



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 07:52 pm GMT

PDB ID : 1SE9
Title : Structure of At3g01050, a ubiquitin-fold protein from Arabidopsis thaliana
Authors : Volkman, B.F.; Lytle, B.L.; Peterson, F.C.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2004-02-16

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 ⓘ 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 : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

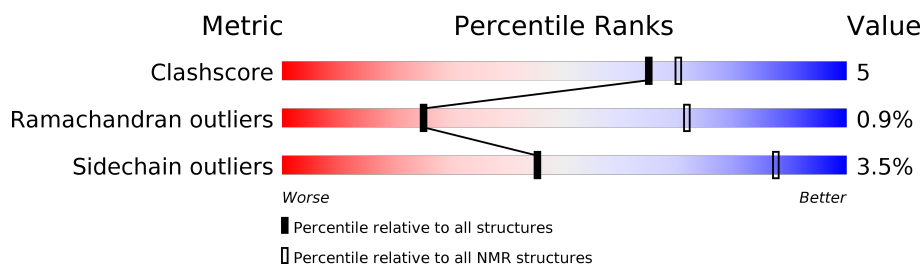
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	126	<div> <div style="width: 59%; background-color: green;"></div> <div style="width: 17%; background-color: cyan;"></div> <div style="width: 20%; background-color: grey;"></div> </div> <div>59% . 17% 20%</div>

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:7-A:75, A:85-A:94 (79)	0.52	19

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1583 atoms, of which 805 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called ubiquitin family.

Mol	Chain	Residues	Atoms						Trace
1	A	101	Total	C	H	N	O	S	0
			1583	490	805	133	154	1	

There are 10 discrepancies between the modelled and reference sequences:

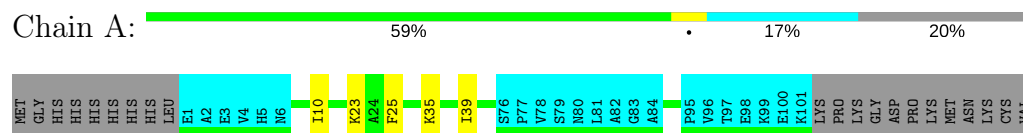
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	INSERTION	UNP Q9MAB9
A	-7	GLY	-	INSERTION	UNP Q9MAB9
A	-6	HIS	-	INSERTION	UNP Q9MAB9
A	-5	HIS	-	INSERTION	UNP Q9MAB9
A	-4	HIS	-	INSERTION	UNP Q9MAB9
A	-3	HIS	-	INSERTION	UNP Q9MAB9
A	-2	HIS	-	INSERTION	UNP Q9MAB9
A	-1	HIS	-	INSERTION	UNP Q9MAB9
A	0	LEU	-	INSERTION	UNP Q9MAB9
A	1	GLU	-	INSERTION	UNP Q9MAB9

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: ubiquitin family

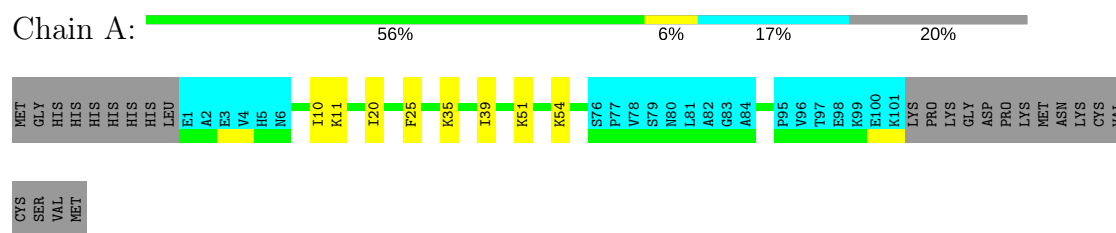


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

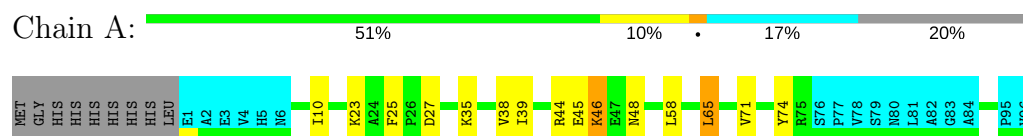
4.2.1 Score per residue for model 1

- Molecule 1: ubiquitin family



4.2.2 Score per residue for model 2

- Molecule 1: ubiquitin family



LYS
PRO
LYS
GLY
GLY
ASP
PRO
LYS
MET
ASN
LYS
CYS
VAL
CYS
SER
VAL
MET

4.2.3 Score per residue for model 3

- Molecule 1: ubiquitin family

Chain A: 54% 9% 17% 20%

MET GLY HIS HIS HIS HIS HIS LEU E1 A2 E3 V4 H5 N6 I10 K11 I20 F25 K35 V38 W42 P50 K51 V71 R75 S76 P77 V78 S79 N80 L81 A82 G83 A84 P95 V96 T97 E98 K99 E100 K101 LYS PRO LYS GLY ASP PRO LYS MET

ASN
LYS
CYS
VAL
SER
VAL
MET

4.2.4 Score per residue for model 4

- Molecule 1: ubiquitin family

Chain A: 51% 11% 17% 20%

MET GLY HIS HIS HIS HIS HIS LEU E1 A2 E3 V4 H5 N6 Q7 L8 E9 I10 K23 A24 F25 K35 I39 E47 N48 K51 L58 I59 L65 S76 P77 V78 S79 N80 L81 A82 G83 A84 M88 I91 P95 V96 T97 E98 K99 E100 K101 LYS

PRO
LYS
GLY
ASP
PRO
LYS
MET
ASN
LYS
CYS
VAL
CYS
SER
VAL
MET

4.2.5 Score per residue for model 5

- Molecule 1: ubiquitin family

Chain A: 48% 14% 17% 20%

MET GLY HIS HIS HIS HIS HIS LEU E1 A2 E3 V4 H5 N6 I10 E9 I11 K11 T15 I20 K23 A24 F25 S32 K35 E36 I39 R44 N48 L65 T70 Y74 R75 S76 P77 V78 S79 N80 L81 A82 G83 A84 M88 H89 P95 V96

T97 E98 K99 E100 K101 LYS PRO LYS ASP PRO LYS MET ASN LYS CYS VAL CYS SER VAL MET

4.2.6 Score per residue for model 6

- Molecule 1: ubiquitin family

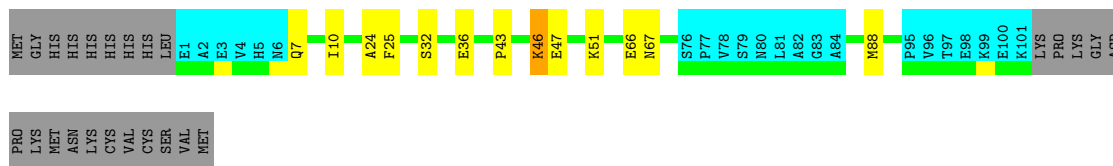
Chain A: 52% 10% 17% 20%



4.2.7 Score per residue for model 7

- Molecule 1: ubiquitin family

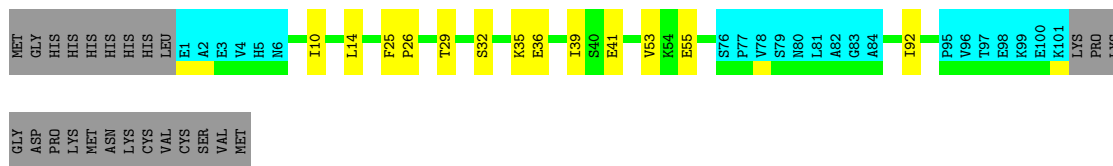
Chain A: 52% 10% 17% 20%



4.2.8 Score per residue for model 8

- Molecule 1: ubiquitin family

Chain A: 52% 10% 17% 20%



4.2.9 Score per residue for model 9

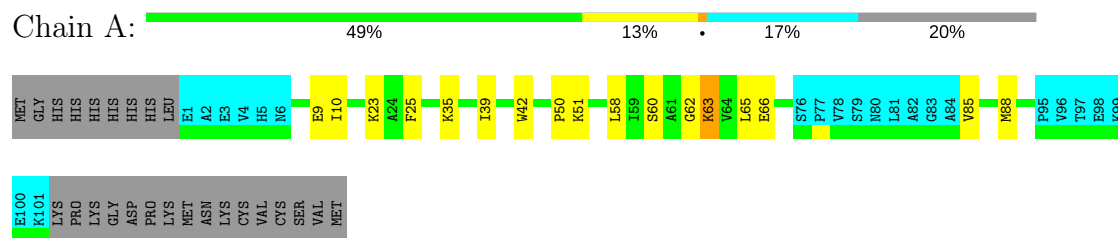
- Molecule 1: ubiquitin family

Chain A: 48% 13% 17% 20%



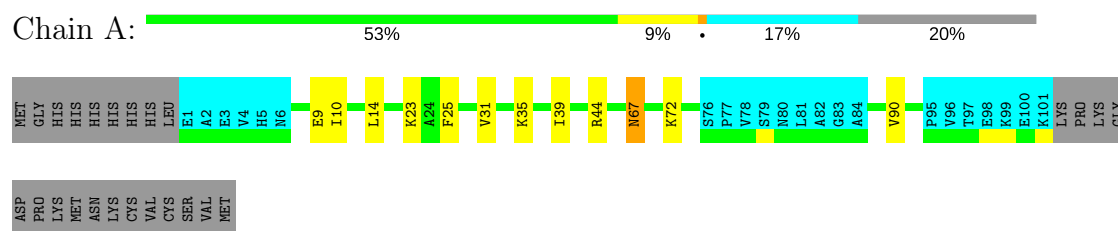
4.2.10 Score per residue for model 10

- Molecule 1: ubiquitin family



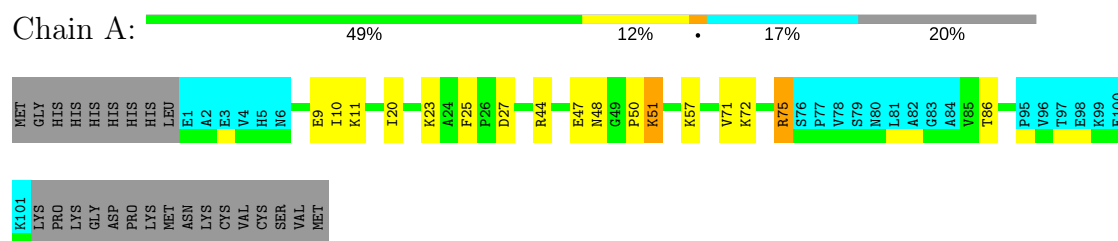
4.2.11 Score per residue for model 11

- Molecule 1: ubiquitin family



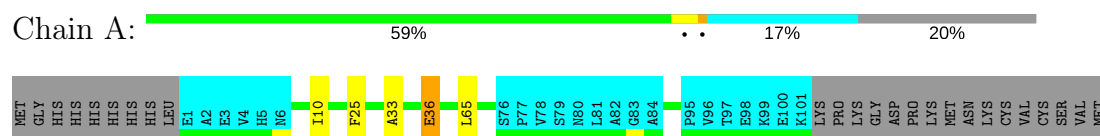
4.2.12 Score per residue for model 12

- Molecule 1: ubiquitin family



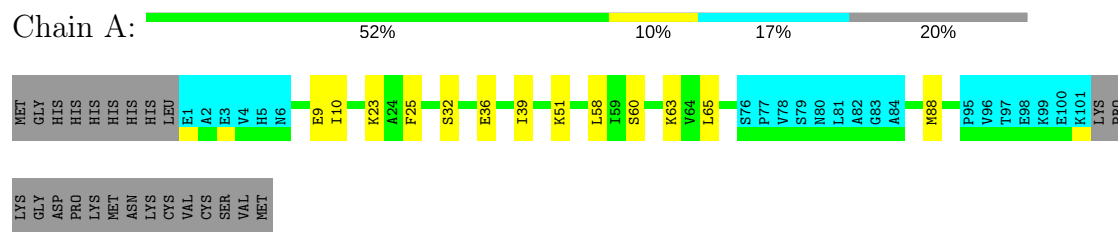
4.2.13 Score per residue for model 13

- Molecule 1: ubiquitin family



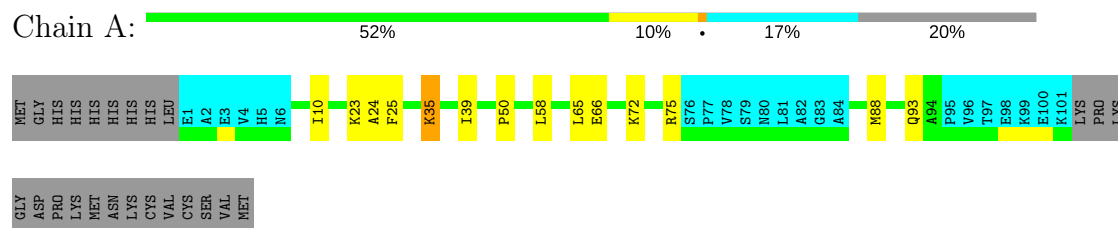
4.2.14 Score per residue for model 14

- Molecule 1: ubiquitin family



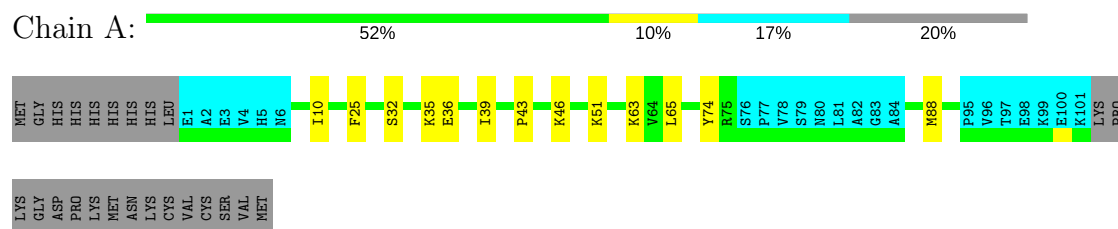
4.2.15 Score per residue for model 15

- Molecule 1: ubiquitin family



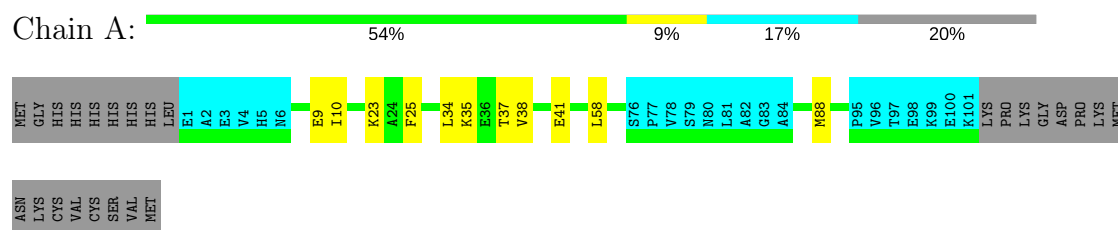
4.2.16 Score per residue for model 16

- Molecule 1: ubiquitin family



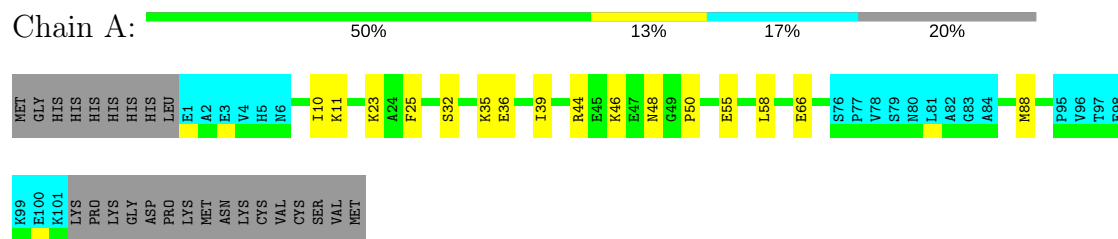
4.2.17 Score per residue for model 17

- Molecule 1: ubiquitin family



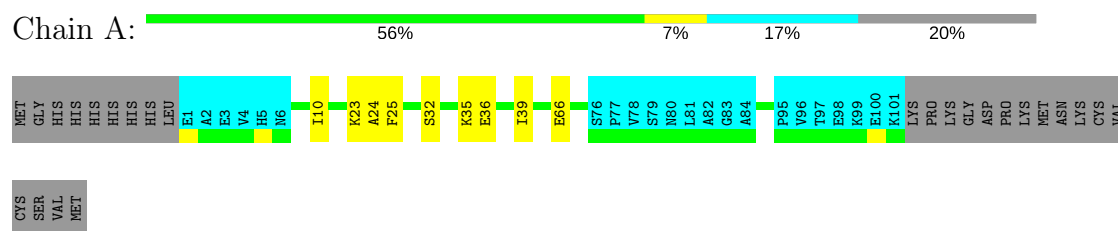
4.2.18 Score per residue for model 18

- Molecule 1: ubiquitin family



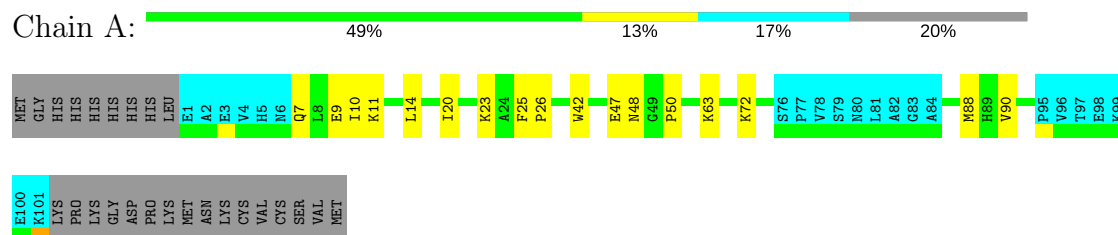
4.2.19 Score per residue for model 19 (medoid)

- Molecule 1: ubiquitin family



4.2.20 Score per residue for model 20

- Molecule 1: ubiquitin family



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics followed by cartesian molecular dynamics in explicit solvent*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	refinement	1.0.6
XPLOR-NIH	refinement	2.0.6

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 6128
Number of chemical shift lists	1
Total number of shifts	1287
Number of shifts mapped to atoms	1287
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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.

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 [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	617	648	647	6±2
All	All	12340	12960	12940	122

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ASP:O	1:A:71:VAL:HB	0.64	1.93	2	1
1:A:58:LEU:HD11	1:A:88:MET:SD	0.62	2.35	10	3
1:A:10:ILE:HB	1:A:25:PHE:CE1	0.60	2.32	7	20
1:A:11:LYS:HB2	1:A:20:ILE:O	0.55	2.02	12	5
1:A:35:LYS:CD	1:A:53:VAL:HG13	0.55	2.31	9	2
1:A:9:GLU:HA	1:A:23:LYS:O	0.54	2.03	12	10
1:A:33:ALA:O	1:A:36:GLU:HG3	0.52	2.04	13	1
1:A:35:LYS:O	1:A:38:VAL:HG12	0.52	2.04	2	2
1:A:72:LYS:O	1:A:75:ARG:HG2	0.52	2.05	15	1
1:A:65:LEU:HB3	1:A:74:TYR:CE1	0.51	2.41	2	1
1:A:10:ILE:HA	1:A:86:THR:O	0.51	2.05	12	1
1:A:34:LEU:O	1:A:38:VAL:HG23	0.50	2.06	17	1
1:A:35:LYS:O	1:A:39:ILE:HG12	0.50	2.06	2	5
1:A:10:ILE:HB	1:A:25:PHE:CD1	0.50	2.40	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LYS:O	1:A:39:ILE:HG13	0.50	2.07	8	7
1:A:39:ILE:HG12	1:A:51:LYS:O	0.50	2.07	16	2
1:A:69:LYS:HA	1:A:69:LYS:HE3	0.50	1.84	9	1
1:A:35:LYS:HD2	1:A:53:VAL:HG13	0.49	1.85	8	2
1:A:65:LEU:HD12	1:A:74:TYR:CD1	0.48	2.43	5	1
1:A:32:SER:O	1:A:36:GLU:HG2	0.48	2.08	7	7
1:A:31:VAL:HB	1:A:67:ASN:HA	0.48	1.86	11	3
1:A:42:TRP:CD1	1:A:50:PRO:HG3	0.48	2.43	10	1
1:A:65:LEU:HG	1:A:74:TYR:CE2	0.48	2.44	16	1
1:A:71:VAL:O	1:A:75:ARG:HG3	0.47	2.08	3	2
1:A:23:LYS:HD3	1:A:24:ALA:N	0.47	2.24	15	2
1:A:58:LEU:HB3	1:A:88:MET:SD	0.47	2.50	17	2
1:A:35:LYS:HA	1:A:38:VAL:HG12	0.46	1.86	3	2
1:A:15:THR:HA	1:A:89:HIS:NE2	0.46	2.25	5	1
1:A:44:ARG:O	1:A:51:LYS:HE2	0.46	2.11	12	1
1:A:43:PRO:O	1:A:46:LYS:HD2	0.45	2.10	9	1
1:A:27:ASP:O	1:A:72:LYS:HB2	0.45	2.11	12	1
1:A:58:LEU:HD12	1:A:65:LEU:HD12	0.45	1.88	14	1
1:A:93:GLN:HA	1:A:93:GLN:OE1	0.45	2.12	15	1
1:A:44:ARG:HD2	1:A:45:GLU:N	0.44	2.28	2	1
1:A:47:GLU:HG2	1:A:48:ASN:N	0.44	2.28	4	1
1:A:14:LEU:HA	1:A:90:VAL:CG1	0.43	2.43	20	1
1:A:9:GLU:O	1:A:85:VAL:HA	0.43	2.13	10	1
1:A:72:LYS:HA	1:A:72:LYS:HE3	0.43	1.88	6	1
1:A:23:LYS:HB3	1:A:25:PHE:CE1	0.43	2.48	18	1
1:A:37:THR:O	1:A:41:GLU:HG2	0.43	2.14	17	1
1:A:7:GLN:OE1	1:A:26:PRO:HA	0.43	2.13	20	1
1:A:46:LYS:HA	1:A:46:LYS:HE3	0.43	1.89	2	1
1:A:43:PRO:HB2	1:A:46:LYS:CG	0.42	2.44	16	1
1:A:42:TRP:CZ2	1:A:50:PRO:HD2	0.42	2.50	20	2
1:A:26:PRO:HD2	1:A:29:THR:OG1	0.42	2.14	9	2
1:A:43:PRO:O	1:A:46:LYS:HB3	0.42	2.15	7	1
1:A:59:ILE:HD12	1:A:91:ILE:HD12	0.41	1.92	4	1
1:A:62:GLY:C	1:A:63:LYS:HE3	0.41	2.35	10	1
1:A:71:VAL:O	1:A:75:ARG:HD2	0.41	2.16	12	1
1:A:14:LEU:HD13	1:A:90:VAL:CG1	0.41	2.46	11	1
1:A:7:GLN:HG3	1:A:24:ALA:HB1	0.41	1.92	7	1
1:A:71:VAL:O	1:A:75:ARG:HG2	0.41	2.15	6	1
1:A:60:SER:HB3	1:A:88:MET:SD	0.41	2.55	14	1
1:A:60:SER:OG	1:A:65:LEU:HD11	0.41	2.16	10	1
1:A:50:PRO:O	1:A:51:LYS:HD3	0.40	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HG	1:A:74:TYR:CE1	0.40	2.51	9	1
1:A:14:LEU:HD22	1:A:92:ILE:HD11	0.40	1.93	8	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	79/126 (63%)	76±1 (96±1%)	3±1 (3±1%)	1±1 (1±1%)	25	72
All	All	1580/2520 (63%)	1514 (96%)	52 (3%)	14 (1%)	25	72

All 6 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	51	LYS	5
1	A	50	PRO	3
1	A	48	ASN	3
1	A	43	PRO	1
1	A	7	GLN	1
1	A	47	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	70/111 (63%)	68±1 (96±2%)	2±1 (4±2%)	45	87
All	All	1400/2220 (63%)	1351 (96%)	49 (4%)	45	87

All 23 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	66	GLU	5
1	A	65	LEU	4
1	A	63	LYS	4
1	A	46	LYS	4
1	A	88	MET	4
1	A	72	LYS	3
1	A	44	ARG	3
1	A	55	GLU	3
1	A	48	ASN	2
1	A	35	LYS	2
1	A	47	GLU	2
1	A	67	ASN	2
1	A	75	ARG	1
1	A	23	LYS	1
1	A	69	LYS	1
1	A	11	LYS	1
1	A	54	LYS	1
1	A	57	LYS	1
1	A	13	ARG	1
1	A	41	GLU	1
1	A	70	THR	1
1	A	36	GLU	1
1	A	58	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6128

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	1287
Number of shifts mapped to atoms	1287
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

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	-0.33 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	111	-0.21 ± 0.21	None needed (< 0.5 ppm)
$^{13}\text{C}'$	116	-0.05 ± 0.13	None needed (< 0.5 ppm)
^{15}N	108	-0.60 ± 0.41	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 90%, i.e. 884 atoms were assigned a chemical shift out of a possible 979. 12 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	387/387 (100%)	154/154 (100%)	158/158 (100%)	75/75 (100%)
Sidechain	465/546 (85%)	285/318 (90%)	176/205 (86%)	4/23 (17%)

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	Total	^1H	^{13}C	^{15}N
Aromatic	32/46 (70%)	20/24 (83%)	11/19 (58%)	1/3 (33%)
Overall	884/979 (90%)	459/496 (93%)	345/382 (90%)	80/101 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1097 atoms were assigned a chemical shift out of a possible 1225. 13 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	493/493 (100%)	196/196 (100%)	202/202 (100%)	95/95 (100%)
Sidechain	572/678 (84%)	348/395 (88%)	218/256 (85%)	6/27 (22%)
Aromatic	32/54 (59%)	20/28 (71%)	11/21 (52%)	1/5 (20%)
Overall	1097/1225 (90%)	564/619 (91%)	431/479 (90%)	102/127 (80%)

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 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:

