Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2L5Q
Title	:	Solution NMR Structure of BVU_3817 from Bacteroides vulgatus, Northeast Structural Genomics Consortium Target BvR159
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Deposited on	:	2010-11-03

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 (i)) were used in the production of this report:

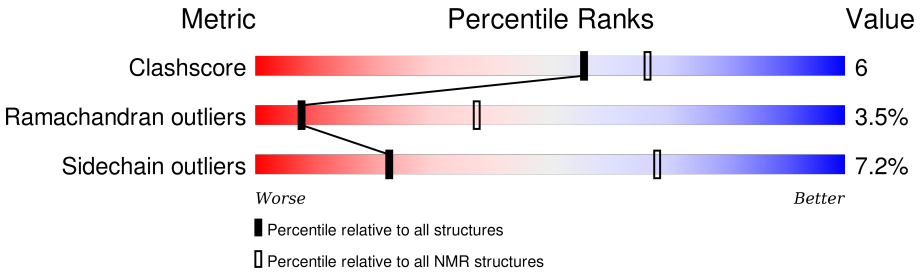
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 82%.

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	142	77% 14% 8%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:1-A:130 (130)	0.79	4

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 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2259 atoms, of which 1140 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2259	716	1140	193	207	3	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	LEU	-	EXPRESSION TAG	UNP A6L6W4
A	136	GLU	-	EXPRESSION TAG	UNP A6L6W4
A	137	HIS	-	EXPRESSION TAG	UNP A6L6W4
A	138	HIS	-	EXPRESSION TAG	UNP A6L6W4
A	139	HIS	-	EXPRESSION TAG	UNP A6L6W4
A	140	HIS	-	EXPRESSION TAG	UNP A6L6W4
A	141	HIS	-	EXPRESSION TAG	UNP A6L6W4
A	142	HIS	-	EXPRESSION TAG	UNP A6L6W4

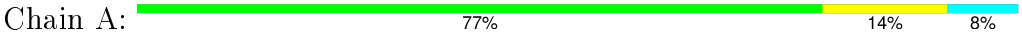
4 Residue-property plots (i)

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: Uncharacterized protein

Chain A:



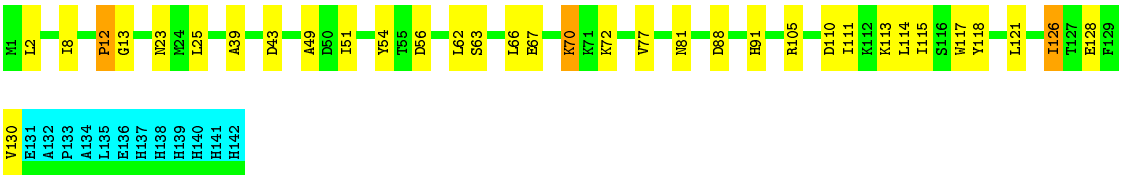
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Uncharacterized protein

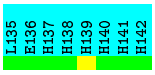
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Uncharacterized protein

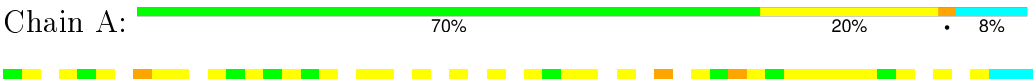
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Uncharacterized protein

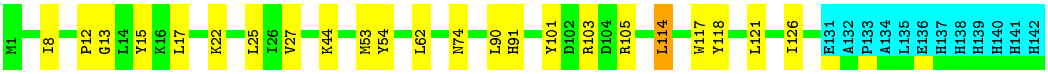
Chain A:



4.2.4 Score per residue for model 4 (medoid)

• Molecule 1: Uncharacterized protein

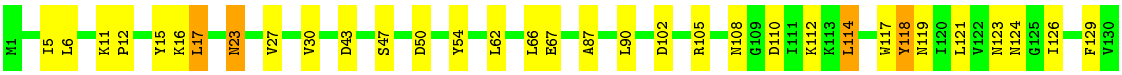
Chain A:

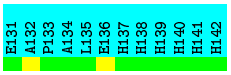


4.2.5 Score per residue for model 5

• Molecule 1: Uncharacterized protein

Chain A:

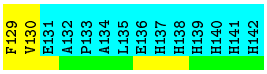




4.2.6 Score per residue for model 6

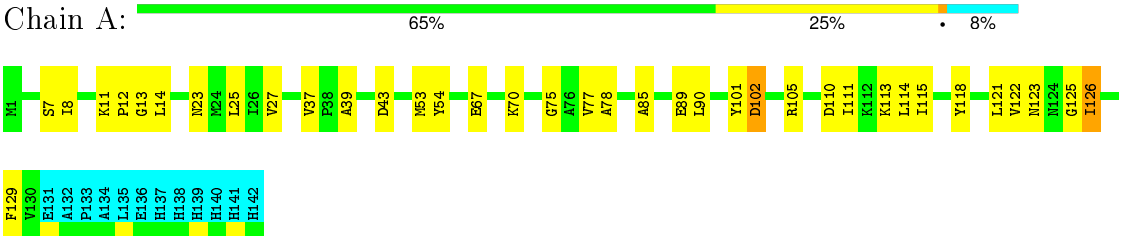
• Molecule 1: Uncharacterized protein

Chain A:



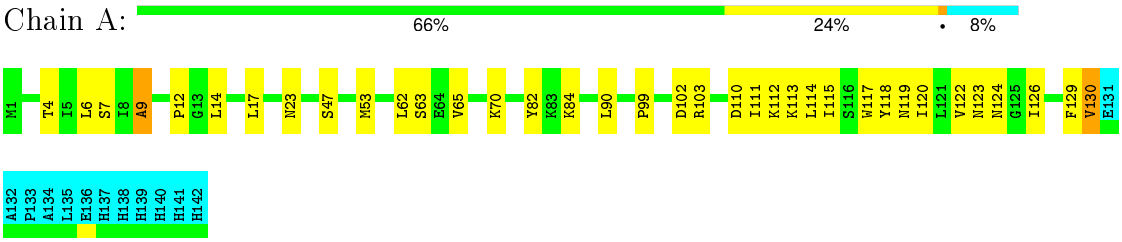
4.2.7 Score per residue for model 7

• Molecule 1: Uncharacterized protein



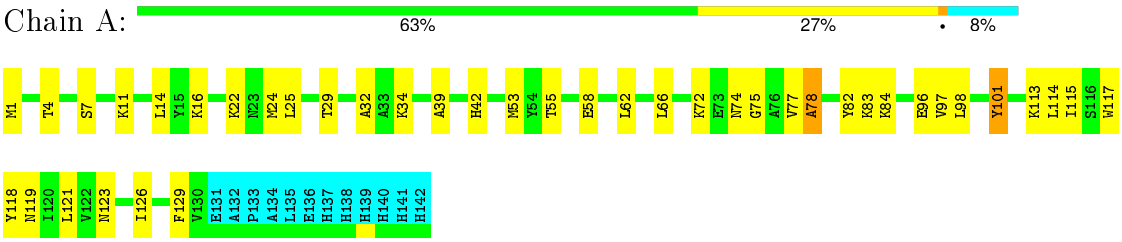
4.2.8 Score per residue for model 8

• Molecule 1: Uncharacterized protein



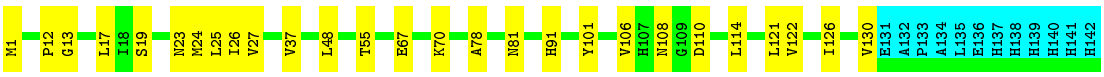
4.2.9 Score per residue for model 9

• Molecule 1: Uncharacterized protein



4.2.10 Score per residue for model 10

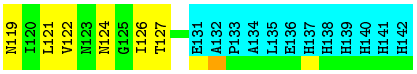
• Molecule 1: Uncharacterized protein



4.2.11 Score per residue for model 11

• Molecule 1: Uncharacterized protein

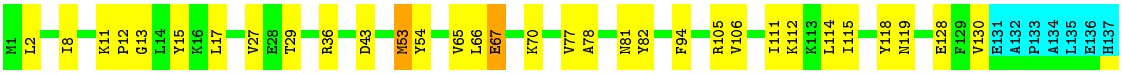
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Uncharacterized protein

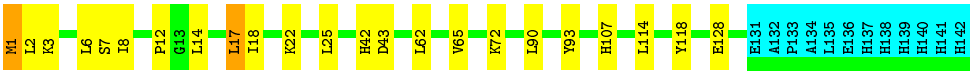
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Uncharacterized protein

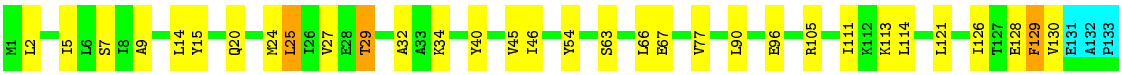
Chain A:

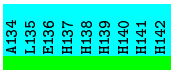


4.2.14 Score per residue for model 14

• Molecule 1: Uncharacterized protein

Chain A:

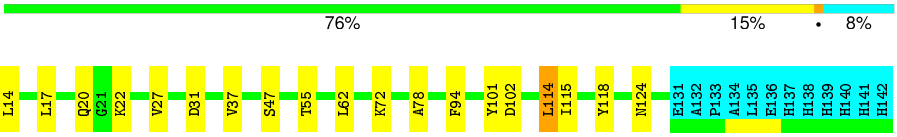




4.2.15 Score per residue for model 15

• Molecule 1: Uncharacterized protein

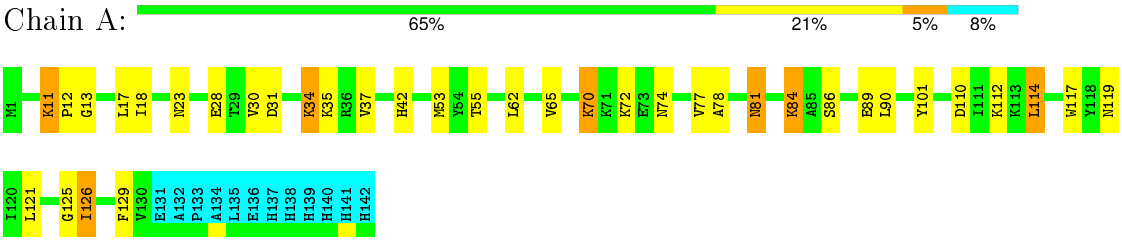
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Uncharacterized protein

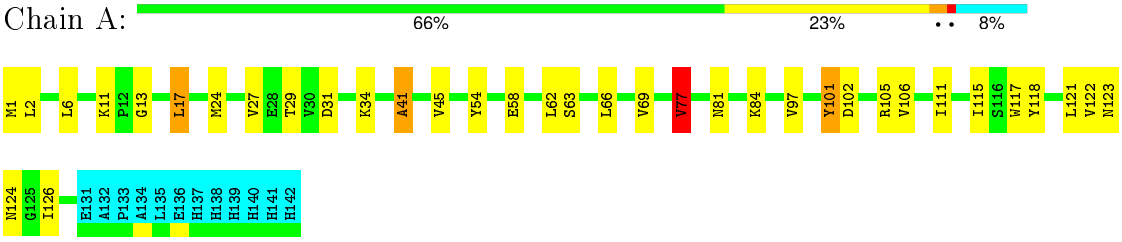
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Uncharacterized protein

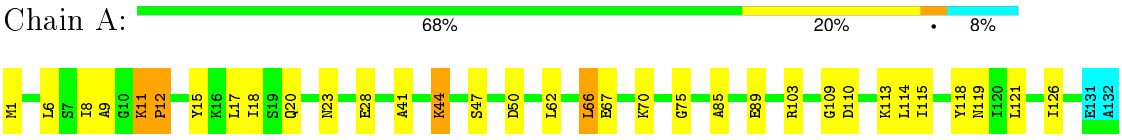
Chain A:

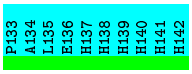


4.2.18 Score per residue for model 18

• Molecule 1: Uncharacterized protein

Chain A:

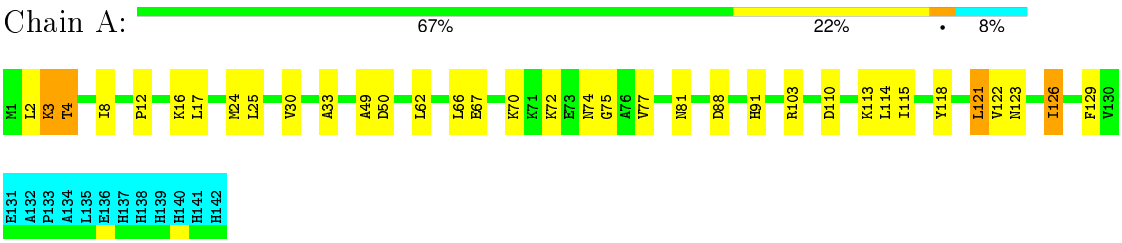




4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

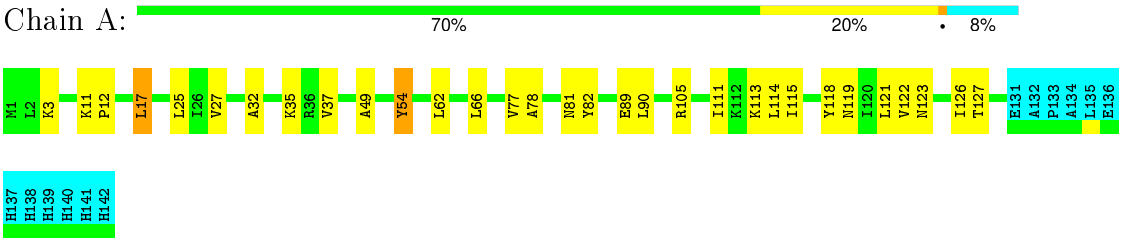
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein

Chain A:



5 Refinement protocol and experimental data overview

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
CNS	refinement	
CNS	structure solution	
CNS	geometry optimization	
CYANA	refinement	3.0
CYANA	geometry optimization	3.0
CYANA	structure solution	3.0
TALOS+	geometry optimization	
PALES	geometry optimization	

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 17280
Number of chemical shift lists	1
Total number of shifts	1566
Number of shifts mapped to atoms	1566
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

6 Model quality

6.1 Standard geometry

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	0.46±0.01	0±0/1034 (0.0±0.0%)	0.60±0.02	0±0/1400 (0.0±0.0%)
All	All	0.46	0/20680 (0.0%)	0.60	3/28000 (0.0%)

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	A	118	TYR	CB-CG-CD1	5.74	124.44	121.00	7	1
1	A	118	TYR	CB-CG-CD2	-5.60	117.64	121.00	7	2

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	1016	1052	1049	13±3
All	All	20320	21040	20980	263

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:GLU:HG2	1:A:130:VAL:HA	0.79	1.53	1	2
1:A:54:TYR:HB2	1:A:105:ARG:HB3	0.79	1.53	12	7
1:A:82:TYR:HB3	1:A:115:ILE:HB	0.78	1.54	9	5
1:A:62:LEU:HD11	1:A:114:LEU:HD12	0.74	1.58	4	9
1:A:70:LYS:HA	1:A:70:LYS:HE3	0.71	1.60	1	2
1:A:121:LEU:HG	1:A:126:ILE:HG13	0.70	1.64	16	1
1:A:1:MET:HA	1:A:128:GLU:HB3	0.69	1.65	13	2
1:A:15:TYR:HB3	1:A:27:VAL:HB	0.68	1.64	3	5
1:A:63:SER:HA	1:A:66:LEU:HD12	0.67	1.67	1	3
1:A:54:TYR:HB3	1:A:105:ARG:HB3	0.67	1.65	20	1
1:A:110:ASP:HA	1:A:113:LYS:HE2	0.67	1.67	18	4
1:A:90:LEU:HG	1:A:112:LYS:HG2	0.67	1.65	2	2
1:A:121:LEU:HA	1:A:126:ILE:HD12	0.65	1.69	18	9
1:A:90:LEU:HG	1:A:112:LYS:HE3	0.64	1.70	3	1
1:A:5:ILE:HG13	1:A:126:ILE:HG23	0.64	1.68	5	1
1:A:17:LEU:HA	1:A:27:VAL:HG12	0.64	1.69	10	4
1:A:54:TYR:HB2	1:A:105:ARG:HD3	0.64	1.70	1	2
1:A:77:VAL:HG13	1:A:122:VAL:HB	0.63	1.70	7	2
1:A:2:LEU:H	1:A:128:GLU:HB3	0.62	1.53	12	1
1:A:70:LYS:HE2	1:A:122:VAL:HG21	0.62	1.70	8	1
1:A:118:TYR:HA	1:A:121:LEU:HD12	0.62	1.70	1	2
1:A:27:VAL:HG23	1:A:37:VAL:HG23	0.61	1.71	7	2
1:A:6:LEU:HG	1:A:47:SER:HA	0.60	1.72	15	1
1:A:55:THR:HA	1:A:101:TYR:HA	0.60	1.73	9	2
1:A:7:SER:HA	1:A:14:LEU:HD23	0.60	1.74	14	6
1:A:85:ALA:HB1	1:A:89:GLU:HG2	0.59	1.73	7	1
1:A:53:MET:HE1	1:A:110:ASP:HB3	0.58	1.75	16	1
1:A:9:ALA:HB2	1:A:44:LYS:H	0.58	1.59	18	1
1:A:67:GLU:HG3	1:A:130:VAL:HB	0.58	1.75	12	1
1:A:106:VAL:HG13	1:A:110:ASP:HB2	0.57	1.76	6	1
1:A:73:GLU:HG3	1:A:76:ALA:HB3	0.57	1.76	6	1
1:A:8:ILE:HG21	1:A:12:PRO:HG2	0.57	1.77	1	3
1:A:62:LEU:O	1:A:66:LEU:HG	0.57	1.99	1	6
1:A:11:LYS:HB3	1:A:12:PRO:HD3	0.56	1.77	16	3
1:A:70:LYS:HE2	1:A:122:VAL:HG22	0.56	1.77	10	1
1:A:5:ILE:HB	1:A:128:GLU:HG3	0.56	1.76	14	1
1:A:121:LEU:HD12	1:A:126:ILE:HD12	0.56	1.76	6	1
1:A:67:GLU:CG	1:A:130:VAL:HA	0.56	2.31	10	1
1:A:29:THR:O	1:A:34:LYS:HA	0.55	2.01	11	2
1:A:6:LEU:HD13	1:A:47:SER:HA	0.55	1.79	8	2
1:A:47:SER:HB3	1:A:50:ASP:HB2	0.55	1.77	5	1
1:A:115:ILE:HA	1:A:118:TYR:CD2	0.54	2.37	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HB2	1:A:39:ALA:HB3	0.54	1.80	11	4
1:A:70:LYS:HD2	1:A:130:VAL:HB	0.54	1.79	8	1
1:A:121:LEU:HD23	1:A:126:ILE:HG13	0.53	1.79	7	2
1:A:121:LEU:HD23	1:A:126:ILE:HD12	0.53	1.79	4	2
1:A:48:LEU:HA	1:A:51:ILE:HD12	0.53	1.78	2	1
1:A:69:VAL:HA	1:A:97:VAL:HG21	0.53	1.79	17	1
1:A:78:ALA:HA	1:A:118:TYR:HD2	0.53	1.62	11	1
1:A:19:SER:HB2	1:A:26:ILE:HB	0.52	1.79	10	1
1:A:3:LYS:HA	1:A:49:ALA:HB2	0.52	1.80	19	1
1:A:82:TYR:HA	1:A:90:LEU:HD21	0.52	1.81	11	1
1:A:17:LEU:HD21	1:A:20:GLN:HG3	0.52	1.80	11	1
1:A:55:THR:HA	1:A:102:ASP:HB2	0.52	1.80	15	1
1:A:117:TRP:O	1:A:121:LEU:HB2	0.52	2.05	16	1
1:A:3:LYS:H	1:A:49:ALA:HB2	0.52	1.64	20	1
1:A:67:GLU:OE1	1:A:130:VAL:HB	0.52	2.05	14	1
1:A:30:VAL:HG21	1:A:126:ILE:HD13	0.51	1.83	16	1
1:A:95:ALA:HA	1:A:98:LEU:O	0.51	2.06	6	1
1:A:90:LEU:HD21	1:A:111:ILE:HB	0.51	1.81	14	2
1:A:35:LYS:HE2	1:A:37:VAL:HG22	0.50	1.82	16	3
1:A:14:LEU:HD13	1:A:121:LEU:HD13	0.50	1.81	3	1
1:A:31:ASP:HA	1:A:34:LYS:HE2	0.50	1.83	16	1
1:A:8:ILE:HG13	1:A:15:TYR:HD2	0.50	1.67	12	4
1:A:8:ILE:HG13	1:A:15:TYR:CD2	0.50	2.42	4	2
1:A:66:LEU:HB3	1:A:114:LEU:HD11	0.49	1.84	12	1
1:A:66:LEU:HD13	1:A:114:LEU:HG	0.49	1.84	9	1
1:A:6:LEU:HD22	1:A:17:LEU:HG	0.49	1.84	13	1
1:A:117:TRP:O	1:A:121:LEU:HG	0.49	2.07	5	5
1:A:86:SER:HB3	1:A:89:GLU:HG2	0.49	1.85	16	1
1:A:101:TYR:HD1	1:A:106:VAL:HB	0.49	1.68	17	1
1:A:78:ALA:HA	1:A:118:TYR:CD1	0.48	2.43	9	1
1:A:62:LEU:HD12	1:A:65:VAL:HB	0.48	1.85	8	1
1:A:77:VAL:HG12	1:A:119:ASN:HA	0.48	1.84	16	2
1:A:85:ALA:HB1	1:A:89:GLU:HB2	0.48	1.85	18	1
1:A:119:ASN:O	1:A:123:ASN:HB2	0.48	2.08	20	4
1:A:77:VAL:HG23	1:A:119:ASN:HA	0.48	1.84	12	1
1:A:65:VAL:HB	1:A:94:PHE:CE1	0.48	2.44	12	1
1:A:62:LEU:HG	1:A:114:LEU:HD12	0.47	1.85	2	1
1:A:111:ILE:O	1:A:115:ILE:HG12	0.47	2.09	8	7
1:A:115:ILE:HA	1:A:118:TYR:HB2	0.47	1.84	2	1
1:A:11:LYS:HB2	1:A:12:PRO:HD3	0.47	1.86	11	1
1:A:9:ALA:HB3	1:A:12:PRO:HD2	0.47	1.86	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HA	1:A:126:ILE:CG1	0.47	2.40	5	3
1:A:17:LEU:HD11	1:A:20:GLN:HG3	0.47	1.86	18	2
1:A:70:LYS:HG2	1:A:75:GLY:HA2	0.47	1.85	7	2
1:A:16:LYS:HE3	1:A:30:VAL:HG13	0.47	1.87	5	1
1:A:67:GLU:HB2	1:A:129:PHE:HD2	0.47	1.68	5	2
1:A:77:VAL:HA	1:A:122:VAL:HG21	0.47	1.86	17	2
1:A:87:ALA:HA	1:A:108:ASN:ND2	0.47	2.25	3	1
1:A:62:LEU:HD12	1:A:65:VAL:HG23	0.46	1.86	16	1
1:A:6:LEU:HD11	1:A:17:LEU:HD13	0.46	1.87	11	2
1:A:62:LEU:HD21	1:A:114:LEU:HB2	0.46	1.88	15	1
1:A:82:TYR:HB3	1:A:115:ILE:CB	0.46	2.36	9	1
1:A:7:SER:HB2	1:A:46:ILE:HB	0.46	1.87	14	1
1:A:117:TRP:HA	1:A:120:ILE:HD12	0.46	1.87	8	1
1:A:25:LEU:HD11	1:A:45:VAL:HG11	0.46	1.86	14	1
1:A:31:ASP:HB2	1:A:124:ASN:HD21	0.46	1.71	17	2
1:A:81:ASN:HB3	1:A:84:LYS:HE3	0.46	1.87	16	1
1:A:51:ILE:HG21	1:A:62:LEU:HD22	0.46	1.88	1	1
1:A:66:LEU:HD12	1:A:114:LEU:HG	0.46	1.86	11	1
1:A:2:LEU:HD23	1:A:2:LEU:H	0.45	1.71	19	1
1:A:88:ASP:HA	1:A:91:HIS:CE1	0.45	2.46	1	2
1:A:70:LYS:HE2	1:A:122:VAL:CG2	0.45	2.40	8	1
1:A:91:HIS:HA	1:A:101:TYR:OH	0.45	2.11	4	2
1:A:1:MET:HG2	1:A:2:LEU:H	0.45	1.72	17	1
1:A:90:LEU:HD23	1:A:112:LYS:HA	0.45	1.87	16	1
1:A:66:LEU:HD21	1:A:121:LEU:HD21	0.45	1.87	6	1
1:A:18:ILE:HD11	1:A:28:GLU:HB3	0.45	1.87	16	2
1:A:90:LEU:HA	1:A:93:TYR:CE2	0.45	2.46	13	1
1:A:4:THR:O	1:A:16:LYS:HA	0.45	2.11	9	2
1:A:55:THR:OG1	1:A:101:TYR:HA	0.44	2.12	10	1
1:A:78:ALA:HB2	1:A:118:TYR:CD2	0.44	2.47	15	1
1:A:77:VAL:HA	1:A:122:VAL:HB	0.44	1.89	20	1
1:A:106:VAL:HG23	1:A:108:ASN:H	0.44	1.72	10	1
1:A:65:VAL:HB	1:A:94:PHE:HE1	0.44	1.71	12	2
1:A:62:LEU:O	1:A:66:LEU:HB3	0.44	2.12	11	2
1:A:41:ALA:HA	1:A:45:VAL:HB	0.44	1.90	17	1
1:A:69:VAL:HG11	1:A:94:PHE:HA	0.44	1.89	11	1
1:A:6:LEU:HD13	1:A:17:LEU:HD12	0.44	1.87	13	2
1:A:70:LYS:HE3	1:A:75:GLY:HA2	0.44	1.88	18	1
1:A:63:SER:HA	1:A:129:PHE:CE1	0.43	2.48	8	1
1:A:44:LYS:HE3	1:A:44:LYS:HA	0.43	1.89	18	1
1:A:14:LEU:HD11	1:A:117:TRP:HB3	0.43	1.89	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:THR:HG22	1:A:58:GLU:HB2	0.43	1.90	9	1
1:A:6:LEU:HD21	1:A:45:VAL:HG13	0.43	1.90	2	2
1:A:13:GLY:HA3	1:A:120:ILE:HD13	0.43	1.91	3	1
1:A:78:ALA:HA	1:A:118:TYR:CE2	0.43	2.49	12	1
1:A:29:THR:HB	1:A:34:LYS:HA	0.42	1.91	14	1
1:A:121:LEU:HB3	1:A:129:PHE:CE2	0.42	2.48	14	1
1:A:6:LEU:HB2	1:A:17:LEU:HB2	0.42	1.91	2	1
1:A:102:ASP:HB3	1:A:105:ARG:HB2	0.42	1.90	7	1
1:A:62:LEU:HA	1:A:65:VAL:HG22	0.42	1.92	13	1
1:A:6:LEU:HD22	1:A:47:SER:HA	0.42	1.90	5	1
1:A:113:LYS:HD3	1:A:117:TRP:CH2	0.42	2.49	9	1
1:A:53:MET:HB2	1:A:106:VAL:HA	0.42	1.90	12	1
1:A:70:LYS:HB2	1:A:118:TYR:HE1	0.42	1.75	12	1
1:A:20:GLN:HA	1:A:25:LEU:HB3	0.41	1.90	14	1
1:A:2:LEU:HB3	1:A:49:ALA:HA	0.41	1.91	1	1
1:A:121:LEU:HA	1:A:126:ILE:HG12	0.41	1.91	16	1
1:A:7:SER:HB2	1:A:117:TRP:CZ2	0.41	2.51	3	1
1:A:6:LEU:HG	1:A:17:LEU:HB2	0.41	1.91	5	1
1:A:82:TYR:HB2	1:A:112:LYS:HD3	0.41	1.92	12	1
1:A:90:LEU:HD12	1:A:112:LYS:HE3	0.41	1.92	8	1
1:A:24:MET:HB3	1:A:40:TYR:CD1	0.41	2.51	14	1
1:A:18:ILE:HD11	1:A:28:GLU:HG3	0.41	1.92	6	1
1:A:97:VAL:HG23	1:A:98:LEU:HG	0.41	1.92	9	1
1:A:114:LEU:HD23	1:A:115:ILE:HD13	0.41	1.91	19	1
1:A:27:VAL:HG23	1:A:37:VAL:HB	0.41	1.92	15	1
1:A:47:SER:HB2	1:A:50:ASP:HB2	0.41	1.92	18	1
1:A:16:LYS:HE2	1:A:30:VAL:HG13	0.40	1.93	19	1
1:A:90:LEU:HD12	1:A:111:ILE:HG22	0.40	1.93	7	1
1:A:72:LYS:HG2	1:A:96:GLU:HG3	0.40	1.93	9	1
1:A:87:ALA:HA	1:A:90:LEU:HB2	0.40	1.93	5	1
1:A:114:LEU:O	1:A:118:TYR:HB2	0.40	2.16	20	1
1:A:8:ILE:HG23	1:A:43:ASP:HB3	0.40	1.92	13	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	129/142 (91%)	109±3 (85±3%)	15±3 (12±2%)	5±2 (3±2%)	8 37
All	All	2580/2840 (91%)	2189 (85%)	301 (12%)	90 (3%)	8 37

All 25 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	13	GLY	9
1	A	23	ASN	9
1	A	12	PRO	9
1	A	81	ASN	7
1	A	78	ALA	7
1	A	11	LYS	6
1	A	126	ILE	6
1	A	32	ALA	5
1	A	74	ASN	3
1	A	129	PHE	3
1	A	77	VAL	3
1	A	42	HIS	3
1	A	41	ALA	2
1	A	22	LYS	2
1	A	108	ASN	2
1	A	130	VAL	2
1	A	3	LYS	2
1	A	102	ASP	2
1	A	9	ALA	2
1	A	107	HIS	1
1	A	33	ALA	1
1	A	75	GLY	1
1	A	34	LYS	1
1	A	109	GLY	1
1	A	58	GLU	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	109/119 (92%)	101±2 (93±2%)	8±2 (7±2%)	23 68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2180/2380 (92%)	2024 (93%)	156 (7%)	23 68

All 55 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	114	LEU	12
1	A	118	TYR	8
1	A	25	LEU	8
1	A	17	LEU	8
1	A	53	MET	6
1	A	110	ASP	5
1	A	29	THR	5
1	A	84	LYS	5
1	A	72	LYS	5
1	A	101	TYR	5
1	A	123	ASN	4
1	A	24	MET	4
1	A	67	GLU	4
1	A	43	ASP	4
1	A	113	LYS	4
1	A	103	ARG	4
1	A	1	MET	4
1	A	22	LYS	3
1	A	44	LYS	3
1	A	124	ASN	3
1	A	102	ASP	3
1	A	77	VAL	3
1	A	2	LEU	3
1	A	81	ASN	2
1	A	96	GLU	2
1	A	98	LEU	2
1	A	129	PHE	2
1	A	23	ASN	2
1	A	70	LYS	2
1	A	66	LEU	2
1	A	36	ARG	2
1	A	119	ASN	2
1	A	89	GLU	2
1	A	4	THR	2
1	A	11	LYS	1
1	A	69	VAL	1

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Mol	Chain	Res	Type	Models (Total)
1	A	83	LYS	1
1	A	56	ASP	1
1	A	99	PRO	1
1	A	108	ASN	1
1	A	31	ASP	1
1	A	128	GLU	1
1	A	48	LEU	1
1	A	74	ASN	1
1	A	50	ASP	1
1	A	18	ILE	1
1	A	94	PHE	1
1	A	107	HIS	1
1	A	90	LEU	1
1	A	121	LEU	1
1	A	34	LYS	1
1	A	5	ILE	1
1	A	54	TYR	1
1	A	3	LYS	1
1	A	12	PRO	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

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 82% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17280

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	1566
Number of shifts mapped to atoms	1566
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	131	0.06 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	125	0.42 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	130	-0.01 ± 0.16	None needed (< 0.5 ppm)
^{15}N	117	0.55 ± 0.47	None needed (imprecise)

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 82%, i.e. 1303 atoms were assigned a chemical shift out of a possible 1594. 20 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	593/642 (92%)	235/256 (92%)	247/260 (95%)	111/126 (88%)
Sidechain	643/842 (76%)	387/488 (79%)	249/322 (77%)	7/32 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	67/110 (61%)	43/56 (77%)	23/47 (49%)	1/7 (14%)
Overall	1303/1594 (82%)	665/800 (83%)	519/629 (83%)	119/165 (72%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 78%, i.e. 1367 atoms were assigned a chemical shift out of a possible 1754. 21 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	625/700 (89%)	247/279 (89%)	261/284 (92%)	117/137 (85%)
Sidechain	675/896 (75%)	406/521 (78%)	262/343 (76%)	7/32 (22%)
Aromatic	67/158 (42%)	43/80 (54%)	23/59 (39%)	1/19 (5%)
Overall	1367/1754 (78%)	696/880 (79%)	546/686 (80%)	125/188 (66%)

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	89	GLU	CG	25.31	42.24 – 29.94	-8.8

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: