Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 03:21 PM BST

PDB ID	:	1KLQ
Title	:	The Mad2 Spindle Checkpoint Protein Undergoes Similar Major Conformational Changes upon Binding to Either Mad1 or Cdc20
Authors	:	Luo, X.; Tang, Z.; Rizo, J.; Yu, H.
Deposited on	:	2001-12-12

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:

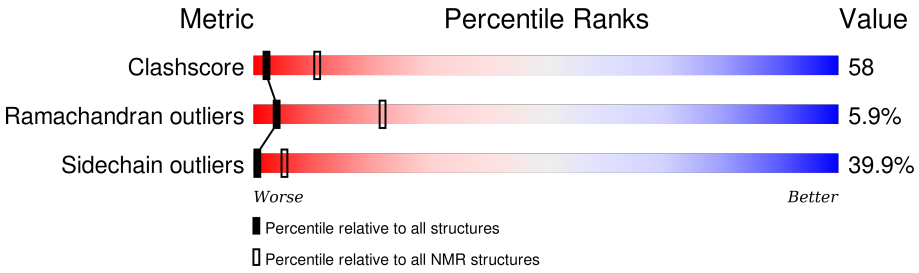
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 76%.

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	197	28% 47% 24% .
2	B	12	25% 42% 17% 17%

2 Ensemble composition and analysis (i)

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3371 atoms, of which 1691 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A.

Mol	Chain	Residues	Atoms						Trace
1	A	197	Total	C	H	N	O	S	0
			3198	1018	1609	258	309	4	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	GLY	GLN	EXPRESSION TAG	UNP Q13257
A	12	SER	GLY	EXPRESSION TAG	UNP Q13257

- Molecule 2 is a protein called Mad2-binding peptide.

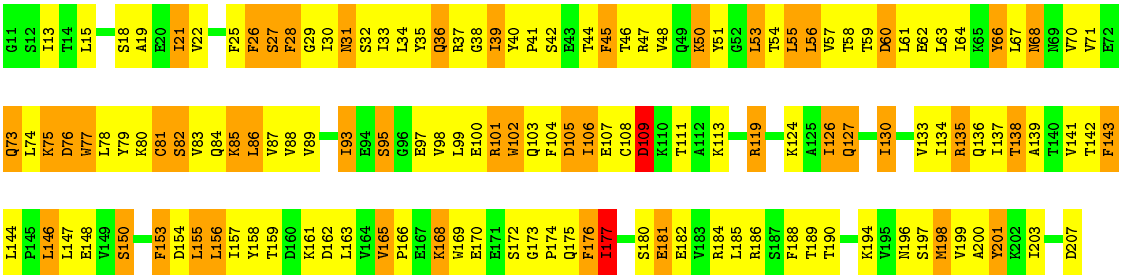
Mol	Chain	Residues	Atoms					Trace
2	B	10	Total	C	H	N	O	0
			173	61	82	15	15	

4 Residue-property plots (i)

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.

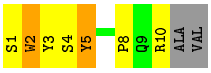
- Molecule 1: MITOTIC SPINDLE ASSEMBLY CHECKPOINT PROTEIN MAD2A

Chain A:



- Molecule 2: Mad2-binding peptide

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 1 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
CNS	structure solution	0.9a
CNS	refinement	0.9a

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 5299
Number of chemical shift lists	2
Total number of shifts	2145
Number of shifts mapped to atoms	2145
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

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

6 Model quality

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1589	1609	1605	195
2	B	91	82	82	39
All	All	1680	1691	1687	196

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 58.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:19:ALA:HB2	1:A:79:TYR:CE2	0.92	1.99
1:A:45:PHE:HB2	1:A:56:LEU:HD21	0.91	1.40
1:A:53:LEU:HD22	1:A:55:LEU:CD2	0.86	1.99
1:A:45:PHE:CB	1:A:56:LEU:HD21	0.86	1.99
1:A:34:LEU:HD21	1:A:153:PHE:CZ	0.86	2.05
1:A:126:ILE:O	1:A:130:ILE:HG22	0.83	1.72
1:A:137:ILE:O	1:A:141:VAL:HG23	0.80	1.76
1:A:77:TRP:CZ2	2:B:3:TYR:CD2	0.79	2.70
1:A:156:LEU:HD22	2:B:2:TRP:CE3	0.78	2.14
1:A:66:TYR:O	1:A:70:VAL:HG23	0.78	1.79
1:A:28:PHE:CE1	1:A:55:LEU:HD12	0.78	2.14
1:A:42:SER:HA	1:A:45:PHE:CZ	0.76	2.15
1:A:77:TRP:CZ2	1:A:157:ILE:HG21	0.75	2.17
1:A:158:TYR:OH	2:B:2:TRP:CH2	0.74	2.40

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:28:PHE:CD1	1:A:55:LEU:HD12	0.74	2.17
1:A:156:LEU:HD23	2:B:3:TYR:O	0.74	1.83
1:A:35:TYR:HD2	1:A:56:LEU:HD22	0.72	1.44
1:A:105:ASP:C	1:A:106:ILE:HD13	0.72	2.05
1:A:86:LEU:HB2	1:A:106:ILE:HD11	0.71	1.63
1:A:98:VAL:HG11	1:A:177:ILE:HG23	0.70	1.62
1:A:169:TRP:CE3	2:B:5:TYR:CD1	0.70	2.80
1:A:70:VAL:HG12	1:A:74:LEU:HD13	0.70	1.62
1:A:67:LEU:O	1:A:71:VAL:HG23	0.70	1.86
1:A:185:LEU:HD11	1:A:199:VAL:HG12	0.69	1.65
1:A:29:GLY:O	1:A:33:ILE:HG12	0.69	1.87
1:A:158:TYR:CE1	2:B:2:TRP:CE3	0.68	2.82
1:A:21:ILE:O	1:A:25:PHE:HB2	0.67	1.88
1:A:18:SER:O	1:A:22:VAL:HG23	0.67	1.89
1:A:36:GLN:CB	1:A:137:ILE:HG22	0.67	2.19
1:A:40:TYR:CE2	1:A:58:THR:HG21	0.67	2.25
1:A:165:VAL:HB	2:B:3:TYR:CE1	0.67	2.24
1:A:34:LEU:HD22	1:A:39:ILE:HG13	0.66	1.66
1:A:42:SER:HA	1:A:45:PHE:CE2	0.66	2.25
1:A:163:LEU:HG	2:B:3:TYR:CZ	0.65	2.25
1:A:55:LEU:HB3	1:A:134:ILE:HD12	0.65	1.68
1:A:136:GLN:HB2	1:A:185:LEU:HD22	0.65	1.67
1:A:77:TRP:CZ2	2:B:3:TYR:HD2	0.65	2.09
1:A:106:ILE:HD13	1:A:106:ILE:N	0.64	2.07
1:A:163:LEU:CG	2:B:3:TYR:CZ	0.64	2.80
1:A:102:TRP:CZ2	1:A:137:ILE:HG12	0.64	2.27
1:A:86:LEU:HD13	1:A:104:PHE:CE2	0.64	2.28
1:A:35:TYR:CG	1:A:45:PHE:CE2	0.63	2.85
1:A:28:PHE:CE1	1:A:57:VAL:HG22	0.63	2.29
1:A:60:ASP:OD2	1:A:63:LEU:HD22	0.63	1.94
1:A:189:THR:HG23	1:A:194:LYS:HB2	0.62	1.71
1:A:34:LEU:HD11	1:A:63:LEU:HD11	0.62	1.70
1:A:165:VAL:CG2	2:B:3:TYR:CZ	0.61	2.82
1:A:70:VAL:HG22	2:B:5:TYR:CE2	0.60	2.32
1:A:66:TYR:C	1:A:66:TYR:CD1	0.60	2.75
1:A:99:LEU:HD21	1:A:147:LEU:HD21	0.60	1.74
1:A:158:TYR:HA	2:B:2:TRP:HB3	0.59	1.74
1:A:168:LYS:HD3	1:A:169:TRP:NE1	0.59	2.12
1:A:77:TRP:CH2	1:A:157:ILE:HG21	0.59	2.31
1:A:165:VAL:HG23	2:B:3:TYR:CZ	0.59	2.32
1:A:73:GLN:O	1:A:77:TRP:N	0.59	2.34
1:A:78:LEU:HD22	1:A:83:VAL:CB	0.59	2.27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:40:TYR:CZ	1:A:58:THR:HG21	0.58	2.34
1:A:70:VAL:O	1:A:74:LEU:HB2	0.58	1.99
1:A:78:LEU:HD11	1:A:157:ILE:HG23	0.57	1.74
1:A:78:LEU:HD22	1:A:83:VAL:HB	0.57	1.76
1:A:163:LEU:HD21	2:B:3:TYR:CE2	0.57	2.35
1:A:93:ILE:HB	1:A:150:SER:O	0.57	2.00
1:A:163:LEU:HG	2:B:3:TYR:CE1	0.57	2.35
1:A:77:TRP:CZ2	2:B:3:TYR:CE2	0.57	2.93
1:A:101:ARG:HH11	1:A:177:ILE:HD11	0.57	1.59
1:A:157:ILE:O	2:B:2:TRP:CB	0.57	2.52
1:A:26:PHE:CE1	1:A:67:LEU:HD22	0.56	2.35
1:A:89:VAL:HG22	1:A:101:ARG:HD2	0.56	1.77
1:A:144:LEU:HD21	1:A:201:TYR:CE2	0.56	2.35
1:A:53:LEU:CD1	1:A:53:LEU:N	0.56	2.69
1:A:28:PHE:CE1	1:A:57:VAL:CG2	0.56	2.88
1:A:26:PHE:CD1	1:A:26:PHE:C	0.56	2.79
1:A:40:TYR:OH	1:A:58:THR:HG21	0.55	2.00
1:A:35:TYR:CD2	1:A:56:LEU:HD22	0.55	2.31
1:A:35:TYR:CD1	1:A:45:PHE:CE2	0.55	2.94
1:A:35:TYR:CD2	1:A:45:PHE:CD2	0.55	2.95
1:A:53:LEU:HD13	1:A:53:LEU:N	0.55	2.17
1:A:54:THR:C	1:A:55:LEU:HD23	0.54	2.23
1:A:173:GLY:HA3	2:B:2:TRP:CD2	0.54	2.37
1:A:86:LEU:HD22	1:A:104:PHE:CZ	0.54	2.37
1:A:51:TYR:HB3	1:A:130:ILE:HG21	0.54	1.78
1:A:53:LEU:H	1:A:53:LEU:HD13	0.54	1.63
1:A:133:VAL:O	1:A:137:ILE:HG13	0.53	2.03
1:A:78:LEU:HD11	1:A:157:ILE:CG2	0.53	2.34
1:A:25:PHE:CE2	1:A:130:ILE:HB	0.52	2.39
1:A:35:TYR:CD2	1:A:45:PHE:CE2	0.52	2.98
2:B:2:TRP:CD1	2:B:2:TRP:N	0.52	2.76
1:A:66:TYR:CE1	1:A:155:LEU:HD11	0.52	2.39
1:A:26:PHE:CD1	1:A:27:SER:N	0.52	2.78
1:A:40:TYR:OH	1:A:58:THR:OG1	0.52	2.19
1:A:169:TRP:CD2	2:B:5:TYR:CD1	0.52	2.97
1:A:101:ARG:NH1	1:A:177:ILE:HD11	0.51	2.20
1:A:74:LEU:O	1:A:78:LEU:CB	0.51	2.58
1:A:77:TRP:O	1:A:77:TRP:CE3	0.51	2.64
1:A:45:PHE:CG	1:A:56:LEU:HD21	0.51	2.40
1:A:163:LEU:HD21	2:B:3:TYR:CZ	0.51	2.41
1:A:84:GLN:HA	1:A:106:ILE:O	0.51	2.06
1:A:98:VAL:HG11	1:A:177:ILE:CG2	0.50	2.36

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:169:TRP:CZ3	2:B:5:TYR:CD1	0.50	2.99
1:A:88:VAL:O	1:A:101:ARG:HA	0.50	2.06
1:A:163:LEU:CD2	2:B:3:TYR:CE1	0.50	2.95
1:A:85:LYS:HB2	1:A:158:TYR:CG	0.50	2.42
1:A:25:PHE:CE2	1:A:126:ILE:HD13	0.50	2.42
1:A:36:GLN:HG3	1:A:138:THR:HA	0.50	1.83
1:A:77:TRP:CZ3	1:A:163:LEU:HD11	0.50	2.41
1:A:66:TYR:CE1	1:A:155:LEU:CD1	0.50	2.94
1:A:173:GLY:N	1:A:174:PRO:CD	0.49	2.74
1:A:66:TYR:CZ	1:A:67:LEU:CD2	0.49	2.95
1:A:36:GLN:HG2	1:A:137:ILE:HG22	0.49	1.82
1:A:102:TRP:CZ2	1:A:137:ILE:CG1	0.49	2.94
1:A:25:PHE:CZ	1:A:130:ILE:HB	0.49	2.42
1:A:36:GLN:CG	1:A:137:ILE:HG22	0.49	2.37
1:A:163:LEU:CD2	2:B:3:TYR:CZ	0.48	2.97
1:A:77:TRP:CH2	1:A:157:ILE:CG2	0.48	2.96
1:A:106:ILE:N	1:A:106:ILE:CD1	0.48	2.75
1:A:136:GLN:CD	1:A:185:LEU:HD13	0.48	2.29
1:A:165:VAL:CB	2:B:3:TYR:CE1	0.48	2.97
1:A:66:TYR:CE1	1:A:67:LEU:HD23	0.48	2.43
1:A:158:TYR:CZ	2:B:2:TRP:CE3	0.48	3.01
1:A:34:LEU:CD1	1:A:63:LEU:HD11	0.47	2.39
1:A:53:LEU:CD2	1:A:55:LEU:CD2	0.47	2.84
1:A:75:LYS:O	1:A:79:TYR:HB2	0.47	2.10
1:A:31:ASN:OD1	1:A:58:THR:N	0.47	2.47
1:A:163:LEU:HD21	2:B:3:TYR:CD2	0.47	2.45
1:A:144:LEU:HD21	1:A:201:TYR:CD2	0.47	2.45
1:A:77:TRP:C	1:A:77:TRP:CE3	0.46	2.88
1:A:77:TRP:CZ3	1:A:163:LEU:CD1	0.46	2.99
1:A:155:LEU:HB2	2:B:5:TYR:CB	0.46	2.40
1:A:135:ARG:O	1:A:139:ALA:N	0.46	2.40
1:A:159:THR:CG2	1:A:163:LEU:HD22	0.46	2.41
1:A:182:GLU:HA	1:A:200:ALA:HB2	0.46	1.87
1:A:57:VAL:HG12	1:A:58:THR:N	0.46	2.26
1:A:156:LEU:HD22	2:B:2:TRP:HE3	0.46	1.64
1:A:158:TYR:CZ	2:B:2:TRP:CZ3	0.46	3.04
1:A:177:ILE:HD12	1:A:180:SER:HB2	0.46	1.87
1:A:78:LEU:HD13	1:A:83:VAL:HB	0.45	1.88
1:A:165:VAL:CG2	2:B:3:TYR:CE1	0.45	2.98
1:A:53:LEU:HD22	1:A:55:LEU:HD23	0.45	1.82
1:A:66:TYR:CZ	1:A:155:LEU:HD11	0.45	2.47
1:A:181:GLU:N	1:A:203:ILE:HG23	0.45	2.27

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:34:LEU:CD1	1:A:63:LEU:CD1	0.44	2.96
1:A:46:THR:N	1:A:57:VAL:O	0.44	2.43
1:A:34:LEU:HD13	1:A:39:ILE:CG2	0.44	2.43
1:A:136:GLN:OE1	1:A:185:LEU:HD13	0.44	2.12
1:A:26:PHE:CZ	1:A:67:LEU:HD22	0.44	2.48
1:A:26:PHE:CE2	1:A:30:ILE:HG13	0.44	2.48
1:A:33:ILE:HA	1:A:137:ILE:HG21	0.44	1.89
1:A:70:VAL:O	1:A:74:LEU:N	0.44	2.49
1:A:51:TYR:HD1	1:A:55:LEU:HD11	0.44	1.73
1:A:39:ILE:CD1	1:A:153:PHE:CD1	0.44	3.01
1:A:157:ILE:O	2:B:2:TRP:CA	0.44	2.66
1:A:51:TYR:CB	1:A:130:ILE:HG21	0.43	2.43
1:A:40:TYR:OH	1:A:58:THR:CG2	0.43	2.67
1:A:26:PHE:O	1:A:30:ILE:CG1	0.43	2.66
1:A:156:LEU:HA	2:B:3:TYR:O	0.43	2.13
1:A:175:GLN:O	1:A:176:PHE:C	0.43	2.56
1:A:48:VAL:O	1:A:55:LEU:N	0.43	2.42
1:A:74:LEU:O	1:A:78:LEU:HB2	0.43	2.12
1:A:146:LEU:O	1:A:147:LEU:HD13	0.43	2.14
1:A:50:LYS:HB3	1:A:55:LEU:HD11	0.43	1.90
1:A:34:LEU:HD21	1:A:153:PHE:CE1	0.43	2.46
1:A:88:VAL:N	1:A:102:TRP:O	0.43	2.51
1:A:77:TRP:HE3	1:A:77:TRP:O	0.43	1.94
1:A:36:GLN:CB	1:A:141:VAL:HG21	0.43	2.44
1:A:133:VAL:O	1:A:136:GLN:HG2	0.43	2.13
1:A:155:LEU:HB2	2:B:5:TYR:HB3	0.43	1.90
1:A:201:TYR:CD1	1:A:201:TYR:N	0.43	2.85
1:A:81:CYS:O	1:A:82:SER:CB	0.43	2.67
1:A:28:PHE:CE2	1:A:50:LYS:CD	0.42	3.02
1:A:50:LYS:O	1:A:53:LEU:HD13	0.42	2.14
1:A:36:GLN:HB3	1:A:141:VAL:HG21	0.42	1.91
1:A:87:VAL:O	1:A:156:LEU:HB2	0.42	2.14
1:A:15:LEU:HD23	1:A:109:ASP:OD1	0.42	2.15
1:A:34:LEU:O	1:A:38:GLY:N	0.42	2.52
1:A:25:PHE:CE2	1:A:126:ILE:CD1	0.42	3.03
1:A:158:TYR:CE1	2:B:2:TRP:CZ3	0.42	3.07
1:A:103:GLN:O	1:A:198:MET:O	0.42	2.38
1:A:60:ASP:CG	1:A:63:LEU:HB3	0.42	2.34
1:A:77:TRP:CZ2	1:A:157:ILE:CG2	0.41	2.98
1:A:40:TYR:OH	1:A:58:THR:CB	0.41	2.67
1:A:143:PHE:CE1	1:A:201:TYR:OH	0.41	2.73
1:A:77:TRP:CH2	2:B:3:TYR:CE2	0.41	3.09

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:42:SER:CA	1:A:45:PHE:CE2	0.41	3.02
1:A:53:LEU:HD12	1:A:127:GLN:NE2	0.41	2.31
1:A:127:GLN:HA	1:A:130:ILE:CG2	0.41	2.46
1:A:60:ASP:OD1	1:A:60:ASP:N	0.41	2.54
1:A:70:VAL:CG1	1:A:74:LEU:HD13	0.41	2.40
1:A:76:ASP:O	1:A:80:LYS:CB	0.41	2.69
1:A:55:LEU:HB3	1:A:134:ILE:HG21	0.41	1.91
1:A:102:TRP:CD1	1:A:199:VAL:CG2	0.41	3.04
1:A:158:TYR:CZ	2:B:2:TRP:CD2	0.41	3.09
1:A:64:ILE:O	1:A:68:ASN:HB2	0.41	2.16
1:A:26:PHE:HE1	1:A:67:LEU:HD22	0.40	1.76
1:A:40:TYR:HB2	1:A:41:PRO:HD2	0.40	1.92
1:A:157:ILE:CD1	1:A:169:TRP:CH2	0.40	3.05
1:A:157:ILE:O	2:B:2:TRP:HB3	0.40	2.16

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	195/197 (99%)	161 (83%)	23 (12%)	11 (6%)	4 23
2	B	8/12 (67%)	6 (75%)	1 (12%)	1 (12%)	1 7
All	All	203/209 (97%)	167 (82%)	24 (12%)	12 (6%)	4 22

All 12 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	176	PHE
1	A	119	ARG
1	A	95	SER
1	A	166	PRO
1	A	146	LEU
1	A	97	GLU
1	A	111	THR
1	A	172	SER

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Mol	Chain	Res	Type
1	A	177	ILE
2	B	8	PRO
1	A	148	GLU
1	A	109	ASP

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	183/183 (100%)	111 (61%)	72 (39%)	1 6
2	B	10/11 (91%)	5 (50%)	5 (50%)	0 1
All	All	193/194 (99%)	116 (60%)	77 (40%)	1 5

All 77 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	A	102	TRP
1	A	197	SER
1	A	55	LEU
1	A	161	LYS
1	A	127	GLN
1	A	44	THR
1	A	126	ILE
1	A	32	SER
1	A	113	LYS
1	A	142	THR
1	A	106	ILE
1	A	181	GLU
1	A	53	LEU
1	A	85	LYS
1	A	82	SER
1	A	177	ILE
1	A	107	GLU
2	B	2	TRP
1	A	13	ILE
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	45	PHE
1	A	162	ASP
1	A	56	LEU
1	A	119	ARG
1	A	156	LEU
2	B	5	TYR
1	A	75	LYS
1	A	26	PHE
1	A	81	CYS
1	A	47	ARG
1	A	76	ASP
1	A	73	GLN
1	A	77	TRP
1	A	168	LYS
1	A	198	MET
1	A	36	GLN
1	A	27	SER
1	A	109	ASP
1	A	135	ARG
1	A	39	ILE
1	A	201	TYR
1	A	28	PHE
1	A	165	VAL
2	B	1	SER
1	A	108	CYS
1	A	62	GLU
1	A	186	ARG
1	A	153	PHE
1	A	155	LEU
1	A	66	TYR
2	B	4	SER
2	B	10	ARG
1	A	184	ARG
1	A	86	LEU
1	A	150	SER
1	A	130	ILE
1	A	154	ASP
1	A	101	ARG
1	A	188	PHE
1	A	170	GLU
1	A	93	ILE
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	143	PHE
1	A	100	GLU
1	A	196	ASN
1	A	95	SER
1	A	105	ASP
1	A	50	LYS
1	A	37	ARG
1	A	61	LEU
1	A	59	THR
1	A	124	LYS
1	A	31	ASN
1	A	190	THR
1	A	207	ASP
1	A	138	THR
1	A	60	ASP

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 76% for the well-defined parts and 76% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5299

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	2075
Number of shifts mapped to atoms	2075
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	11

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	194	-0.24 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	179	0.29 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	181	-0.70 ± 0.09	Should be applied
^{15}N	189	0.27 ± 0.28	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 73%, i.e. 1927 atoms were assigned a chemical shift out of a possible 2623. 26 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	942/1017 (93%)	378/405 (93%)	375/414 (91%)	189/198 (95%)
Sidechain	882/1397 (63%)	543/815 (67%)	325/522 (62%)	14/60 (23%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	103/209 (49%)	85/109 (78%)	15/94 (16%)	3/6 (50%)
Overall	1927/2623 (73%)	1006/1329 (76%)	715/1030 (69%)	206/264 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1927 atoms were assigned a chemical shift out of a possible 2623. 26 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	942/1017 (93%)	378/405 (93%)	375/414 (91%)	189/198 (95%)
Sidechain	882/1397 (63%)	543/815 (67%)	325/522 (62%)	14/60 (23%)
Aromatic	103/209 (49%)	85/109 (78%)	15/94 (16%)	3/6 (50%)
Overall	1927/2623 (73%)	1006/1329 (76%)	715/1030 (69%)	206/264 (78%)

7.1.4 Statistically unusual chemical shifts (i)

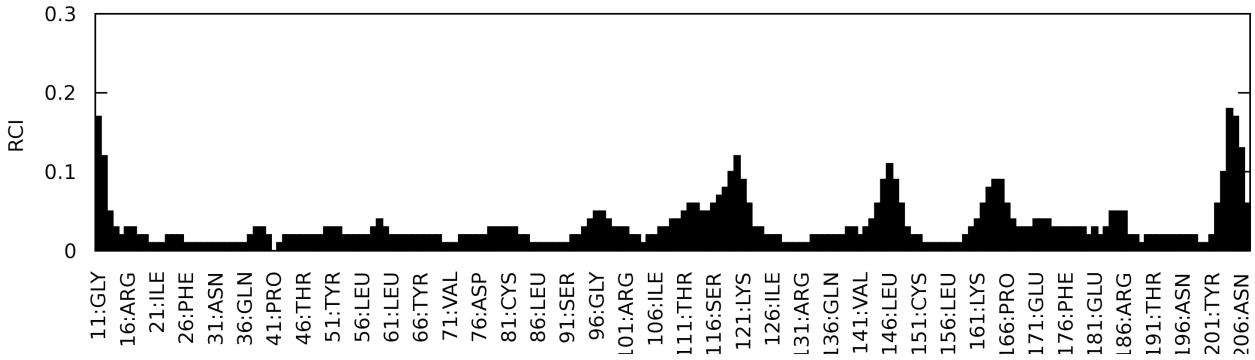
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	130	ILE	HB	-1.28	3.24 – 0.34	-10.6
1	A	161	LYS	CG	36.22	30.67 – 19.17	9.8
1	A	50	LYS	HD2	-0.61	2.76 – 0.46	-9.7
1	A	174	PRO	CD	42.09	55.31 – 45.41	-8.4
1	A	73	GLN	HG2	0.13	3.67 – 0.97	-8.1
1	A	33	ILE	CG1	17.22	36.54 – 18.94	-6.0
1	A	50	LYS	CD	22.33	34.86 – 23.06	-5.6
1	A	33	ILE	HG12	-0.80	3.27 – -0.73	-5.2
1	A	73	GLN	HE21	4.85	9.53 – 4.93	-5.2
1	A	77	TRP	HH2	5.01	8.94 – 5.04	-5.1
1	A	32	SER	HB2	5.18	5.18 – 2.58	5.0

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: BMRB entry 5299

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	70
Number of shifts mapped to atoms	70
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	5	0.19 ± 1.91	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	2	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	6	-1.96 ± 1.80	None needed (imprecise)

7.2.3 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 3%, i.e. 74 atoms were assigned a chemical shift out of a possible 2623. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	24/1017 (2%)	13/405 (3%)	5/414 (1%)	6/198 (3%)
Sidechain	22/1397 (2%)	20/815 (2%)	2/522 (0%)	0/60 (0%)
Aromatic	28/209 (13%)	14/109 (13%)	13/94 (14%)	1/6 (17%)
Overall	74/2623 (3%)	47/1329 (4%)	20/1030 (2%)	7/264 (3%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 3%, i.e. 74 atoms were assigned a chemical shift out of a possible 2623. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	24/1017 (2%)	13/405 (3%)	5/414 (1%)	6/198 (3%)
Sidechain	22/1397 (2%)	20/815 (2%)	2/522 (0%)	0/60 (0%)
Aromatic	28/209 (13%)	14/109 (13%)	13/94 (14%)	1/6 (17%)
Overall	74/2623 (3%)	47/1329 (4%)	20/1030 (2%)	7/264 (3%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B: