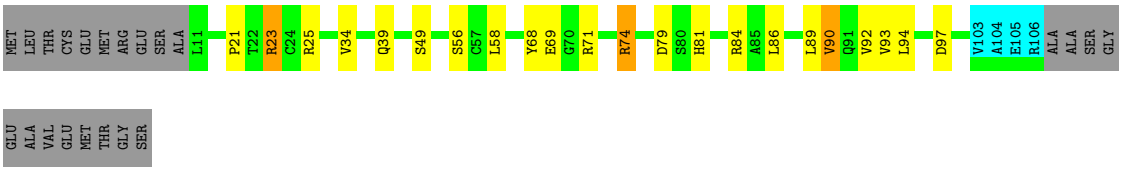
Chain B:



4.2.18 Score per residue for model 18

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



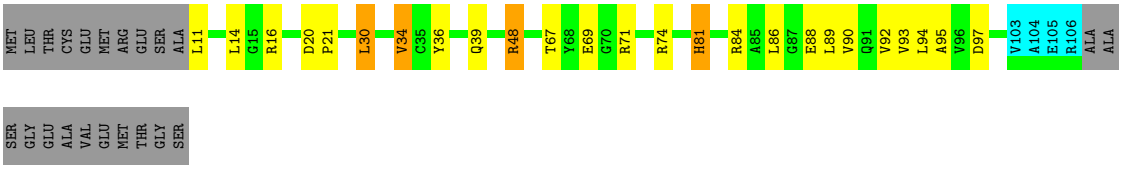
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

4.2.19 Score per residue for model 19

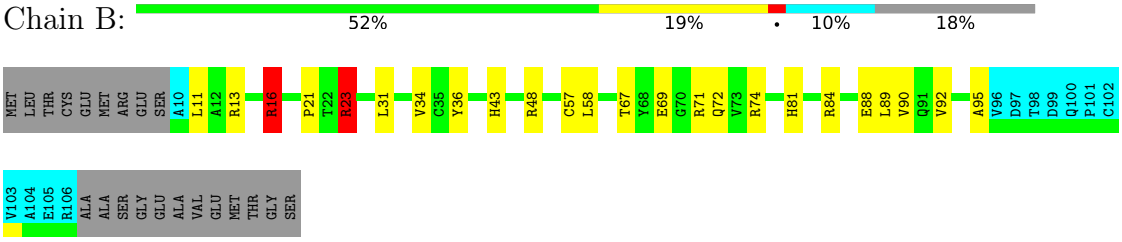
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

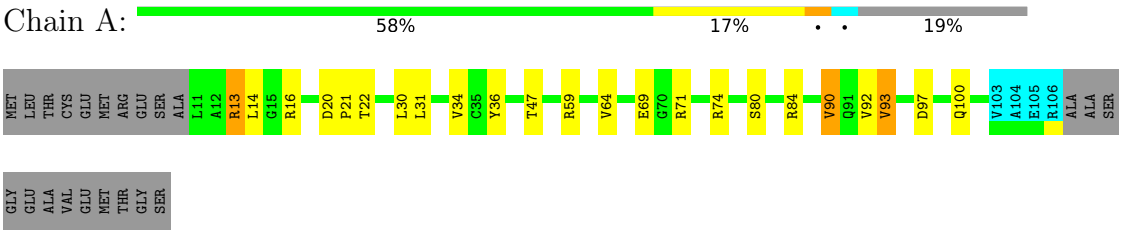
Chain B:



4.2.20 Score per residue for model 20

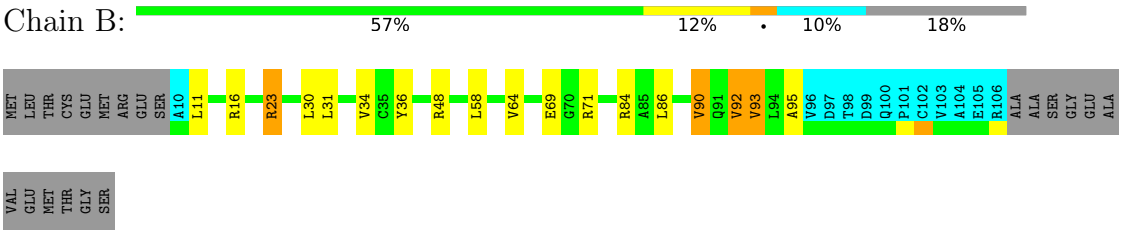
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

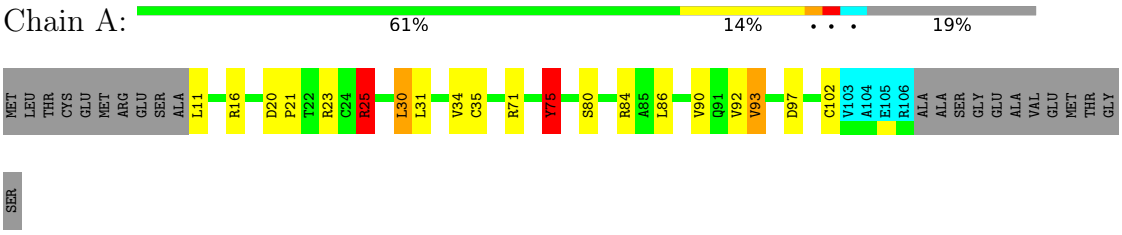
Chain B:



4.2.21 Score per residue for model 21

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



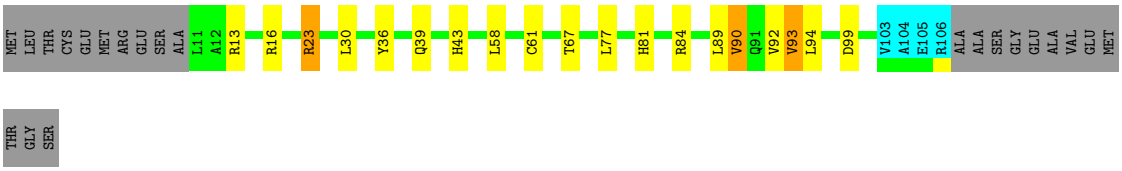
• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

4.2.22 Score per residue for model 22

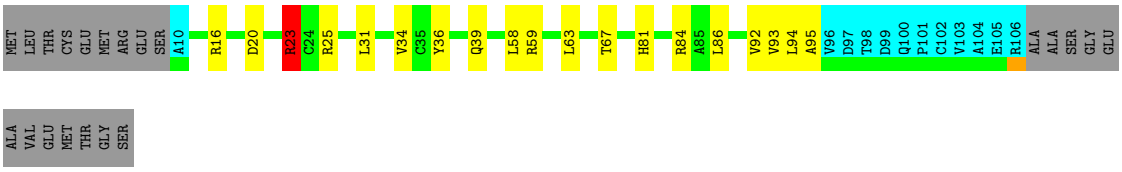
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

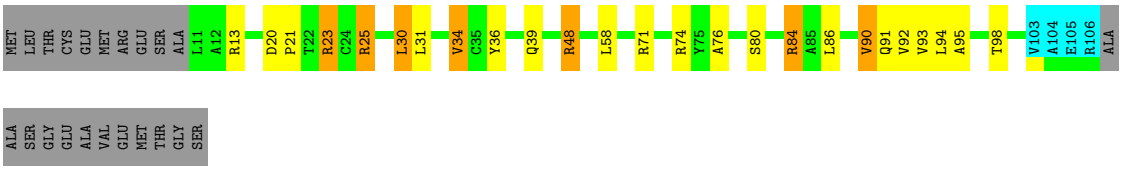
Chain B:



4.2.23 Score per residue for model 23

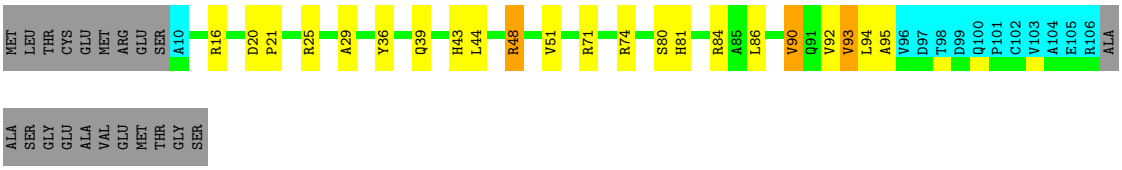
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

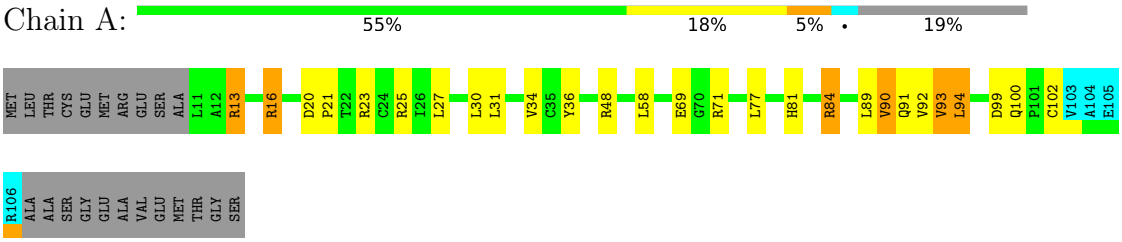
Chain B:



4.2.24 Score per residue for model 24

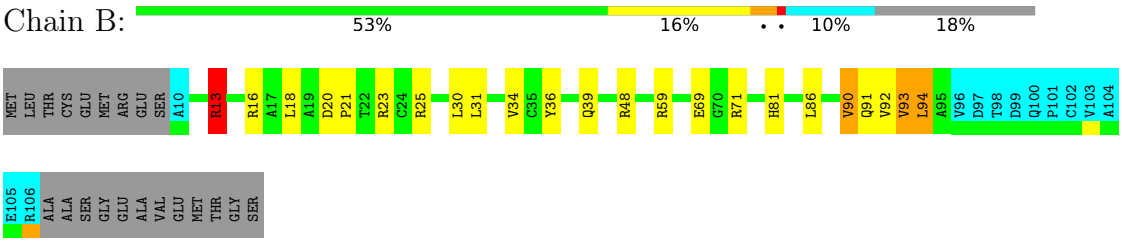
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

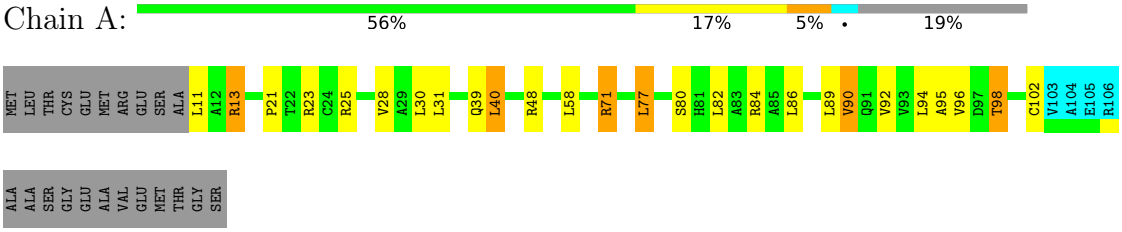
Chain B:



4.2.25 Score per residue for model 25

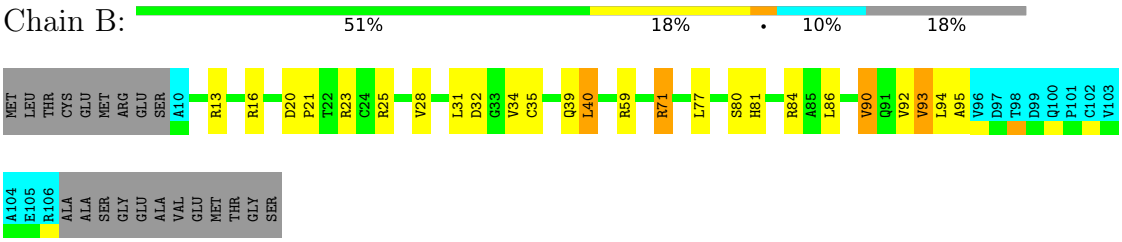
- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A:



- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:



4.2.26 Score per residue for model 26

- Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 58% 19% • • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 R16 D20 P21 R25 V34 C35 Y36 Q39 L40 H43 V64 R71 Q72 R84 A85 L86 L89 V90 Q91 V92 V93 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA

VAL GLU MET THR GLY SER

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 58% 12% • • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 L14 P21 R25 L30 L31 V34 C35 Y36 H43 R59 V64 Q72 H81 R84 A85 L86 V90 Q91 V92 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL

GLU MET THR GLY SER

4.2.27 Score per residue for model 27

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 61% 16% • • 19%

MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 D20 P21 T22 R25 L30 L31 V34 Q39 R59 T67 Y68 E69 Q72 V73 R74 H81 R84 V92 V93 L94 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET THR GLY

SER

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B: 53% 18% • 10% 18%

MET LEU THR CYS GLU MET ARG GLU SER A10 R13 P21 T22 R23 C24 R25 I26 L27 L31 C35 Y36 C57 L58 R59 L63 V64 T67 Y68 E69 Q72 V73 R74 L77 S80 H81 V92 V93 V96 D97 T98 D99 Q100 P101 C102 V103 A104 E105 R106

ALA ALA SER GLY GLU ALA VAL GLU MET THR GLY SER

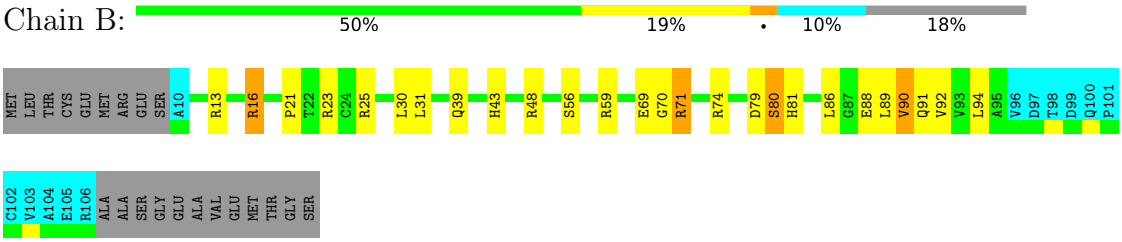
4.2.28 Score per residue for model 28

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain A: 56% 19% • • 19%

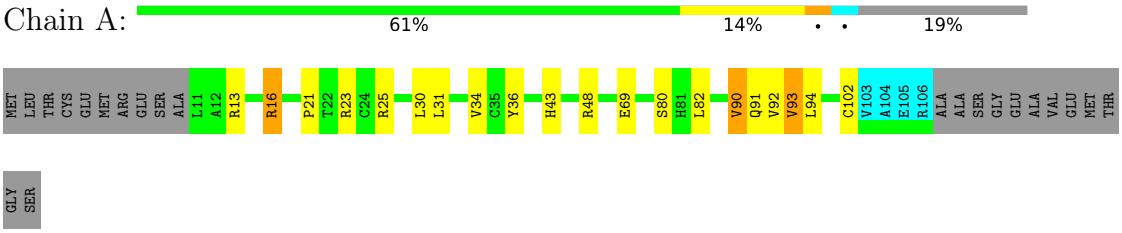
MET LEU THR CYS GLU MET ARG GLU SER ALA L11 A12 R13 R16 D20 P21 T22 R23 C24 R25 L30 L31 V34 C35 Y36 Q39 E69 G70 R71 R74 Y75 D79 S80 H81 E88 L89 V90 Q91 V92 V93 L94 T98 D99 Q100 V103 A104 E105 R106 ALA

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

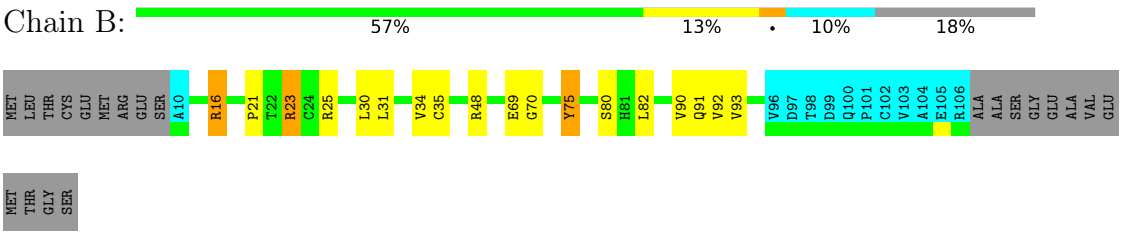


4.2.29 Score per residue for model 29

• Molecule 1: Transcriptional regulator Rv1994c/MT2050

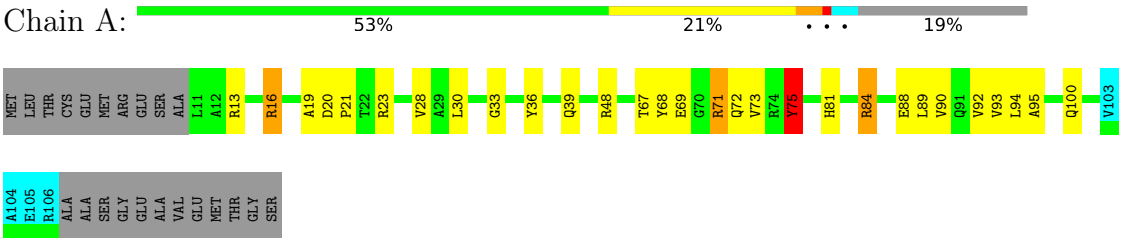


• Molecule 1: Transcriptional regulator Rv1994c/MT2050



4.2.30 Score per residue for model 30

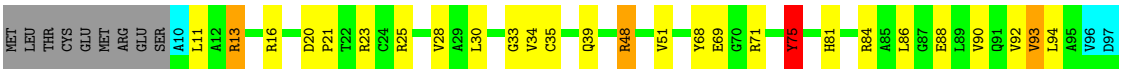
• Molecule 1: Transcriptional regulator Rv1994c/MT2050



• Molecule 1: Transcriptional regulator Rv1994c/MT2050

Chain B:

49%
19%
10%
18%


MET LEU THR CYS GLU MET ARG GLU SER A10 L11 A12 R13 R16 D20 P21 T22 R23 C24 R25 V28 A29 L30 G33 V34 C35 Q39 R48 V51 Y68 E69 G70 R71 Y75 H81 R84 A85 L86 G87 E88 L89 V90 Q91 V92 V93 L94 A95 V96 D97

T98 D99 Q100 P101 C102 V103 A104 E105 R106 ALA ALA SER GLY GLU ALA VAL GLU MET THR GLY SER

5 Refinement protocol and experimental data overview (i)

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.

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(^{o})	Ideal(^{o})	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(^{o})	Ideal(^{o})	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(^{o})	Ideal(^{o})	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	16	ARG	Sidechain	2
1	A	59	ARG	Sidechain	2
1	B	59	ARG	Sidechain	2
1	B	13	ARG	Sidechain	2
1	B	74	ARG	Sidechain	2
1	A	75	TYR	Sidechain	2
1	B	75	TYR	Sidechain	2
1	B	71	ARG	Sidechain	1
1	A	48	ARG	Sidechain	1
1	B	48	ARG	Sidechain	1
1	B	36	TYR	Sidechain	1
1	B	16	ARG	Sidechain	1
1	A	84	ARG	Sidechain	1
1	B	84	ARG	Sidechain	1
1	A	36	TYR	Sidechain	1
1	B	43	HIS	Sidechain	1

6.2 Too-close contacts (i)

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:HD12	1:A:40:LEU:H	0.51	1.64	7	4
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:HD12	1:A:58:LEU:H	0.46	1.68	23	1
1:B:40:LEU:H	1:B:40:LEU:HD12	0.46	1.69	25	3
1:A:34:VAL:HG12	1:A:76:ALA:HA	0.46	1.88	10	2
1:A:82:LEU:H	1:A:82:LEU:HD22	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
1:A:67:THR:HG22	1:A:68:TYR:H	0.44	1.71	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
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 (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	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%)	2	17
All	All	5309/7080 (75%)	4293 (81%)	615 (12%)	401 (8%)	2	15

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

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Mol	Chain	Res	Type	Models (Total)
1	A	35	CYS	1
1	A	100	GLN	1
1	A	19	ALA	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	72/91 (79%)	60±3 (84±4%)	12±3 (16±4%)	5 42
1	B	65/91 (71%)	55±2 (84±4%)	10±2 (16±4%)	5 42
All	All	4110/5460 (75%)	3457 (84%)	653 (16%)	5 42

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

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Mol	Chain	Res	Type	Models (Total)
1	A	30	LEU	9
1	A	67	THR	8
1	A	72	GLN	8
1	A	84	ARG	8
1	B	88	GLU	8
1	A	81	HIS	8
1	B	35	CYS	8
1	B	30	LEU	8
1	B	71	ARG	8
1	A	22	THR	7
1	A	98	THR	7
1	A	97	ASP	7
1	A	102	CYS	7
1	B	64	VAL	7
1	A	88	GLU	7
1	A	13	ARG	7
1	A	80	SER	7
1	B	80	SER	7
1	A	11	LEU	6
1	A	25	ARG	6
1	B	25	ARG	6
1	B	67	THR	6
1	B	72	GLN	6
1	B	22	THR	6
1	B	56	SER	6
1	A	28	VAL	6
1	B	68	TYR	6
1	A	68	TYR	6
1	A	40	LEU	5
1	A	64	VAL	5
1	B	13	ARG	5
1	A	48	ARG	5
1	B	11	LEU	5
1	B	48	ARG	5
1	B	84	ARG	4
1	A	58	LEU	4
1	A	96	VAL	4
1	B	28	VAL	4
1	B	14	LEU	3
1	B	40	LEU	3
1	B	43	HIS	3
1	B	94	LEU	3

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

No chemical shift data were provided