Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	1YXR
Title	:	NMR Structure of VPS4A MIT Domain
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Deposited on	:	2005-02-22

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:

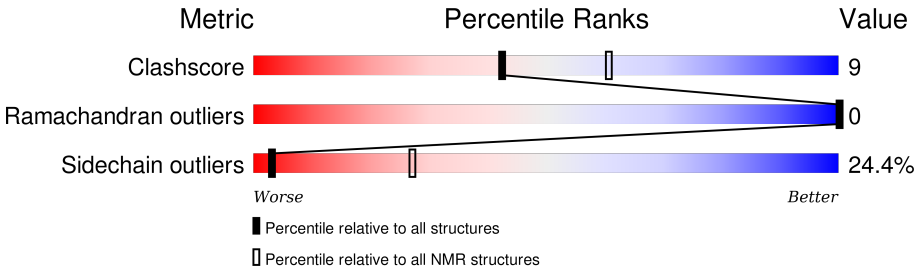
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal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

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	77	57% 35% • 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 18 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:5-A:76 (72)	0.18	15

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 2 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1285 atoms, of which 649 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called vacuolar protein sorting factor 4A.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	77	1285	401	649	110	123	2	0

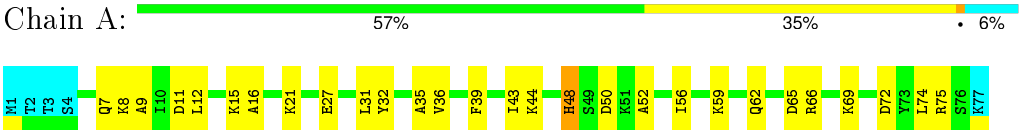
4 Residue-property plots

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: vacuolar protein sorting factor 4A

Chain A:



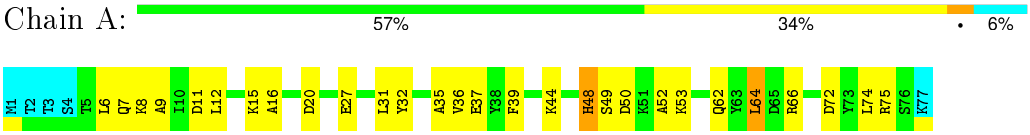
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: vacuolar protein sorting factor 4A

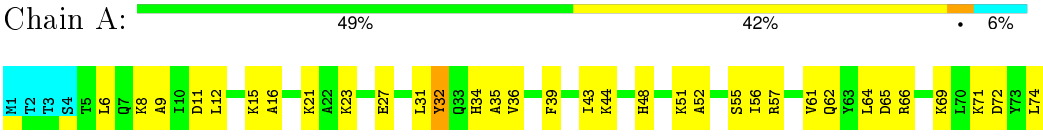
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: vacuolar protein sorting factor 4A

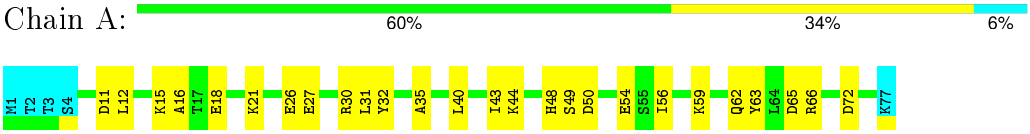
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: vacuolar protein sorting factor 4A

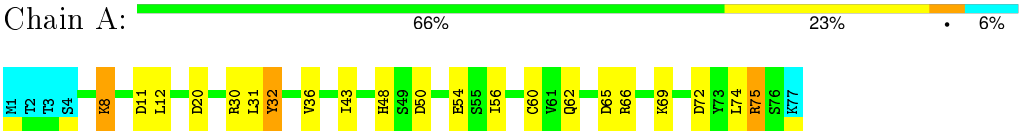
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: vacuolar protein sorting factor 4A

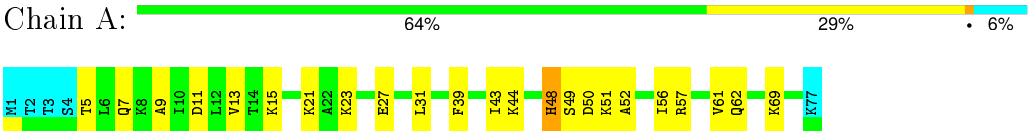
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: vacuolar protein sorting factor 4A

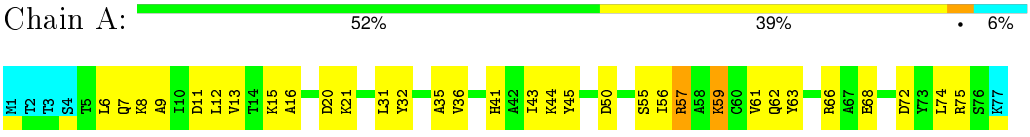
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: vacuolar protein sorting factor 4A

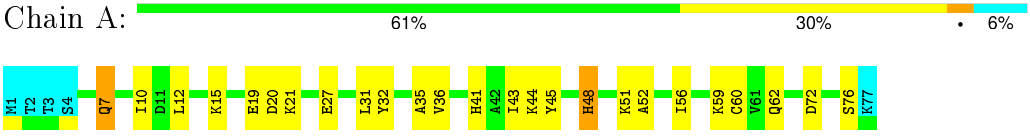
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: vacuolar protein sorting factor 4A

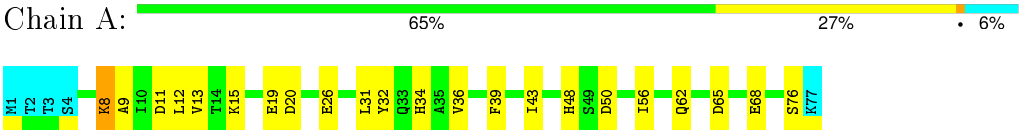
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: vacuolar protein sorting factor 4A

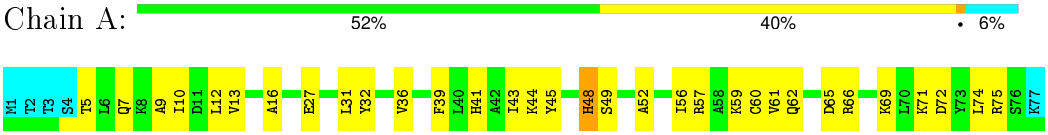
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: vacuolar protein sorting factor 4A

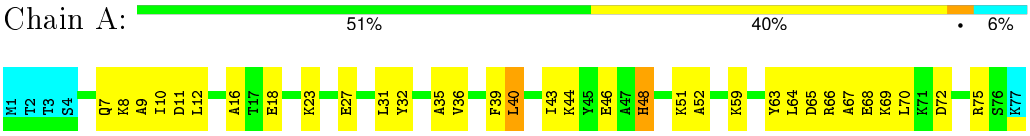
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: vacuolar protein sorting factor 4A

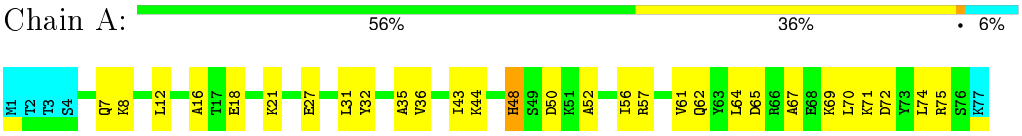
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: vacuolar protein sorting factor 4A

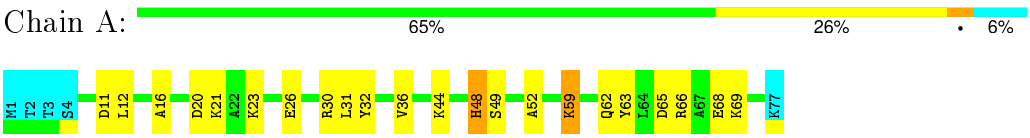
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: vacuolar protein sorting factor 4A

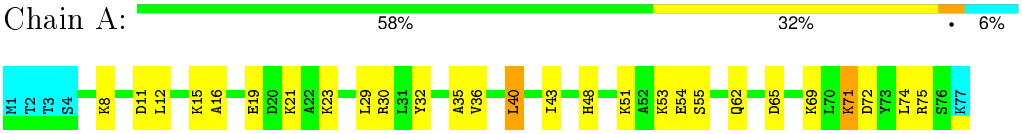
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: vacuolar protein sorting factor 4A

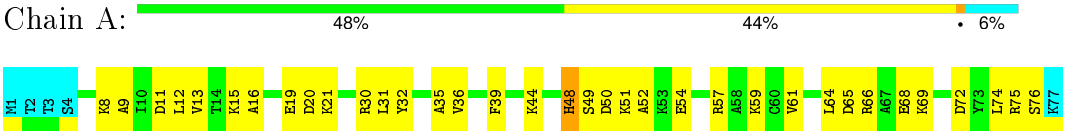
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: vacuolar protein sorting factor 4A

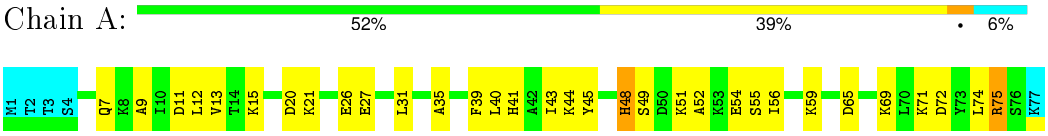
Chain A:



4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: vacuolar protein sorting factor 4A

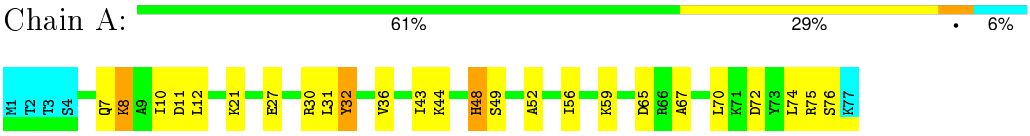
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: vacuolar protein sorting factor 4A

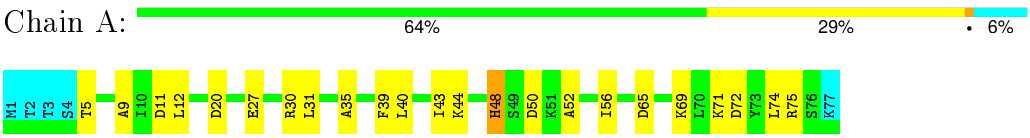
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: vacuolar protein sorting factor 4A

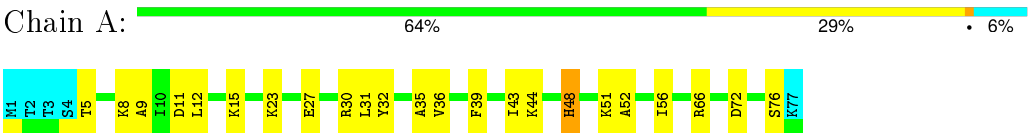
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: vacuolar protein sorting factor 4A

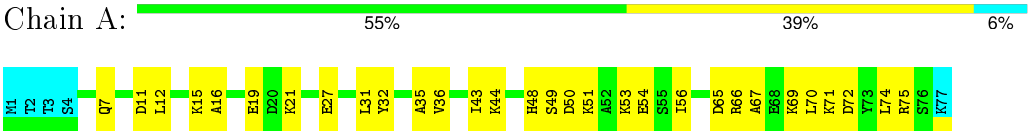
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: vacuolar protein sorting factor 4A

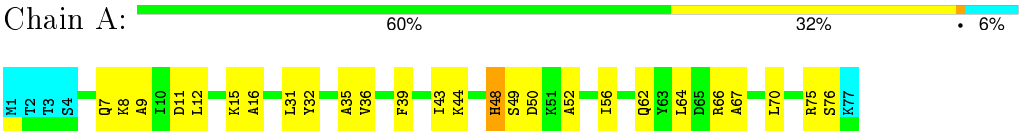
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: vacuolar protein sorting factor 4A

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *automated NOE assignment using CYANA and torsion angle dynamics for structure calculations.*

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
CYANA	structure solution	2.0
CNS	refinement	1.1

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 6573
Number of chemical shift lists	1
Total number of shifts	1402
Number of shifts mapped to atoms	920
Number of unparsed shifts	0
Number of shifts with mapping errors	482
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

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	598	606	603	10±3
All	All	11960	12120	12060	209

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:ILE:HD11	1:A:56:ILE:CG2	0.74	2.11	7	11
1:A:74:LEU:HD12	1:A:75:ARG:N	0.72	1.99	17	12
1:A:57:ARG:O	1:A:61:VAL:HG23	0.72	1.84	5	6
1:A:43:ILE:HD11	1:A:56:ILE:HG22	0.72	1.59	15	15
1:A:8:LYS:O	1:A:12:LEU:HD23	0.71	1.86	2	11
1:A:32:TYR:O	1:A:36:VAL:HG23	0.69	1.87	19	15
1:A:36:VAL:HG11	1:A:64:LEU:HG	0.67	1.67	20	4
1:A:7:GLN:HA	1:A:10:ILE:HD12	0.66	1.65	9	4
1:A:16:ALA:HB1	1:A:32:TYR:CD2	0.65	2.26	11	10
1:A:16:ALA:HB2	1:A:31:LEU:HB3	0.64	1.69	1	7
1:A:12:LEU:HB3	1:A:35:ALA:HB2	0.64	1.69	20	11
1:A:12:LEU:CD1	1:A:31:LEU:HD13	0.64	2.23	15	18
1:A:9:ALA:HB1	1:A:39:PHE:CE2	0.63	2.29	10	11
1:A:12:LEU:HD13	1:A:31:LEU:CD1	0.62	2.25	20	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD13	1:A:31:LEU:HD13	0.61	1.72	1	6
1:A:9:ALA:O	1:A:13:VAL:HG23	0.58	1.98	5	6
1:A:27:GLU:O	1:A:31:LEU:HD23	0.58	1.98	5	1
1:A:67:ALA:HA	1:A:70:LEU:HD12	0.56	1.75	20	5
1:A:12:LEU:CB	1:A:35:ALA:HB2	0.52	2.35	20	6
1:A:36:VAL:HG11	1:A:64:LEU:CG	0.51	2.34	20	1
1:A:36:VAL:HG11	1:A:64:LEU:CD1	0.50	2.37	20	1
1:A:40:LEU:HA	1:A:43:ILE:HD12	0.49	1.84	13	2
1:A:48:HIS:HB3	1:A:52:ALA:HB3	0.48	1.86	20	14
1:A:16:ALA:HB2	1:A:31:LEU:CB	0.46	2.40	1	1
1:A:41:HIS:NE2	1:A:45:TYR:CE1	0.45	2.84	6	4
1:A:41:HIS:CD2	1:A:45:TYR:CD1	0.44	3.05	7	2
1:A:12:LEU:HD12	1:A:31:LEU:HD13	0.44	1.89	8	2
1:A:52:ALA:O	1:A:56:ILE:HD12	0.43	2.13	17	2
1:A:16:ALA:HB1	1:A:32:TYR:CE2	0.43	2.48	13	3
1:A:43:ILE:HD11	1:A:56:ILE:HG21	0.43	1.90	7	1
1:A:29:LEU:HD22	1:A:71:LYS:HB3	0.43	1.90	13	1
1:A:41:HIS:NE2	1:A:45:TYR:CD1	0.41	2.89	9	1
1:A:59:LYS:O	1:A:63:TYR:CD2	0.41	2.74	3	4
1:A:12:LEU:CD1	1:A:31:LEU:CD1	0.40	3.00	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	72/77 (94%)	69±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	100	100
All	All	1440/1540 (94%)	1388 (96%)	52 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	62/67 (93%)	47±2 (76±4%)	15±2 (24±4%)	3 27
All	All	1240/1340 (93%)	938 (76%)	302 (24%)	3 27

All 40 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	48	HIS	18
1	A	44	LYS	17
1	A	11	ASP	17
1	A	72	ASP	16
1	A	65	ASP	14
1	A	15	LYS	13
1	A	62	GLN	13
1	A	69	LYS	12
1	A	66	ARG	12
1	A	27	GLU	12
1	A	21	LYS	12
1	A	50	ASP	11
1	A	49	SER	10
1	A	51	LYS	9
1	A	20	ASP	9
1	A	7	GLN	8
1	A	30	ARG	8
1	A	59	LYS	7
1	A	71	LYS	7
1	A	23	LYS	6
1	A	54	GLU	6
1	A	76	SER	6
1	A	19	GLU	5
1	A	40	LEU	5
1	A	68	GLU	5
1	A	75	ARG	5
1	A	5	THR	4
1	A	8	LYS	4
1	A	26	GLU	4
1	A	55	SER	4
1	A	64	LEU	3
1	A	32	TYR	3
1	A	6	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	53	LYS	3
1	A	60	CYS	3
1	A	18	GLU	3
1	A	34	HIS	2
1	A	46	GLU	1
1	A	37	GLU	1
1	A	57	ARG	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 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 6573

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	1402
Number of shifts mapped to atoms	920
Number of unparsed shifts	0
Number of shifts with mapping errors	482
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 482 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	86	LYS	HG3	1.393	0.008	1
A	116	ALA	CB	19.398	0.011	1
A	121	LYS	N	124.127	0.006	1
A	82	LYS	HB2	1.79	0.003	1
A	108	LYS	HD3	1.672	0.004	1
A	90	SER	HB2	3.864	0.006	1
A	89	GLN	HB2	2.128	0.003	1
A	92	GLY	HA3	3.936	0.006	1
A	120	GLU	CG	36.138	0.0	1
A	93	LYS	HB3	1.752	0.0	1
A	100	GLU	CG	36.27	0.0	1
A	87	GLU	H	8.508	0.004	1
A	101	GLY	CA	45.468	0.048	1
A	107	LYS	HD2	1.654	0.002	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	90	SER	CA	58.859	0.0	1
A	109	LEU	CD2	23.783	0.021	1
A	117	VAL	HG21	0.894	0.004	1
A	118	VAL	H	8.198	0.005	1
A	80	HIS	HD2	7.216	0.001	1
A	94	GLY	HA3	3.98	0.002	1
A	94	GLY	CA	45.291	0.003	1
A	107	LYS	HE3	2.958	0.006	1
A	91	GLU	CB	30.191	0.032	1
A	93	LYS	H	8.185	0.002	1
A	118	VAL	CB	32.844	0.0	1
A	119	MET	N	124.928	0.006	1
A	100	GLU	HA	4.28	0.003	1
A	98	ASP	HB3	2.656	0.001	1
A	102	ASP	CB	41.29	0.025	1
A	86	LYS	HE3	2.968	0.008	1
A	120	GLU	HB2	1.896	0.002	1
A	88	ASN	HB3	2.821	0.003	1
A	122	PRO	CB	32.089	0.009	1
A	103	ASN	ND2	113.35	0.006	1
A	89	GLN	N	120.919	0.012	1
A	121	LYS	HG3	1.442	0.003	1
A	112	GLN	HB3	2.077	0.007	1
A	102	ASP	H	8.187	0.006	1
A	79	LYS	CE	42.2	0.0	1
A	121	LYS	HA	4.561	0.004	1
A	106	LYS	CA	57.69	0.088	1
A	122	PRO	HD3	3.599	0.007	1
A	108	LYS	HG3	1.432	0.01	1
A	82	LYS	HA	4.315	0.01	1
A	113	LEU	HD21	0.817	0.002	1
A	99	SER	N	115.931	0.043	1
A	122	PRO	HB3	1.854	0.003	1
A	104	PRO	CD	50.872	0.058	1
A	112	GLN	HA	4.222	0.008	1
A	110	GLN	HB3	2.082	0.004	1
A	106	LYS	HB2	1.832	0.009	1
A	85	VAL	CG1	20.726	0.055	1
A	117	VAL	HG11	0.894	0.004	1
A	83	LYS	N	124.586	0.003	1
A	84	PRO	HG3	1.99	0.004	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	99	SER	CB	63.91	0.054	1
A	98	ASP	CB	41.233	0.063	1
A	79	LYS	HB3	1.716	0.006	1
A	87	GLU	CA	56.858	0.081	1
A	78	GLU	CG	36.27	0.0	1
A	106	LYS	N	120.859	0.001	1
A	108	LYS	CG	24.958	0.0	1
A	96	ASP	HA	4.635	0.004	1
A	82	LYS	HE2	2.974	0.001	1
A	108	LYS	HB3	1.794	0.007	1
A	79	LYS	HD2	1.625	0.002	1
A	113	LEU	HA	4.262	0.011	1
A	80	HIS	CD2	120.163	0.016	1
A	109	LEU	CG	27.15	0.0	1
A	86	LYS	H	8.325	0.001	1
A	97	SER	HA	4.408	0.004	1
A	107	LYS	N	120.714	0.052	1
A	105	GLU	CG	36.39	0.0	1
A	115	GLY	HA2	3.916	0.006	1
A	118	VAL	HG13	0.885	0.009	1
A	110	GLN	NE2	111.911	0.009	1
A	86	LYS	CE	42.15	0.0	1
A	114	MET	CG	32.166	0.078	1
A	95	SER	CA	58.343	0.0	1
A	109	LEU	HD13	0.895	0.001	1
A	104	PRO	HB3	1.956	0.004	1
A	78	GLU	HA	4.176	0.004	1
A	122	PRO	HA	4.212	0.005	1
A	121	LYS	HB3	1.712	0.001	1
A	84	PRO	HD2	3.813	0.003	1
A	103	ASN	HB2	2.78	0.003	1
A	102	ASP	HB3	2.576	0.006	1
A	121	LYS	CE	42.26	0.0	1
A	111	GLU	HB2	2.019	0.003	1
A	80	HIS	HB2	3.281	0.008	1
A	91	GLU	HG3	2.249	0.004	1
A	114	MET	HB3	2.048	0.007	1
A	98	ASP	N	122.449	0.008	1
A	95	SER	N	115.809	0.021	1
A	111	GLU	H	8.229	0.007	1
A	78	GLU	H	7.911	0.006	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	84	PRO	CA	63.05	0.007	1
A	105	GLU	N	118.894	0.009	1
A	80	HIS	HE1	8.308	0.001	1
A	82	LYS	HE3	2.974	0.001	1
A	93	LYS	HG2	1.415	0.001	1
A	104	PRO	CG	27.412	0.032	1
A	105	GLU	CB	29.42	0.0	1
A	103	ASN	N	119.537	0.017	1
A	104	PRO	HG3	2.014	0.003	1
A	117	VAL	HG13	0.894	0.004	1
A	87	GLU	HA	4.234	0.007	1
A	107	LYS	HA	4.15	0.012	1
A	121	LYS	HD3	1.664	0.0	1
A	121	LYS	CB	32.6	0.0	1
A	120	GLU	HG3	2.224	0.004	1
A	98	ASP	CA	54.693	0.033	1
A	89	GLN	HG2	2.339	0.008	1
A	95	SER	HB2	3.869	0.008	1
A	108	LYS	HE3	2.943	0.002	1
A	91	GLU	HB2	1.946	0.003	1
A	93	LYS	HB2	1.856	0.007	1
A	78	GLU	CB	29.976	0.0	1
A	100	GLU	CA	57.116	0.0	1
A	113	LEU	HB2	1.68	0.005	1
A	79	LYS	CA	56.645	0.0	1
A	119	MET	CG	32.09	0.0	1
A	97	SER	HB2	3.883	0.003	1
A	80	HIS	CB	29.592	0.056	1
A	109	LEU	HD23	0.859	0.009	1
A	114	MET	H	8.145	0.003	1
A	95	SER	H	8.291	0.002	1
A	107	LYS	HG3	1.411	0.0	1
A	81	GLY	HA2	3.924	0.008	1
A	93	LYS	CD	29.0	0.0	1
A	119	MET	H	8.399	0.006	1
A	89	GLN	HE21	7.518	0.003	1
A	86	LYS	HB3	1.726	0.002	1
A	107	LYS	CB	32.82	0.0	1
A	103	ASN	HA	4.92	0.002	1
A	92	GLY	H	8.412	0.002	1
A	110	GLN	HE21	7.482	0.001	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	78	GLU	HB3	2.001	0.003	1
A	89	GLN	CG	33.9	0.0	1
A	96	ASP	N	122.423	0.019	1
A	116	ALA	CA	52.451	0.0	1
A	80	HIS	N	118.888	0.01	1
A	82	LYS	CG	24.764	0.0	1
A	82	LYS	HB3	1.726	0.004	1
A	101	GLY	HA2	3.912	0.003	1
A	114	MET	CB	32.692	0.03	1
A	91	GLU	N	122.625	0.017	1
A	95	SER	CB	64.15	0.0	1
A	84	PRO	HB3	1.854	0.002	1
A	90	SER	HA	4.409	0.006	1
A	79	LYS	N	121.054	0.01	1
A	88	ASN	H	8.5	0.005	1
A	115	GLY	CA	45.42	0.0	1
A	107	LYS	H	7.971	0.001	1
A	97	SER	CA	58.859	0.0	1
A	110	GLN	HG3	2.39	0.011	1
A	105	GLU	H	8.339	0.007	1
A	103	ASN	CB	39.01	0.019	1
A	118	VAL	CG1	21.209	0.007	1
A	108	LYS	H	7.982	0.004	1
A	118	VAL	HB	2.003	0.002	1
A	86	LYS	CA	56.226	0.042	1
A	88	ASN	ND2	112.994	0.002	1
A	112	GLN	N	119.981	0.012	1
A	99	SER	HB2	3.873	0.01	1
A	78	GLU	N	120.198	0.009	1
A	80	HIS	H	8.343	0.006	1
A	85	VAL	CA	62.338	0.006	1
A	115	GLY	N	109.19	0.022	1
A	97	SER	N	115.59	0.034	1
A	114	MET	HG2	2.539	0.007	1
A	78	GLU	HG2	2.285	0.002	1
A	85	VAL	HG21	0.91	0.004	1
A	98	ASP	HB2	2.696	0.007	1
A	84	PRO	CD	50.744	0.035	1
A	86	LYS	HE2	2.968	0.008	1
A	120	GLU	HB3	1.969	0.005	1
A	87	GLU	CG	36.314	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	103	ASN	H	8.265	0.008	1
A	117	VAL	N	119.559	0.003	1
A	110	GLN	CA	57.42	0.0	1
A	89	GLN	H	8.405	0.003	1
A	113	LEU	CG	26.953	0.0	1
A	87	GLU	HB3	2.009	0.005	1
A	106	LYS	HG3	1.415	0.001	1
A	122	PRO	CA	64.743	0.012	1
A	109	LEU	N	121.809	0.064	1
A	96	ASP	CB	41.111	0.013	1
A	83	LYS	CB	32.6	0.0	1
A	85	VAL	HG13	0.91	0.004	1
A	121	LYS	CA	54.293	0.0	1
A	86	LYS	N	124.883	0.003	1
A	78	GLU	CA	57.261	0.0	1
A	79	LYS	CB	32.8	0.0	1
A	85	VAL	N	120.772	0.008	1
A	106	LYS	CB	32.82	0.0	1
A	122	PRO	HD2	3.7	0.003	1
A	121	LYS	HE2	2.989	0.001	1
A	108	LYS	HG2	1.446	0.003	1
A	93	LYS	CA	56.188	0.019	1
A	89	GLN	HE22	6.838	0.001	1
A	110	GLN	N	119.604	0.004	1
A	87	GLU	N	122.624	0.065	1
A	122	PRO	HB2	2.177	0.005	1
A	111	GLU	HA	4.125	0.003	1
A	109	LEU	HA	4.215	0.008	1
A	83	LYS	H	8.368	0.01	1
A	106	LYS	HB3	1.832	0.009	1
A	107	LYS	CA	57.602	0.0	1
A	107	LYS	CE	42.1	0.0	1
A	117	VAL	HG12	0.894	0.004	1
A	105	GLU	CA	57.996	0.0	1
A	82	LYS	CD	29.102	0.0	1
A	106	LYS	H	7.892	0.0	1
A	96	ASP	HB3	2.659	0.004	1
A	112	GLN	CB	29.191	0.0	1
A	96	ASP	H	8.479	0.008	1
A	117	VAL	CB	32.808	0.036	1
A	111	GLU	HG3	2.316	0.003	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	79	LYS	HD3	1.625	0.002	1
A	119	MET	HB2	2.031	0.003	1
A	93	LYS	HE3	2.99	0.001	1
A	114	MET	N	119.307	0.006	1
A	118	VAL	HG12	0.885	0.009	1
A	118	VAL	HA	4.058	0.004	1
A	106	LYS	HE3	2.967	0.002	1
A	82	LYS	HG3	1.408	0.0	1
A	85	VAL	CB	32.905	0.045	1
A	83	LYS	HB3	1.454	0.0	1
A	117	VAL	H	8.022	0.005	1
A	104	PRO	HB2	2.304	0.006	1
A	109	LEU	CA	56.469	0.079	1
A	91	GLU	H	8.4	0.004	1
A	112	GLN	NE2	111.824	0.007	1
A	81	GLY	H	8.347	0.003	1
A	121	LYS	HB2	1.819	0.006	1
A	84	PRO	CG	27.452	0.044	1
A	80	HIS	CE1	137.2	0.0	1
A	87	GLU	CB	30.304	0.047	1
A	88	ASN	HD22	6.908	0.003	1
A	107	LYS	HB3	1.782	0.0	1
A	120	GLU	H	8.365	0.0	1
A	118	VAL	HG21	0.885	0.009	1
A	104	PRO	HD3	3.787	0.003	1
A	83	LYS	CA	54.324	0.029	1
A	121	LYS	CD	29.26	0.0	1
A	80	HIS	HB3	3.143	0.005	1
A	85	VAL	H	8.212	0.006	1
A	91	GLU	HG2	2.249	0.004	1
A	91	GLU	CG	36.237	0.0	1
A	105	GLU	HB3	2.025	0.002	1
A	117	VAL	CG1	21.217	0.0	1
A	79	LYS	CG	24.899	0.0	1
A	106	LYS	CG	25.31	0.0	1
A	93	LYS	CB	33.15	0.0	1
A	93	LYS	HD2	1.68	0.0	1
A	81	GLY	N	109.734	0.007	1
A	116	ALA	H	7.986	0.002	1
A	109	LEU	HB3	1.593	0.005	1
A	121	LYS	HD2	1.664	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	82	LYS	CA	56.117	0.001	1
A	100	GLU	HG3	2.264	0.003	1
A	120	GLU	HG2	2.224	0.004	1
A	95	SER	HB3	3.825	0.003	1
A	116	ALA	HB3	1.344	0.001	1
A	108	LYS	HE2	2.943	0.002	1
A	112	GLN	CG	33.986	0.0	1
A	91	GLU	HB3	2.067	0.003	1
A	120	GLU	CB	30.455	0.007	1
A	100	GLU	CB	30.179	0.047	1
A	113	LEU	HB3	1.566	0.005	1
A	119	MET	HA	4.468	0.006	1
A	97	SER	HB3	3.843	0.012	1
A	120	GLU	CA	56.621	0.087	1
A	111	GLU	CA	57.793	0.005	1
A	81	GLY	HA3	3.924	0.008	1
A	93	LYS	CE	42.2	0.0	1
A	108	LYS	CA	57.426	0.0	1
A	113	LEU	HD13	0.872	0.002	1
A	97	SER	H	8.208	0.003	1
A	113	LEU	CD2	23.403	0.007	1
A	81	GLY	CA	45.34	0.0	1
A	113	LEU	HG	1.645	0.001	1
A	82	LYS	HD2	1.663	0.0	1
A	86	LYS	HD2	1.699	0.003	1
A	110	GLN	HE22	6.85	0.001	1
A	78	GLU	HB2	2.001	0.003	1
A	79	LYS	HG2	1.368	0.004	1
A	100	GLU	H	8.384	0.006	1
A	99	SER	HA	4.419	0.005	1
A	101	GLY	HA3	3.912	0.003	1
A	114	MET	CA	55.88	0.007	1
A	114	MET	HB2	2.099	0.003	1
A	84	PRO	HB2	2.253	0.003	1
A	100	GLU	HB2	1.962	0.007	1
A	97	SER	CB	63.959	0.014	1
A	110	GLN	HG2	2.39	0.011	1
A	117	VAL	HG23	0.894	0.004	1
A	87	GLU	HG2	2.236	0.006	1
A	111	GLU	N	120.575	0.034	1
A	88	ASN	HD21	7.602	0.002	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	89	GLN	HA	4.337	0.006	1
A	118	VAL	HG22	0.885	0.009	1
A	109	LEU	CB	42.091	0.032	1
A	110	GLN	HA	4.138	0.008	1
A	120	GLU	HA	4.234	0.008	1
A	105	GLU	HG2	2.265	0.007	1
A	98	ASP	HA	4.635	0.003	1
A	99	SER	HB3	3.835	0.005	1
A	100	GLU	N	122.547	0.007	1
A	106	LYS	CD	29.2	0.0	1
A	91	GLU	HA	4.285	0.004	1
A	114	MET	HG3	2.614	0.004	1
A	78	GLU	HG3	2.232	0.004	1
A	85	VAL	HG22	0.91	0.004	1
A	90	SER	N	116.842	0.009	1
A	113	LEU	CA	55.85	0.027	1
A	88	ASN	CB	38.82	0.034	1
A	108	LYS	CD	29.2	0.0	1
A	110	GLN	CB	29.084	0.029	1
A	109	LEU	HD12	0.895	0.001	1
A	79	LYS	HE3	2.945	0.002	1
A	94	GLY	N	110.407	0.031	1
A	87	GLU	HB2	1.903	0.006	1
A	93	LYS	HA	4.341	0.009	1
A	106	LYS	HG2	1.415	0.001	1
A	98	ASP	H	8.33	0.003	1
A	88	ASN	HA	4.647	0.003	1
A	96	ASP	CA	54.615	0.0	1
A	85	VAL	HG12	0.91	0.004	1
A	84	PRO	HA	4.438	0.001	1
A	113	LEU	HD11	0.872	0.002	1
A	119	MET	CA	55.179	0.021	1
A	106	LYS	HD2	1.665	0.006	1
A	89	GLN	NE2	112.527	0.002	1
A	109	LEU	HD21	0.859	0.009	1
A	110	GLN	H	8.202	0.002	1
A	113	LEU	N	121.664	0.004	1
A	121	LYS	HE3	2.989	0.001	1
A	112	GLN	HE21	7.458	0.001	1
A	119	MET	HG3	2.558	0.002	1
A	111	GLU	CB	30.091	0.013	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	113	LEU	HD23	0.817	0.002	1
A	108	LYS	CB	32.65	0.0	1
A	90	SER	H	8.356	0.001	1
A	104	PRO	CB	32.114	0.013	1
A	122	PRO	HG2	1.918	0.005	1
A	89	GLN	CA	56.201	0.0	1
A	82	LYS	CE	42.18	0.0	1
A	108	LYS	HD2	1.672	0.004	1
A	90	SER	HB3	3.838	0.003	1
A	122	PRO	CG	27.434	0.0	1
A	96	ASP	HB2	2.708	0.004	1
A	92	GLY	HA2	3.936	0.006	1
A	103	ASN	CA	51.657	0.01	1
A	107	LYS	HD3	1.654	0.002	1
A	90	SER	CB	63.822	0.023	1
A	103	ASN	HD21	7.742	0.001	1
A	99	SER	CA	58.699	0.021	1
A	108	LYS	CE	42.1	0.0	1
A	94	GLY	HA2	3.98	0.002	1
A	117	VAL	CA	62.456	0.01	1
A	117	VAL	HA	4.056	0.003	1
A	111	GLU	HG2	2.224	0.007	1
A	85	VAL	HA	4.06	0.004	1
A	107	LYS	HE2	2.958	0.006	1
A	119	MET	HB3	1.954	0.004	1
A	108	LYS	HA	4.177	0.013	1
A	93	LYS	HE2	2.99	0.001	1
A	86	LYS	HG2	1.393	0.008	1
A	118	VAL	HG11	0.885	0.009	1
A	106	LYS	HE2	2.967	0.002	1
A	86	LYS	CG	24.699	0.0	1
A	85	VAL	HG11	0.91	0.004	1
A	82	LYS	HG2	1.408	0.0	1
A	118	VAL	CA	62.348	0.013	1
A	83	LYS	HB2	1.454	0.0	1
A	102	ASP	CA	54.208	0.011	1
A	94	GLY	H	8.511	0.007	1
A	93	LYS	N	120.949	0.066	1
A	110	GLN	CG	33.986	0.0	1
A	116	ALA	HA	4.31	0.002	1
A	109	LEU	HD11	0.895	0.001	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	88	ASN	HB2	2.768	0.008	1
A	121	LYS	H	8.311	0.007	1
A	107	LYS	HB2	1.782	0.0	1
A	89	GLN	HB3	1.977	0.004	1
A	104	PRO	HD2	3.787	0.003	1
A	121	LYS	CG	24.664	0.0	1
A	86	LYS	CB	33.034	0.0	1
A	114	MET	HA	4.427	0.004	1
A	95	SER	HA	4.325	0.001	1
A	112	GLN	HG2	2.36	0.01	1
A	121	LYS	HG2	1.442	0.003	1
A	105	GLU	HB2	2.025	0.002	1
A	112	GLN	HB2	2.077	0.007	1
A	79	LYS	CD	29.144	0.0	1
A	83	LYS	HA	4.565	0.004	1
A	118	VAL	N	124.747	0.007	1
A	80	HIS	HA	4.694	0.002	1
A	119	MET	CB	33.206	0.0	1
A	112	GLN	CA	56.891	0.0	1
A	112	GLN	HE22	6.815	0.002	1
A	111	GLU	CG	36.424	0.055	1
A	93	LYS	HD3	1.68	0.0	1
A	120	GLU	N	122.984	0.013	1
A	109	LEU	HG	1.636	0.01	1
A	99	SER	H	8.216	0.008	1
A	110	GLN	HB2	2.082	0.004	1
A	122	PRO	CD	50.358	0.027	1
A	89	GLN	CB	29.417	0.018	1
A	82	LYS	CB	33.09	0.049	1
A	84	PRO	HG2	1.99	0.004	1
A	92	GLY	N	109.956	0.009	1
A	100	GLU	HG2	2.264	0.003	1
A	116	ALA	HB2	1.344	0.001	1
A	79	LYS	HB2	1.808	0.007	1
A	103	ASN	HD22	7.028	0.003	1
A	79	LYS	H	8.095	0.001	1
A	88	ASN	N	119.497	0.012	1
A	117	VAL	HB	2.002	0.006	1
A	107	LYS	CD	29.2	0.0	1
A	101	GLY	H	8.271	0.002	1
A	113	LEU	CD1	25.128	0.0	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	102	ASP	N	120.163	0.037	1
A	108	LYS	HB2	1.794	0.007	1
A	82	LYS	H	8.193	0.002	1
A	82	LYS	HD3	1.663	0.0	1
A	86	LYS	HD3	1.699	0.003	1
A	106	LYS	HA	4.119	0.006	1
A	92	GLY	CA	45.425	0.011	1
A	115	GLY	HA3	3.916	0.006	1
A	86	LYS	CD	29.15	0.0	1
A	86	LYS	HA	4.292	0.004	1
A	100	GLU	HB3	2.073	0.004	1
A	117	VAL	HG22	0.894	0.004	1
A	88	ASN	CA	53.394	0.001	1
A	87	GLU	HG3	2.236	0.006	1
A	84	PRO	HD3	3.617	0.003	1
A	105	GLU	HA	4.14	0.004	1
A	113	LEU	H	8.112	0.001	1
A	103	ASN	HB3	2.857	0.006	1
A	104	PRO	HA	4.315	0.005	1
A	118	VAL	HG23	0.885	0.009	1
A	102	ASP	HB2	2.62	0.003	1
A	116	ALA	N	123.44	0.001	1
A	109	LEU	H	8.001	0.006	1
A	107	LYS	CG	24.958	0.0	1
A	82	LYS	N	121.117	0.016	1
A	91	GLU	CA	56.875	0.001	1
A	105	GLU	HG3	2.265	0.007	1
A	106	LYS	CE	42.1	0.0	1
A	85	VAL	HG23	0.91	0.004	1
A	113	LEU	CB	42.252	0.067	1
A	84	PRO	CB	32.096	0.02	1
A	108	LYS	N	120.799	0.029	1
A	93	LYS	HG3	1.415	0.001	1
A	79	LYS	HE2	2.945	0.002	1
A	104	PRO	HG2	2.014	0.003	1
A	102	ASP	HA	4.583	0.005	1
A	112	GLN	H	8.176	0.001	1
A	112	GLN	HG3	2.36	0.01	1
A	79	LYS	HA	4.209	0.004	1
A	111	GLU	HB3	2.019	0.003	1
A	115	GLY	H	8.171	0.005	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	89	GLN	HG3	2.339	0.008	1
A	116	ALA	HB1	1.344	0.001	1
A	113	LEU	HD12	0.872	0.002	1
A	79	LYS	HG3	1.368	0.004	1
A	106	LYS	HD3	1.665	0.006	1
A	109	LEU	HD22	0.859	0.009	1
A	109	LEU	HB2	1.691	0.003	1
A	101	GLY	N	109.091	0.021	1
A	107	LYS	HG2	1.411	0.0	1
A	119	MET	HG2	2.498	0.002	1
A	93	LYS	CG	24.809	0.0	1
A	113	LEU	HD22	0.817	0.002	1
A	86	LYS	HB2	1.775	0.006	1
A	104	PRO	CA	64.561	0.011	1
A	109	LEU	CD1	24.955	0.0	1
A	85	VAL	HB	2.021	0.004	1
A	122	PRO	HG3	1.918	0.005	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	119	-0.67 ± 0.12	Should be applied
$^{13}C_{\beta}$	117	0.25 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	118	0.05 ± 0.26	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 82%, i.e. 779 atoms were assigned a chemical shift out of a possible 947. 7 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	284/360 (79%)	143/144 (99%)	70/144 (49%)	71/72 (99%)
Sidechain	441/506 (87%)	277/296 (94%)	156/184 (85%)	8/26 (31%)
Aromatic	54/81 (67%)	34/41 (83%)	20/34 (59%)	0/6 (0%)
Overall	779/947 (82%)	454/481 (94%)	246/362 (68%)	79/104 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 824 atoms were assigned a chemical shift out of a possible 1004. 7 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	304/385 (79%)	153/154 (99%)	75/154 (49%)	76/77 (99%)
Sidechain	466/538 (87%)	293/315 (93%)	165/196 (84%)	8/27 (30%)
Aromatic	54/81 (67%)	34/41 (83%)	20/34 (59%)	0/6 (0%)
Overall	824/1004 (82%)	480/510 (94%)	260/384 (68%)	84/110 (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 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: