



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 18, 2018 – 07:31 am GMT

PDB ID : 1QTG  
Title : AVERAGED NMR MODEL OF SWITCH ARC, A DOUBLE MUTANT OF ARC REPRESSOR  
Authors : Cordes, M.H.J.; Walsh, N.P.; McKnight, C.J.; Sauer, R.T.  
Deposited on : 1999-06-27

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

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : trunk30686  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

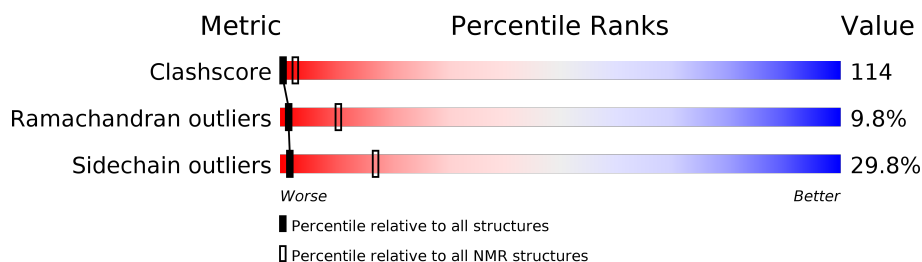
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 54%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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	53	
1	B	53	

## 2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1766 atoms, of which 896 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ARC REPRESSOR.

Mol	Chain	Residues	Atoms						Trace
1	A	53	Total	C	H	N	O	S	0
			883	271	448	82	78	4	
1	B	53	Total	C	H	N	O	S	0
			883	271	448	82	78	4	

There are 4 discrepancies between the modelled and reference sequences:

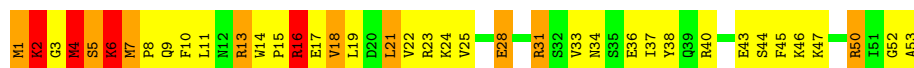
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	LEU	ASN	?	UNP P03050
A	12	ASN	LEU	?	UNP P03050
B	11	LEU	ASN	?	UNP P03050
B	12	ASN	LEU	?	UNP P03050

## 4 Residue-property plots

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: ARC REPRESSOR

Chain A: 



### • Molecule 1: ARC REPRESSOR

Chain B: 



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	BMRB entry 4540
Number of chemical shift lists	1
Total number of shifts	938
Number of shifts mapped to atoms	872
Number of unparsed shifts	0
Number of shifts with mapping errors	66
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	54%

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](#)

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	5
1	B	0	5
All	All	0	10

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	23	ARG	Sidechain
1	A	50	ARG	Sidechain
1	B	31	ARG	Sidechain
1	B	50	ARG	Sidechain
1	B	23	ARG	Sidechain
1	A	13	ARG	Sidechain
1	B	16	ARG	Sidechain
1	A	16	ARG	Sidechain
1	B	13	ARG	Sidechain
1	A	31	ARG	Sidechain

### 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	A	435	448	448	119

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	B	435	448	448	121
All	All	870	896	896	202

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 114.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:2:LYS:CE	1:B:2:LYS:O	1.30	1.79
1:A:2:LYS:O	1:A:2:LYS:CE	1.27	1.80
1:B:3:GLY:O	1:B:5:SER:N	1.26	1.69
1:A:3:GLY:O	1:A:5:SER:N	1.25	1.69
1:B:2:LYS:CD	1:B:2:LYS:O	1.12	1.96
1:A:2:LYS:O	1:A:2:LYS:CD	1.11	1.97
1:B:4:MET:N	1:B:4:MET:HE2	1.10	1.61
1:B:2:LYS:NZ	1:B:2:LYS:O	1.08	1.87
1:A:4:MET:N	1:A:4:MET:CE	1.06	2.18
1:B:1:MET:CA	1:B:5:SER:HB3	1.06	1.81
1:A:4:MET:N	1:A:4:MET:HE2	1.06	1.63
1:A:2:LYS:O	1:A:2:LYS:NZ	1.06	1.87
1:A:1:MET:CA	1:A:5:SER:HB3	1.06	1.81
1:A:4:MET:H	1:A:4:MET:HE2	1.05	0.88
1:B:4:MET:N	1:B:4:MET:CE	1.04	2.18
1:A:2:LYS:HD3	1:A:2:LYS:C	1.04	1.71
1:A:1:MET:HA	1:A:5:SER:HB3	1.04	1.28
1:B:2:LYS:HD3	1:B:2:LYS:C	1.03	1.71
1:B:1:MET:HA	1:B:5:SER:HB3	1.02	1.28
1:B:4:MET:HE2	1:B:4:MET:H	1.01	0.86
1:B:4:MET:CE	1:B:4:MET:H	0.99	1.68
1:B:3:GLY:CA	1:B:4:MET:HE3	0.98	1.88
1:A:4:MET:H	1:A:4:MET:CE	0.97	1.68
1:A:3:GLY:CA	1:A:4:MET:HE3	0.97	1.89
1:A:3:GLY:HA3	1:A:4:MET:HE3	0.96	1.33
1:B:3:GLY:HA3	1:B:4:MET:HE3	0.95	1.33
1:A:1:MET:CG	1:A:2:LYS:H	0.94	1.74
1:B:5:SER:C	1:B:6:LYS:HG3	0.94	1.79
1:A:5:SER:C	1:A:6:LYS:HG3	0.93	1.80
1:B:1:MET:CG	1:B:2:LYS:H	0.93	1.74
1:A:2:LYS:CD	1:A:2:LYS:C	0.91	2.38
1:B:31:ARG:HD2	1:B:36:GLU:OE1	0.86	1.71
1:A:1:MET:HA	1:A:5:SER:CB	0.85	2.01
1:A:31:ARG:HD2	1:A:36:GLU:OE1	0.85	1.71

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:B:1:MET:HA	1:B:5:SER:CB	0.84	2.01
1:B:16:ARG:HH11	1:B:16:ARG:CG	0.84	1.85
1:A:2:LYS:O	1:A:2:LYS:HE2	0.83	1.73
1:A:16:ARG:HH11	1:A:16:ARG:CG	0.82	1.85
1:B:3:GLY:CA	1:B:4:MET:CE	0.82	2.58
1:B:2:LYS:HE2	1:B:2:LYS:O	0.81	1.72
1:A:3:GLY:CA	1:A:4:MET:CE	0.80	2.59
1:A:52:GLY:O	1:A:53:ALA:C	0.79	2.21
1:A:38:TYR:HD1	1:B:14:TRP:CD2	0.78	1.97
1:A:1:MET:SD	1:A:2:LYS:N	0.77	2.56
1:A:14:TRP:CD2	1:B:38:TYR:HD1	0.77	1.97
1:B:1:MET:SD	1:B:2:LYS:N	0.77	2.57
1:A:25:VAL:HG22	1:B:50:ARG:NH1	0.77	1.95
1:B:52:GLY:O	1:B:53:ALA:C	0.77	2.23
1:B:3:GLY:O	1:B:4:MET:C	0.76	2.23
1:A:1:MET:CG	1:A:2:LYS:N	0.76	2.44
1:B:1:MET:CG	1:B:2:LYS:N	0.76	2.44
1:A:3:GLY:O	1:A:4:MET:C	0.75	2.23
1:A:5:SER:N	1:A:6:LYS:HZ3	0.75	1.80
1:A:4:MET:HA	1:A:6:LYS:HE2	0.75	1.57
1:B:4:MET:HA	1:B:6:LYS:HE2	0.74	1.58
1:A:6:LYS:O	1:A:8:PRO:HD3	0.74	1.83
1:B:2:LYS:HD3	1:B:2:LYS:O	0.73	1.67
1:B:6:LYS:O	1:B:8:PRO:HD3	0.73	1.83
1:B:3:GLY:HA3	1:B:4:MET:CE	0.73	2.14
1:A:3:GLY:HA3	1:A:4:MET:CE	0.73	2.14
1:B:1:MET:HG3	1:B:2:LYS:H	0.72	1.42
1:A:1:MET:CE	1:A:2:LYS:HB2	0.71	2.15
1:A:1:MET:HE1	1:A:2:LYS:HB2	0.71	1.62
1:A:1:MET:HG3	1:A:2:LYS:H	0.71	1.42
1:B:1:MET:O	1:B:3:GLY:N	0.71	2.24
1:A:1:MET:O	1:A:3:GLY:N	0.70	2.23
1:A:15:PRO:HG2	1:A:18:VAL:CG2	0.70	2.17
1:B:1:MET:CE	1:B:2:LYS:HB2	0.70	2.15
1:B:15:PRO:HG2	1:B:18:VAL:CG2	0.70	2.16
1:A:38:TYR:CE1	1:B:18:VAL:HG21	0.70	2.21
1:B:6:LYS:O	1:B:8:PRO:CD	0.70	2.40
1:A:2:LYS:O	1:A:2:LYS:HD3	0.70	1.67
1:A:6:LYS:O	1:A:8:PRO:CD	0.69	2.40
1:B:3:GLY:C	1:B:4:MET:HE3	0.68	2.08
1:A:14:TRP:HB2	1:A:19:LEU:HD11	0.68	1.65
1:A:1:MET:CE	1:A:2:LYS:CB	0.68	2.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:3:GLY:C	1:A:4:MET:HE3	0.68	2.08
1:A:14:TRP:CE2	1:B:38:TYR:HD1	0.67	2.07
1:B:1:MET:CE	1:B:2:LYS:CB	0.67	2.71
1:B:18:VAL:O	1:B:21:LEU:N	0.67	2.28
1:A:6:LYS:O	1:A:8:PRO:N	0.67	2.28
1:A:3:GLY:C	1:A:5:SER:N	0.67	2.46
1:A:25:VAL:HG22	1:B:50:ARG:HH11	0.67	1.49
1:A:50:ARG:NH1	1:B:25:VAL:HG22	0.67	2.05
1:B:6:LYS:O	1:B:8:PRO:N	0.67	2.28
1:B:14:TRP:HB2	1:B:19:LEU:HD11	0.66	1.65
1:B:15:PRO:HG2	1:B:18:VAL:HG23	0.66	1.67
1:B:1:MET:HE1	1:B:2:LYS:HB2	0.66	1.66
1:B:44:SER:HA	1:B:47:LYS:HE3	0.66	1.67
1:A:15:PRO:HG2	1:A:18:VAL:HG23	0.66	1.66
1:A:18:VAL:O	1:A:21:LEU:N	0.66	2.28
1:A:18:VAL:O	1:A:19:LEU:C	0.66	2.35
1:B:3:GLY:C	1:B:4:MET:CE	0.66	2.64
1:A:38:TYR:CD1	1:B:14:TRP:CD2	0.65	2.84
1:A:3:GLY:C	1:A:4:MET:CE	0.65	2.65
1:A:44:SER:HA	1:A:47:LYS:HE3	0.65	1.67
1:B:18:VAL:O	1:B:19:LEU:C	0.65	2.35
1:A:14:TRP:CD2	1:B:38:TYR:CD1	0.65	2.84
1:A:18:VAL:HG21	1:B:38:TYR:CE1	0.64	2.28
1:B:1:MET:HG3	1:B:2:LYS:N	0.64	2.07
1:A:10:PHE:HB2	1:B:10:PHE:HB2	0.63	1.69
1:B:5:SER:N	1:B:6:LYS:HZ3	0.63	1.91
1:A:4:MET:O	1:A:6:LYS:N	0.62	2.32
1:A:16:ARG:HH11	1:A:16:ARG:HG2	0.62	1.54
1:B:3:GLY:C	1:B:5:SER:N	0.61	2.47
1:A:38:TYR:HD1	1:B:14:TRP:CE2	0.61	2.12
1:A:14:TRP:HB2	1:A:19:LEU:CD1	0.61	2.25
1:A:16:ARG:NH1	1:A:16:ARG:CG	0.61	2.54
1:B:16:ARG:NH1	1:B:16:ARG:CG	0.61	2.54
1:A:45:PHE:CD2	1:B:21:LEU:HD22	0.61	2.30
1:B:14:TRP:HB2	1:B:19:LEU:CD1	0.61	2.26
1:A:50:ARG:HH11	1:B:25:VAL:HG22	0.60	1.56
1:B:4:MET:O	1:B:6:LYS:N	0.60	2.33
1:A:14:TRP:CE2	1:B:38:TYR:CD1	0.60	2.90
1:B:16:ARG:HH11	1:B:16:ARG:HG2	0.59	1.54
1:A:1:MET:C	1:A:3:GLY:H	0.59	2.01
1:B:1:MET:C	1:B:3:GLY:H	0.59	2.01
1:A:1:MET:HG3	1:A:2:LYS:N	0.59	2.07

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:21:LEU:HD22	1:B:45:PHE:CD2	0.58	2.33
1:A:25:VAL:HA	1:A:28:GLU:OE2	0.58	1.98
1:B:5:SER:C	1:B:6:LYS:CG	0.58	2.66
1:A:5:SER:C	1:A:6:LYS:CG	0.58	2.65
1:B:25:VAL:HA	1:B:28:GLU:OE2	0.58	1.98
1:A:52:GLY:O	1:A:53:ALA:O	0.57	2.22
1:A:11:LEU:HD22	1:A:14:TRP:CE3	0.57	2.34
1:B:1:MET:C	1:B:3:GLY:N	0.57	2.58
1:B:11:LEU:HD22	1:B:14:TRP:CE3	0.56	2.34
1:A:38:TYR:CD1	1:B:14:TRP:CE2	0.55	2.93
1:A:38:TYR:HE1	1:B:18:VAL:HG21	0.55	1.58
1:A:8:PRO:CG	1:A:11:LEU:HD12	0.55	2.32
1:B:8:PRO:CG	1:B:11:LEU:HD12	0.55	2.32
1:A:1:MET:C	1:A:3:GLY:N	0.55	2.58
1:A:21:LEU:O	1:A:25:VAL:HG23	0.54	2.03
1:B:21:LEU:O	1:B:25:VAL:HG23	0.54	2.03
1:B:52:GLY:O	1:B:53:ALA:O	0.53	2.26
1:B:5:SER:N	1:B:6:LYS:NZ	0.53	2.56
1:A:8:PRO:CD	1:A:11:LEU:HD12	0.53	2.34
1:A:25:VAL:CG2	1:B:50:ARG:HH11	0.53	2.16
1:A:1:MET:C	1:A:5:SER:HB3	0.53	2.23
1:A:50:ARG:NH1	1:B:25:VAL:HG13	0.53	2.17
1:A:10:PHE:CE2	1:B:34:ASN:OD1	0.53	2.62
1:B:8:PRO:CD	1:B:11:LEU:HD12	0.53	2.33
1:A:6:LYS:O	1:A:7:MET:C	0.52	2.47
1:B:6:LYS:O	1:B:7:MET:C	0.52	2.47
1:A:34:ASN:OD1	1:B:10:PHE:CE2	0.52	2.63
1:A:50:ARG:HH12	1:B:25:VAL:HG13	0.51	1.65
1:B:1:MET:C	1:B:5:SER:HB3	0.51	2.23
1:A:38:TYR:OH	1:B:18:VAL:HG21	0.51	2.05
1:B:1:MET:HE3	1:B:2:LYS:HB3	0.51	1.83
1:A:3:GLY:C	1:A:5:SER:H	0.51	2.06
1:A:18:VAL:HG21	1:B:38:TYR:HE1	0.50	1.63
1:A:16:ARG:HG3	1:A:16:ARG:HH11	0.50	1.65
1:B:3:GLY:C	1:B:5:SER:H	0.50	2.06
1:A:38:TYR:CE1	1:B:18:VAL:HG11	0.49	2.42
1:A:16:ARG:HG3	1:A:16:ARG:NH1	0.49	2.23
1:A:25:VAL:HG13	1:B:50:ARG:HH12	0.49	1.67
1:B:16:ARG:NH1	1:B:16:ARG:HG3	0.48	2.23
1:A:5:SER:N	1:A:6:LYS:NZ	0.48	2.57
1:B:36:GLU:O	1:B:40:ARG:HG3	0.48	2.09
1:A:25:VAL:HG13	1:B:50:ARG:NH1	0.48	2.23

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:38:TYR:HB2	1:B:14:TRP:CE2	0.48	2.44
1:A:36:GLU:O	1:A:40:ARG:HG3	0.47	2.09
1:A:1:MET:HE3	1:A:2:LYS:HB3	0.47	1.87
1:A:14:TRP:CB	1:A:19:LEU:CD1	0.46	2.93
1:A:38:TYR:CZ	1:B:18:VAL:HG21	0.46	2.45
1:A:50:ARG:HH11	1:B:25:VAL:CG2	0.46	2.24
1:B:1:MET:O	1:B:5:SER:HB3	0.46	2.11
1:A:1:MET:O	1:A:5:SER:HB3	0.46	2.11
1:A:14:TRP:CE2	1:B:38:TYR:HB2	0.45	2.46
1:A:14:TRP:CZ2	1:B:38:TYR:CA	0.45	2.99
1:B:14:TRP:CB	1:B:19:LEU:CD1	0.45	2.94
1:A:18:VAL:HG21	1:B:38:TYR:OH	0.45	2.11
1:B:17:GLU:OE1	1:B:17:GLU:N	0.45	2.50
1:B:22:VAL:CG1	1:B:33:VAL:HG13	0.45	2.42
1:A:17:GLU:N	1:A:17:GLU:OE1	0.44	2.50
1:A:22:VAL:CG1	1:A:33:VAL:HG13	0.44	2.42
1:A:38:TYR:CA	1:B:14:TRP:CZ2	0.44	3.01
1:A:3:GLY:O	1:A:5:SER:CA	0.44	2.62
1:B:1:MET:HE3	1:B:2:LYS:CB	0.43	2.42
1:A:4:MET:HA	1:A:6:LYS:CE	0.43	2.39
1:B:15:PRO:HD2	1:B:18:VAL:HG21	0.43	1.90
1:B:8:PRO:HD2	1:B:11:LEU:HD12	0.43	1.91
1:A:25:VAL:CG2	1:B:50:ARG:NH1	0.42	2.76
1:B:46:LYS:NZ	1:B:53:ALA:OXT	0.42	2.51
1:B:3:GLY:O	1:B:5:SER:CA	0.42	2.62
1:A:8:PRO:HD2	1:A:11:LEU:HD12	0.42	1.91
1:A:15:PRO:HD2	1:A:18:VAL:HG21	0.42	1.91
1:B:15:PRO:O	1:B:16:ARG:C	0.42	2.58
1:A:15:PRO:O	1:A:16:ARG:C	0.42	2.58
1:A:25:VAL:HA	1:A:28:GLU:CD	0.42	2.35
1:B:25:VAL:HA	1:B:28:GLU:CD	0.42	2.35
1:A:38:TYR:OH	1:B:18:VAL:CG2	0.41	2.68
1:B:11:LEU:CD2	1:B:14:TRP:CE3	0.41	3.04
1:B:8:PRO:CG	1:B:11:LEU:CD1	0.41	2.98
1:A:10:PHE:CB	1:B:10:PHE:CG	0.41	3.04
1:B:14:TRP:N	1:B:14:TRP:CD1	0.41	2.87
1:B:24:LYS:HE2	1:B:24:LYS:HB3	0.41	1.46
1:A:14:TRP:N	1:A:14:TRP:CD1	0.41	2.87
1:A:11:LEU:CD2	1:A:14:TRP:CE3	0.41	3.04
1:B:11:LEU:O	1:B:13:ARG:N	0.41	2.54
1:B:4:MET:HA	1:B:6:LYS:CE	0.41	2.40
1:A:8:PRO:HG2	1:A:11:LEU:HG	0.40	1.93

## 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	51/53 (96%)	40 (78%)	6 (12%)	5 (10%)	1	10
1	B	51/53 (96%)	40 (78%)	6 (12%)	5 (10%)	1	10
All	All	102/106 (96%)	80 (78%)	12 (12%)	10 (10%)	1	10

All 10 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	2	LYS
1	A	5	SER
1	B	6	LYS
1	A	7	MET
1	B	7	MET
1	A	4	MET
1	B	4	MET
1	A	6	LYS
1	A	2	LYS
1	B	5	SER

### 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	47/47 (100%)	33 (70%)	14 (30%)	2	17
1	B	47/47 (100%)	33 (70%)	14 (30%)	2	17
All	All	94/94 (100%)	66 (70%)	28 (30%)	2	17

All 28 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	B	2	LYS
1	B	6	LYS
1	B	9	GLN
1	A	16	ARG
1	A	2	LYS
1	A	28	GLU
1	B	46	LYS
1	A	21	LEU
1	B	13	ARG
1	A	24	LYS
1	B	43	GLU
1	B	28	GLU
1	B	24	LYS
1	A	18	VAL
1	B	21	LEU
1	A	4	MET
1	A	46	LYS
1	B	18	VAL
1	B	16	ARG
1	A	13	ARG
1	B	1	MET
1	A	37	ILE
1	B	4	MET
1	A	6	LYS
1	A	1	MET
1	A	9	GLN
1	B	37	ILE
1	A	43	GLU

### 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

There are no ligands in this entry.

## 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 54% for the well-defined parts and 54% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 4540

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	938
Number of shifts mapped to atoms	872
Number of unparsed shifts	0
Number of shifts with mapping errors	66
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 66 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
B	61	ASN	N	120.11	0.1	1
A	60	LYS	HE2	3.1	0.02	1
B	62	GLN	HG3	2.4	0.02	1
A	60	LYS	HG2	1.51	0.02	1
A	60	LYS	HD3	1.79	0.02	1
A	61	ASN	N	120.11	0.1	1
B	64	GLU	H	8.31	0.02	1
A	60	LYS	H	8.66	0.02	1
A	64	GLU	HA	4.26	0.02	1
A	60	LYS	HE3	3.1	0.02	1
B	62	GLN	HG2	2.4	0.02	1
B	64	GLU	N	127.55	0.1	1
B	60	LYS	N	123.36	0.1	1
B	62	GLN	H	8.42	0.02	1

*Continued on next page...*



*Continued from previous page...*

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	63	HIS	N	119.25	0.1	1
A	61	ASN	H	8.74	0.02	1
B	64	GLU	HB2	2.02	0.02	2
A	64	GLU	H	8.31	0.02	1
B	63	HIS	H	8.57	0.02	1
B	60	LYS	HB3	1.88	0.02	1
A	61	ASN	HB2	2.91	0.02	2
B	60	LYS	HD3	1.79	0.02	1
A	62	GLN	HB3	2.14	0.02	2
A	62	GLN	N	120.18	0.1	1
B	60	LYS	HE2	3.1	0.02	1
B	60	LYS	HE3	3.1	0.02	1
A	64	GLU	HG3	2.35	0.02	1
A	64	GLU	HB2	2.02	0.02	2
B	61	ASN	HA	4.78	0.02	1
A	60	LYS	HB2	1.88	0.02	1
B	62	GLN	HB3	2.14	0.02	2
B	63	HIS	N	119.25	0.1	1
B	64	GLU	HB3	2.2	0.02	2
B	62	GLN	HB2	2.04	0.02	2
B	61	ASN	HB2	2.91	0.02	2
A	60	LYS	N	123.36	0.1	1
B	64	GLU	HG2	2.35	0.02	1
B	60	LYS	HD2	1.79	0.02	1
A	60	LYS	HA	4.37	0.02	1
A	61	ASN	HB3	2.99	0.02	2
A	63	HIS	H	8.57	0.02	1
A	62	GLN	HB2	2.04	0.02	2
A	62	GLN	HG2	2.4	0.02	1
A	62	GLN	H	8.42	0.02	1
A	60	LYS	HB3	1.88	0.02	1
B	60	LYS	HA	4.37	0.02	1
B	61	ASN	HB3	2.99	0.02	2
B	62	GLN	N	120.18	0.1	1
A	63	HIS	HA	4.79	0.02	1
B	60	LYS	H	8.66	0.02	1
B	64	GLU	HG3	2.35	0.02	1
A	60	LYS	HD2	1.79	0.02	1
B	62	GLN	HA	4.39	0.02	1
A	62	GLN	HA	4.39	0.02	1
A	64	GLU	N	127.55	0.1	1

*Continued on next page...*

Continued from previous page...

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	62	GLN	HG3	2.4	0.02	1
B	60	LYS	HG2	1.51	0.02	1
A	61	ASN	HA	4.78	0.02	1
B	60	LYS	HB2	1.88	0.02	1
B	61	ASN	H	8.74	0.02	1
A	60	LYS	HG3	1.51	0.02	1
A	64	GLU	HB3	2.2	0.02	2
A	64	GLU	HG2	2.35	0.02	1
B	63	HIS	HA	4.79	0.02	1
B	60	LYS	HG3	1.51	0.02	1
B	64	GLU	HA	4.26	0.02	1

### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	108	$0.50 \pm 0.31$	None needed ( $< 0.5$ ppm)

### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 54%, i.e. 776 atoms were assigned a chemical shift out of a possible 1424. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	300/522 (57%)	202/208 (97%)	0/212 (0%)	98/102 (96%)
Sidechain	434/826 (53%)	412/492 (84%)	0/278 (0%)	22/56 (39%)
Aromatic	42/76 (55%)	40/40 (100%)	0/34 (0%)	2/2 (100%)
Overall	776/1424 (54%)	654/740 (88%)	0/524 (0%)	122/160 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 54%, i.e. 776 atoms were assigned a chemical shift out of a possible 1424. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	300/522 (57%)	202/208 (97%)	0/212 (0%)	98/102 (96%)
Sidechain	434/826 (53%)	412/492 (84%)	0/278 (0%)	22/56 (39%)
Aromatic	42/76 (55%)	40/40 (100%)	0/34 (0%)	2/2 (100%)
Overall	776/1424 (54%)	654/740 (88%)	0/524 (0%)	122/160 (76%)

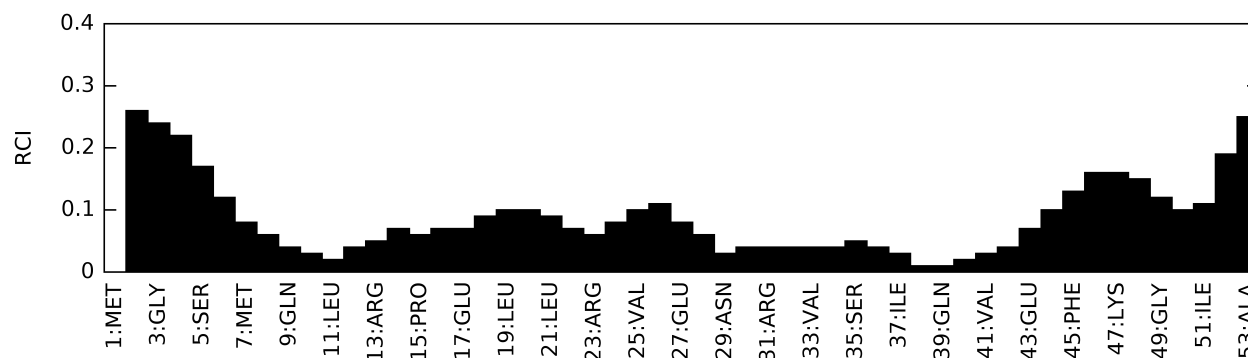
### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 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:

