Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 04:05 AM BST

PDB ID	:	2MVW
Title	:	Solution structure of the TRIM19 B-box1 (B1) of human promyelocytic leukemia (PML)
Authors	:	Huang, S.; Naik, M.T.; Fan, P.; Wang, Y.; Chang, C.; Huang, T.
Deposited on	:	2014-10-17

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

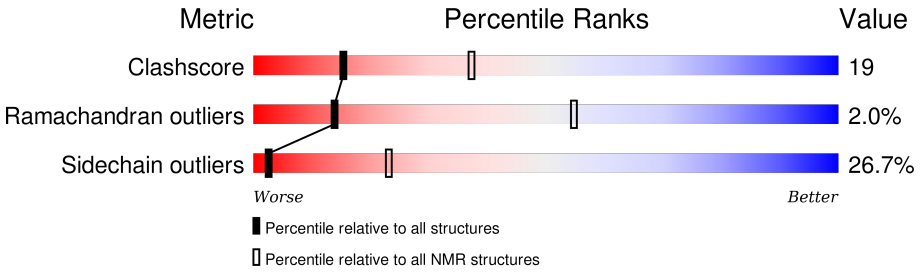
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	51	49% 24% 8% 20%
1	B	51	39% 27% 10% • 22%

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 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:127-A:167, B:127-B:166 (81)	0.29	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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1602 atoms, of which 770 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein PML.

Mol	Chain	Residues	Atoms						Trace
1	A	51	Total	C	H	N	O	S	0
			799	260	385	73	75	6	
1	B	51	Total	C	H	N	O	S	0
			799	260	385	73	75	6	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	GLY	-	EXPRESSION TAG	UNP P29590
A	119	SER	-	EXPRESSION TAG	UNP P29590
B	118	GLY	-	EXPRESSION TAG	UNP P29590
B	119	SER	-	EXPRESSION TAG	UNP P29590

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	B	2	Total	Zn
			2	2
2	A	2	Total	Zn
			2	2

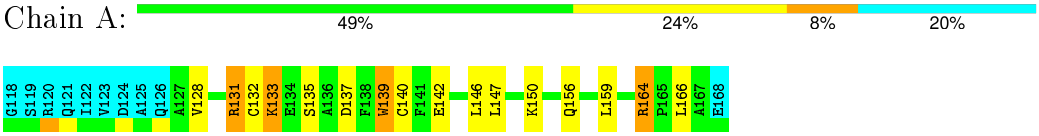
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

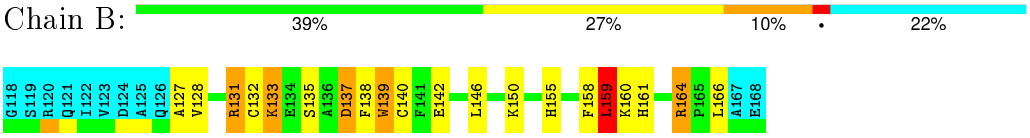
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

Chain B:



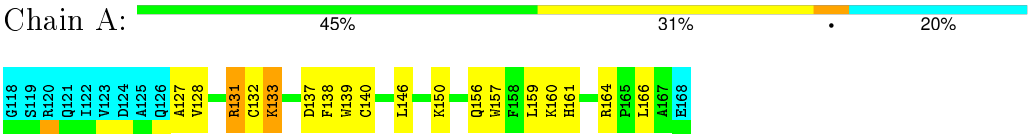
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

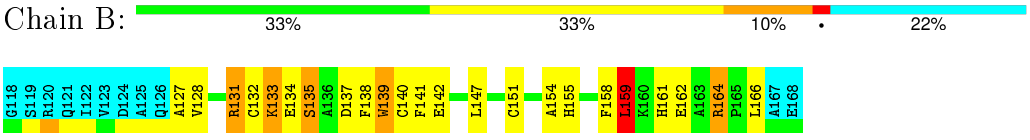
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

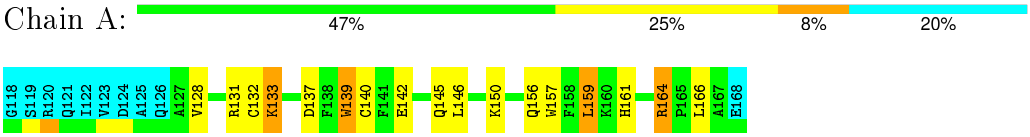
Chain B:



4.2.2 Score per residue for model 2 (medoid)

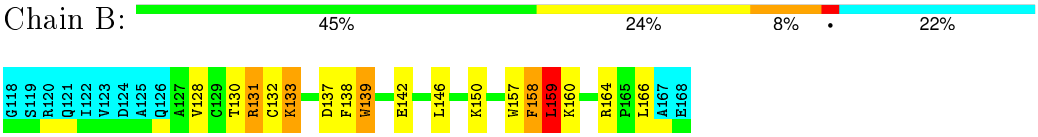
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

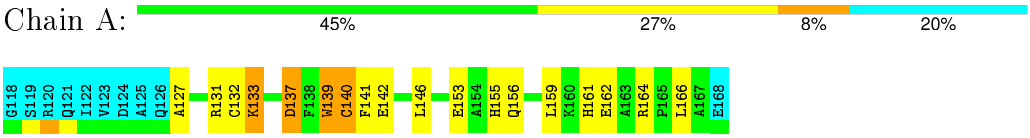
Chain B:



4.2.3 Score per residue for model 3

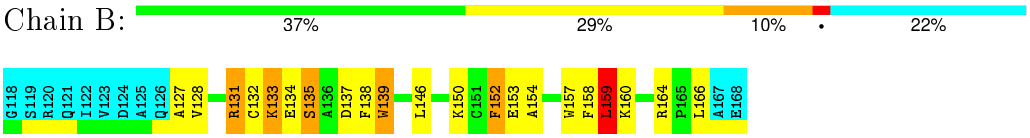
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

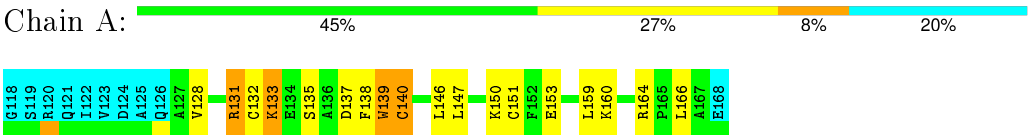
Chain B:



4.2.4 Score per residue for model 4

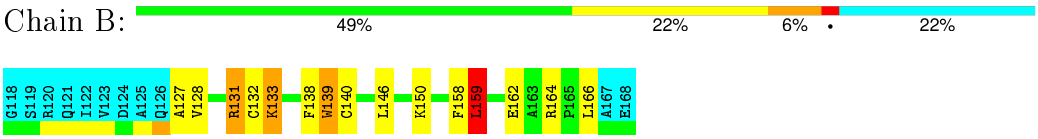
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

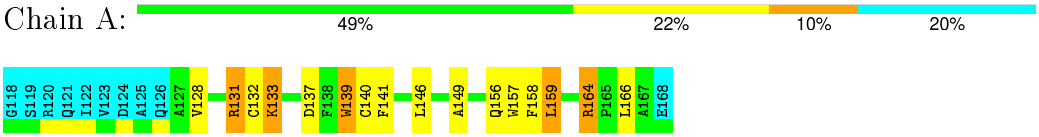
Chain B:



4.2.5 Score per residue for model 5

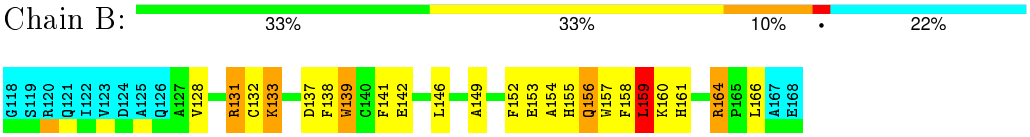
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

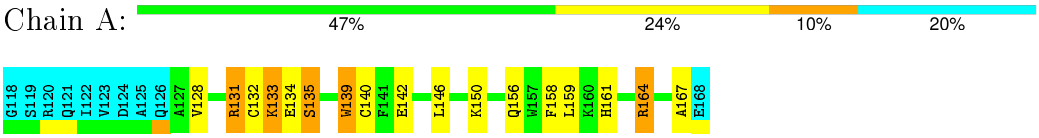
Chain B:



4.2.6 Score per residue for model 6

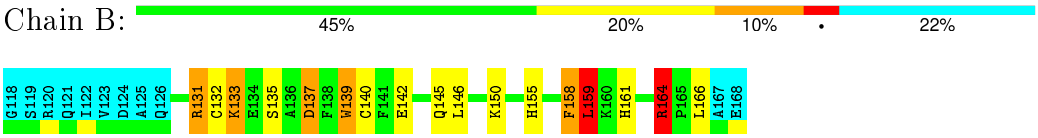
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

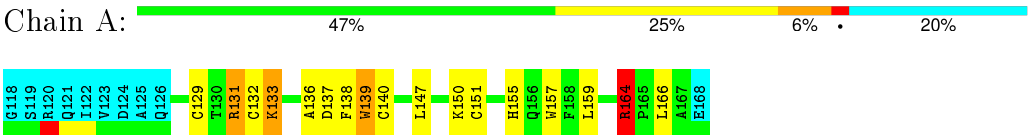
Chain B:



4.2.7 Score per residue for model 7

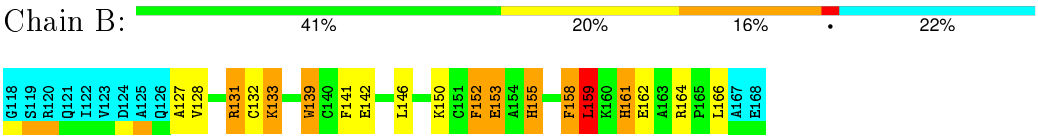
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

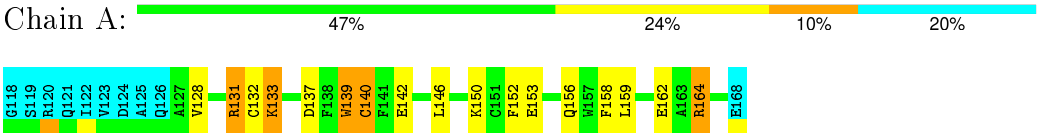
Chain B:



4.2.8 Score per residue for model 8

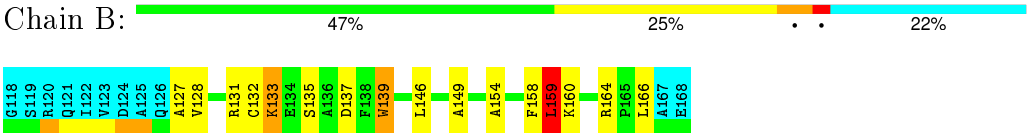
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

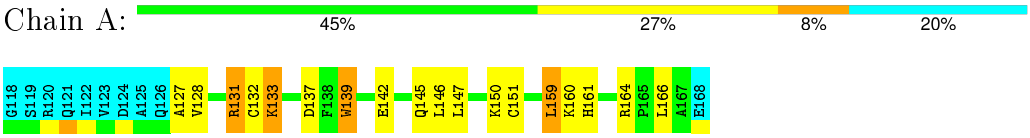
Chain B:



4.2.9 Score per residue for model 9

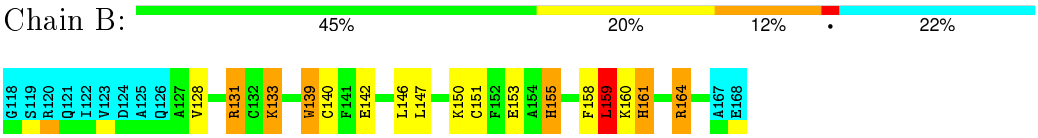
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

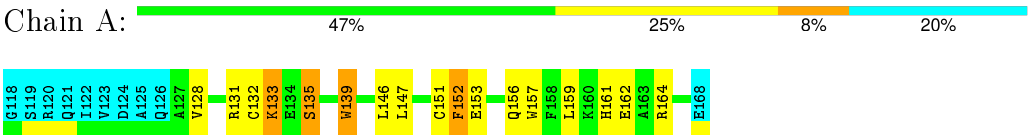
Chain B:



4.2.10 Score per residue for model 10

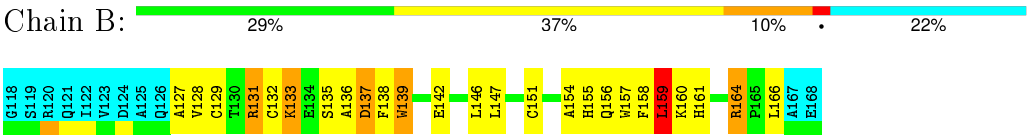
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

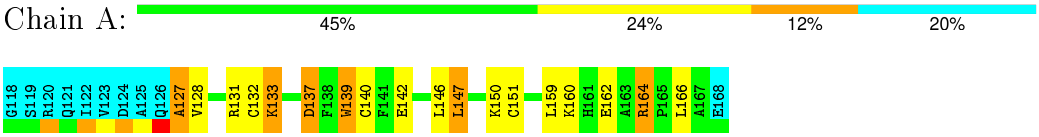
Chain B:



4.2.11 Score per residue for model 11

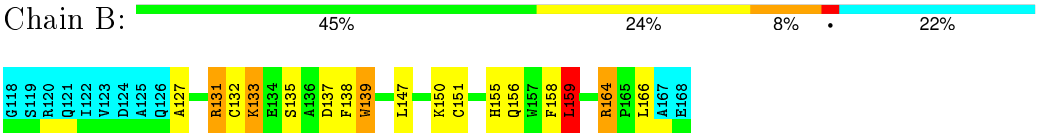
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

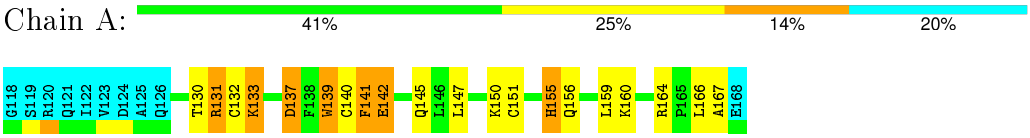
Chain B:



4.2.12 Score per residue for model 12

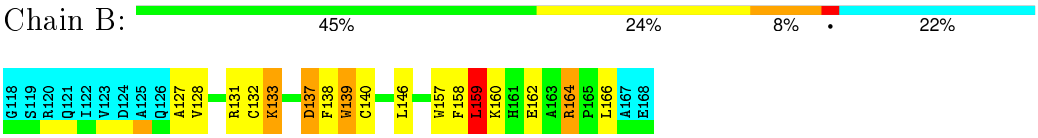
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

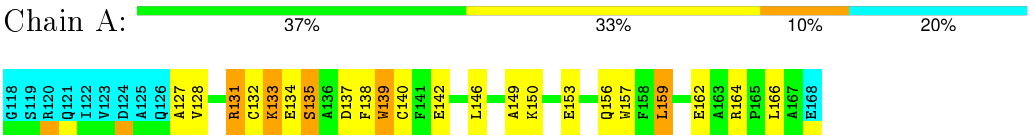
Chain B:



4.2.13 Score per residue for model 13

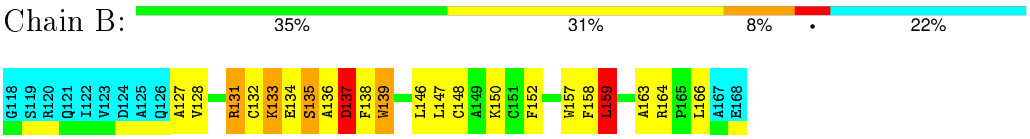
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

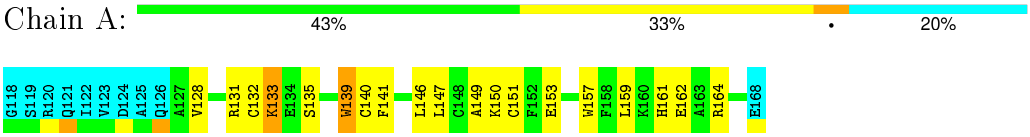
Chain B:



4.2.14 Score per residue for model 14

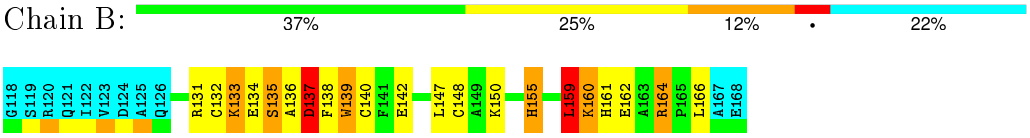
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

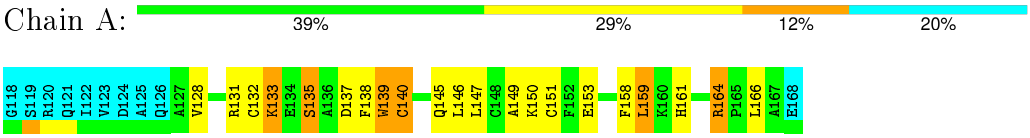
Chain B:



4.2.15 Score per residue for model 15

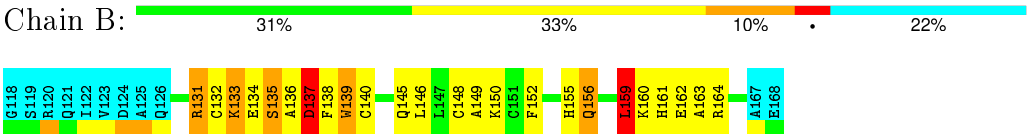
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

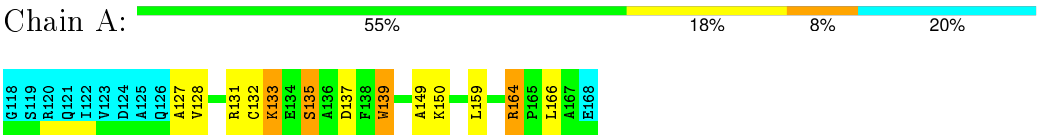
Chain B:



4.2.16 Score per residue for model 16

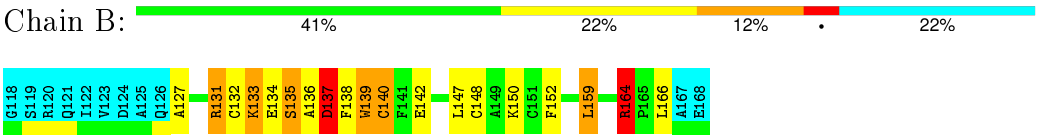
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

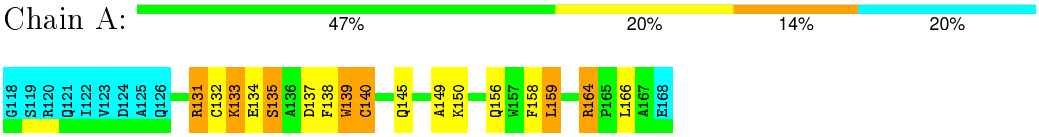
Chain B:



4.2.17 Score per residue for model 17

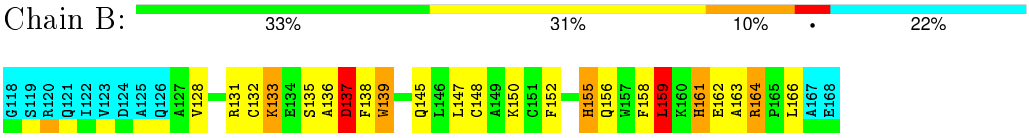
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

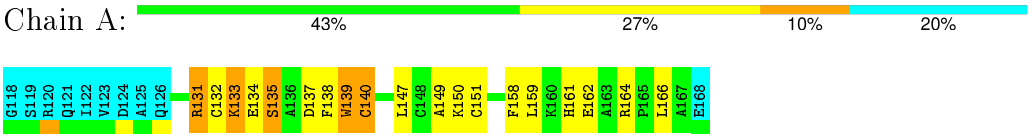
Chain B:



4.2.18 Score per residue for model 18

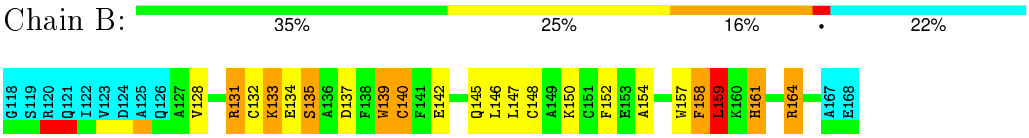
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

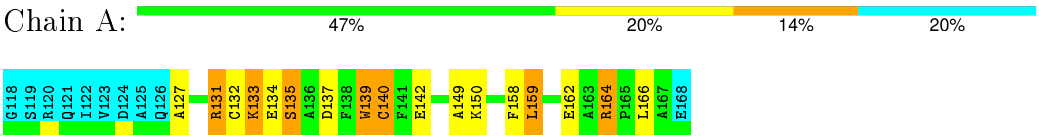
Chain B:



4.2.19 Score per residue for model 19

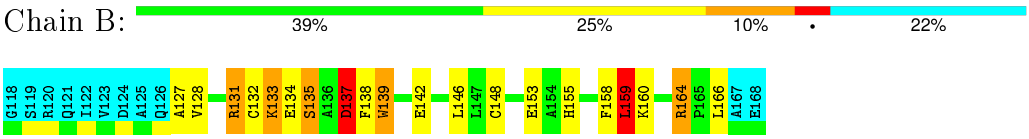
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

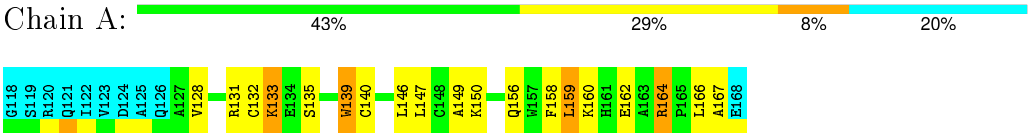
Chain B:



4.2.20 Score per residue for model 20

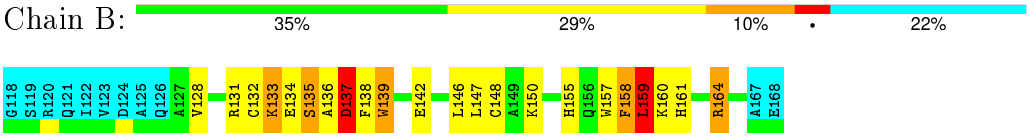
- Molecule 1: Protein PML

Chain A:



- Molecule 1: Protein PML

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	geometry optimization	3.9
X-PLOR NIH	refinement	2.26

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)	2mvw_cs.str
Number of chemical shift lists	1
Total number of shifts	1168
Number of shifts mapped to atoms	1168
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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

6 Model quality

6.1 Standard geometry

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

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

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	2.0±0.0
1	B	0.0±0.0	2.0±0.0
All	All	0	80

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	131	ARG	Sidechain	20
1	B	164	ARG	Sidechain	20
1	B	131	ARG	Sidechain	20
1	A	164	ARG	Sidechain	20

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	337	311	311	13±3
1	B	332	306	306	14±4
All	All	13460	12340	12346	497

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:127:ALA:HB1	1:B:166:LEU:HD23	0.88	1.45	10	5
1:A:127:ALA:HB1	1:A:166:LEU:HD23	0.87	1.46	9	4
1:A:149:ALA:HB3	1:B:137:ASP:HB3	0.81	1.53	18	9
1:B:128:VAL:N	1:B:146:LEU:HD22	0.71	1.99	3	5
1:B:137:ASP:HA	1:B:166:LEU:HD22	0.70	1.63	6	3
1:A:137:ASP:C	1:A:166:LEU:HD13	0.69	2.07	1	1
1:A:137:ASP:HA	1:A:166:LEU:HD12	0.68	1.65	4	7
1:B:158:PHE:HB3	1:B:159:LEU:HD23	0.68	1.66	6	12
1:A:127:ALA:HB1	1:A:166:LEU:CD2	0.66	2.19	13	2
1:A:147:LEU:HD22	1:A:151:CYS:HB3	0.66	1.66	7	6
1:B:147:LEU:HD22	1:B:151:CYS:HB3	0.66	1.68	10	4
1:A:128:VAL:O	1:A:146:LEU:HD22	0.66	1.90	2	5
1:A:149:ALA:HB3	1:B:137:ASP:CB	0.66	2.21	20	8
1:A:137:ASP:HA	1:A:166:LEU:HD22	0.64	1.68	9	6
1:A:137:ASP:HB3	1:B:149:ALA:HB3	0.61	1.72	8	3
1:A:149:ALA:HB1	1:B:138:PHE:CE2	0.61	2.30	13	4
1:A:128:VAL:N	1:A:146:LEU:HD22	0.61	2.10	1	7
1:B:128:VAL:O	1:B:146:LEU:HD13	0.61	1.95	12	3
1:A:138:PHE:N	1:A:166:LEU:HD13	0.61	2.10	1	1
1:B:146:LEU:C	1:B:147:LEU:HD12	0.61	2.16	13	2
1:B:137:ASP:HA	1:B:166:LEU:HD12	0.61	1.73	2	2
1:A:146:LEU:C	1:A:147:LEU:HD12	0.60	2.16	20	1
1:A:128:VAL:O	1:A:146:LEU:HD13	0.59	1.97	4	3
1:A:159:LEU:HD12	1:A:159:LEU:C	0.58	2.19	11	8
1:B:152:PHE:CE1	1:B:163:ALA:HB3	0.58	2.34	15	3
1:A:159:LEU:C	1:A:159:LEU:HD12	0.58	2.20	6	10
1:A:155:HIS:ND1	1:A:159:LEU:HD11	0.56	2.15	12	1
1:B:139:TRP:HB3	1:B:166:LEU:HD21	0.55	1.77	13	6
1:B:158:PHE:CD2	1:B:159:LEU:HD23	0.54	2.37	5	2
1:A:139:TRP:HB3	1:A:166:LEU:HD21	0.53	1.79	11	2
1:B:127:ALA:O	1:B:128:VAL:HG13	0.53	2.04	8	5
1:B:128:VAL:H	1:B:146:LEU:HD13	0.52	1.64	20	1
1:A:159:LEU:O	1:A:159:LEU:HD12	0.52	2.05	15	3
1:B:155:HIS:NE2	1:B:161:HIS:CG	0.52	2.78	1	1
1:B:152:PHE:CZ	1:B:156:GLN:NE2	0.52	2.78	17	3
1:B:139:TRP:CZ3	1:B:164:ARG:CB	0.52	2.93	16	2
1:A:139:TRP:CZ3	1:A:164:ARG:CB	0.52	2.93	8	2
1:B:146:LEU:N	1:B:146:LEU:HD23	0.52	2.18	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:152:PHE:CD2	1:B:153:GLU:N	0.52	2.77	3	2
1:B:159:LEU:HD12	1:B:160:LYS:N	0.52	2.20	19	10
1:A:127:ALA:O	1:A:128:VAL:HG13	0.51	2.05	9	2
1:A:137:ASP:CA	1:A:166:LEU:HD12	0.51	2.33	4	2
1:A:127:ALA:HB1	1:A:166:LEU:HD13	0.50	1.83	19	2
1:B:139:TRP:HB2	1:B:146:LEU:HD23	0.50	1.82	15	1
1:B:155:HIS:CD2	1:B:161:HIS:CG	0.50	2.99	1	5
1:B:136:ALA:HB1	1:B:147:LEU:O	0.49	2.08	20	5
1:B:138:PHE:CA	1:B:166:LEU:HD13	0.49	2.38	10	2
1:A:149:ALA:HB1	1:B:138:PHE:HE2	0.49	1.66	13	1
1:B:128:VAL:N	1:B:146:LEU:HD13	0.49	2.22	20	1
1:B:138:PHE:N	1:B:166:LEU:HD13	0.49	2.23	1	3
1:B:146:LEU:HD23	1:B:166:LEU:HD21	0.49	1.85	8	2
1:B:152:PHE:CG	1:B:153:GLU:N	0.48	2.79	3	2
1:A:146:LEU:HD23	1:A:166:LEU:HD11	0.48	1.84	3	1
1:B:155:HIS:CE1	1:B:159:LEU:HD21	0.48	2.43	19	1
1:B:137:ASP:O	1:B:138:PHE:CG	0.48	2.67	13	6
1:B:137:ASP:O	1:B:138:PHE:CD2	0.48	2.67	14	5
1:B:139:TRP:CD1	1:B:140:CYS:O	0.47	2.67	15	5
1:B:139:TRP:CZ3	1:B:164:ARG:HB2	0.47	2.44	16	9
1:A:127:ALA:HB1	1:A:166:LEU:HB3	0.47	1.85	11	1
1:A:139:TRP:CD1	1:A:140:CYS:O	0.47	2.68	17	11
1:A:139:TRP:CG	1:A:139:TRP:O	0.47	2.67	9	3
1:B:138:PHE:CD2	1:B:152:PHE:CD2	0.47	3.03	13	1
1:B:139:TRP:CG	1:B:139:TRP:O	0.47	2.67	20	3
1:A:139:TRP:CH2	1:A:164:ARG:HB2	0.46	2.46	8	5
1:A:147:LEU:HD23	1:A:151:CYS:HB3	0.46	1.87	11	3
1:B:139:TRP:O	1:B:139:TRP:CG	0.46	2.67	17	6
1:B:146:LEU:CD2	1:B:166:LEU:HD21	0.46	2.39	7	1
1:A:137:ASP:O	1:A:138:PHE:CD1	0.46	2.69	7	4
1:A:139:TRP:CH2	1:A:164:ARG:CB	0.46	2.98	8	1
1:A:159:LEU:HD12	1:A:159:LEU:O	0.45	2.11	1	3
1:B:133:LYS:CD	1:B:133:LYS:O	0.45	2.65	5	11
1:B:133:LYS:O	1:B:133:LYS:CD	0.45	2.64	15	9
1:A:149:ALA:HB3	1:B:137:ASP:HB2	0.45	1.88	14	2
1:A:139:TRP:CZ3	1:A:164:ARG:HB2	0.45	2.47	15	7
1:A:139:TRP:CD1	1:A:140:CYS:N	0.45	2.85	14	1
1:B:128:VAL:H	1:B:146:LEU:HD22	0.45	1.71	19	1
1:B:127:ALA:HB1	1:B:166:LEU:HD22	0.45	1.88	12	1
1:A:128:VAL:H	1:A:146:LEU:HD22	0.45	1.69	11	2
1:A:157:TRP:CE3	1:A:157:TRP:O	0.45	2.69	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ALA:CB	1:A:166:LEU:HD23	0.45	2.41	13	1
1:A:137:ASP:O	1:A:138:PHE:CD2	0.45	2.70	13	1
1:B:139:TRP:CH2	1:B:164:ARG:HB2	0.45	2.47	17	4
1:A:138:PHE:CA	1:A:166:LEU:HD13	0.45	2.42	17	2
1:B:152:PHE:CE2	1:B:153:GLU:HG2	0.45	2.47	7	1
1:B:139:TRP:C	1:B:139:TRP:CD1	0.45	2.89	14	7
1:A:133:LYS:O	1:A:133:LYS:CD	0.44	2.66	8	13
1:B:158:PHE:CB	1:B:159:LEU:HD23	0.44	2.42	8	1
1:B:137:ASP:CA	1:B:166:LEU:HD12	0.44	2.42	2	2
1:A:139:TRP:CD1	1:A:139:TRP:C	0.44	2.90	6	5
1:A:137:ASP:CA	1:A:166:LEU:HD22	0.44	2.41	18	1
1:B:139:TRP:CD1	1:B:139:TRP:C	0.44	2.90	19	6
1:A:133:LYS:CD	1:A:133:LYS:O	0.44	2.65	17	7
1:A:139:TRP:C	1:A:139:TRP:CD1	0.44	2.90	4	6
1:A:152:PHE:CG	1:A:153:GLU:N	0.44	2.83	10	1
1:B:129:CYS:N	1:B:136:ALA:HB3	0.44	2.28	10	1
1:B:140:CYS:SG	1:B:161:HIS:CD2	0.43	3.10	18	1
1:A:159:LEU:H	1:A:159:LEU:HD12	0.43	1.72	9	1
1:A:132:CYS:O	1:A:133:LYS:CG	0.43	2.66	5	20
1:B:153:GLU:O	1:B:157:TRP:CB	0.43	2.66	5	1
1:B:155:HIS:CE1	1:B:161:HIS:ND1	0.43	2.87	14	1
1:A:129:CYS:N	1:A:136:ALA:HB3	0.43	2.28	7	1
1:B:132:CYS:O	1:B:133:LYS:CG	0.43	2.66	8	19
1:B:134:GLU:O	1:B:135:SER:CB	0.43	2.67	1	9
1:B:137:ASP:C	1:B:166:LEU:HD13	0.43	2.33	1	1
1:B:132:CYS:O	1:B:133:LYS:CB	0.43	2.67	2	14
1:A:130:THR:CG2	1:A:131:ARG:N	0.43	2.80	12	1
1:A:135:SER:HA	1:B:135:SER:CA	0.43	2.44	15	2
1:B:162:GLU:O	1:B:162:GLU:CG	0.43	2.66	14	1
1:B:137:ASP:O	1:B:138:PHE:CD1	0.43	2.72	1	3
1:A:140:CYS:SG	1:A:155:HIS:CD2	0.43	3.12	3	1
1:A:132:CYS:O	1:A:133:LYS:CB	0.43	2.67	11	11
1:A:128:VAL:O	1:A:146:LEU:CB	0.43	2.67	10	4
1:A:130:THR:HG23	1:A:131:ARG:N	0.43	2.29	12	1
1:B:146:LEU:H	1:B:146:LEU:HD12	0.43	1.74	5	1
1:A:135:SER:CB	1:B:136:ALA:O	0.42	2.67	16	2
1:A:135:SER:CA	1:B:135:SER:HA	0.42	2.44	14	8
1:A:139:TRP:CZ3	1:A:164:ARG:HB3	0.42	2.49	8	1
1:B:127:ALA:HB1	1:B:166:LEU:HD13	0.42	1.91	12	1
1:B:154:ALA:O	1:B:158:PHE:N	0.42	2.52	10	3
1:B:129:CYS:H	1:B:136:ALA:HB3	0.42	1.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:LEU:HD22	1:A:151:CYS:CB	0.42	2.41	15	1
1:B:127:ALA:O	1:B:128:VAL:CG1	0.42	2.67	8	5
1:B:154:ALA:O	1:B:158:PHE:CD1	0.42	2.72	1	2
1:B:155:HIS:NE2	1:B:161:HIS:CD2	0.42	2.88	17	1
1:A:152:PHE:CD2	1:A:153:GLU:N	0.42	2.87	10	1
1:B:128:VAL:O	1:B:146:LEU:CB	0.42	2.68	12	2
1:B:155:HIS:NE2	1:B:161:HIS:CE1	0.42	2.88	7	1
1:A:134:GLU:O	1:A:135:SER:CB	0.41	2.67	17	5
1:A:153:GLU:O	1:A:157:TRP:CB	0.41	2.68	10	1
1:A:141:PHE:CD2	1:A:142:GLU:N	0.41	2.88	12	1
1:A:139:TRP:NE1	1:A:140:CYS:O	0.41	2.53	14	1
1:A:162:GLU:CG	1:A:162:GLU:O	0.41	2.68	13	1
1:B:127:ALA:CA	1:B:166:LEU:HD23	0.41	2.45	8	1
1:A:152:PHE:CE1	1:A:156:GLN:HG3	0.41	2.51	8	1
1:A:135:SER:HA	1:B:135:SER:HA	0.41	1.92	10	1
1:B:159:LEU:HD12	1:B:160:LYS:H	0.41	1.76	5	1
1:A:127:ALA:O	1:A:128:VAL:CG1	0.41	2.69	9	1
1:B:154:ALA:O	1:B:158:PHE:CB	0.40	2.69	5	1
1:A:146:LEU:HD23	1:A:166:LEU:HD21	0.40	1.93	20	1
1:A:157:TRP:CD2	1:A:157:TRP:C	0.40	2.95	7	1
1:A:159:LEU:N	1:A:159:LEU:HD12	0.40	2.31	9	1
1:A:155:HIS:CE1	1:A:159:LEU:HD11	0.40	2.52	12	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	41/51 (80%)	38±1 (93±2%)	3±1 (6±2%)	0±0 (0±1%)	43 81
1	B	40/51 (78%)	37±1 (92±2%)	2±1 (5±2%)	1±1 (4±2%)	7 36
All	All	1620/2040 (79%)	1499 (93%)	89 (5%)	32 (2%)	14 55

All 5 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	159	LEU	20
1	B	137	ASP	7
1	A	167	ALA	2
1	B	127	ALA	2
1	A	127	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	35/43 (81%)	26±1 (74±4%)	9±1 (26±4%)	3 25
1	B	35/43 (81%)	25±2 (72±5%)	10±2 (28±5%)	2 21
All	All	1400/1720 (81%)	1026 (73%)	374 (27%)	2 23

All 47 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	139	TRP	20
1	B	133	LYS	20
1	A	139	TRP	20
1	A	133	LYS	20
1	B	159	LEU	20
1	A	150	LYS	17
1	B	131	ARG	15
1	B	150	LYS	14
1	B	135	SER	12
1	B	142	GLU	12
1	A	131	ARG	11
1	B	137	ASP	11
1	A	140	CYS	11
1	A	156	GLN	10
1	A	135	SER	9
1	A	161	HIS	9
1	A	159	LEU	9
1	A	142	GLU	9
1	A	162	GLU	8
1	B	148	CYS	8

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Mol	Chain	Res	Type	Models (Total)
1	A	158	PHE	8
1	B	158	PHE	7
1	B	157	TRP	7
1	B	155	HIS	7
1	B	161	HIS	6
1	A	153	GLU	6
1	B	162	GLU	6
1	A	160	LYS	6
1	B	140	CYS	5
1	A	157	TRP	5
1	A	145	GLN	5
1	B	156	GLN	4
1	B	152	PHE	4
1	A	141	PHE	4
1	B	145	GLN	4
1	A	137	ASP	4
1	B	164	ARG	4
1	B	153	GLU	3
1	B	141	PHE	3
1	A	155	HIS	2
1	B	160	LYS	2
1	A	164	ARG	2
1	A	146	LEU	1
1	A	152	PHE	1
1	A	147	LEU	1
1	A	166	LEU	1
1	B	130	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no carbohydrates in this entry.

6.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: 2mvw_cs.str

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	1168
Number of shifts mapped to atoms	1168
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	102	-0.27 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	100	-0.48 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	94	0.04 ± 0.46	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 85%, i.e. 878 atoms were assigned a chemical shift out of a possible 1039. 1 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	312/401 (78%)	154/160 (96%)	81/162 (50%)	77/79 (97%)
Sidechain	432/490 (88%)	273/293 (93%)	153/175 (87%)	6/22 (27%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	134/148 (91%)	70/80 (88%)	60/60 (100%)	4/8 (50%)
Overall	878/1039 (85%)	497/533 (93%)	294/397 (74%)	87/109 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1068 atoms were assigned a chemical shift out of a possible 1284. 1 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	388/506 (77%)	192/202 (95%)	102/204 (50%)	94/100 (94%)
Sidechain	546/630 (87%)	344/374 (92%)	192/224 (86%)	10/32 (31%)
Aromatic	134/148 (91%)	70/80 (88%)	60/60 (100%)	4/8 (50%)
Overall	1068/1284 (83%)	606/656 (92%)	354/488 (73%)	108/140 (77%)

7.1.4 Statistically unusual chemical shifts (i)

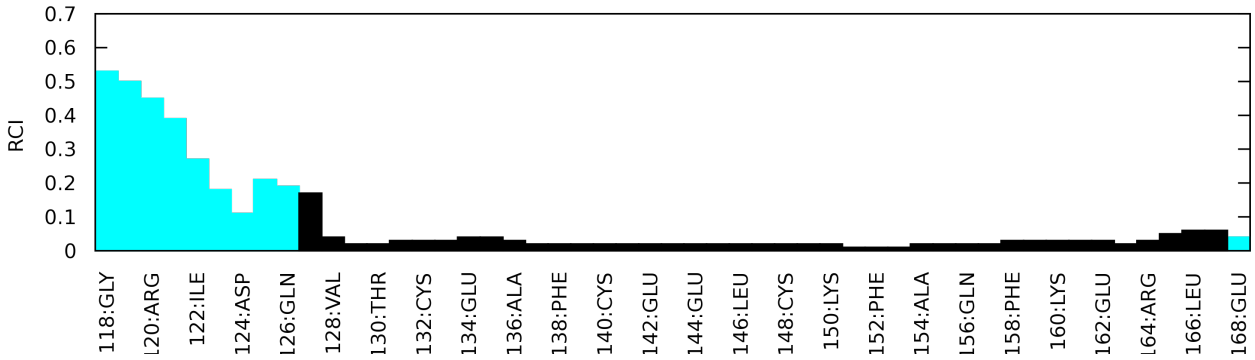
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	142	GLU	HB3	0.89	3.10 – 0.90	-5.0
1	B	142	GLU	HB3	0.89	3.10 – 0.90	-5.0

7.1.5 Random Coil Index (RCI) plots (i)

The images below report *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:



Random coil index (RCI) for chain B: