Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 11:24 PM BST

PDB ID	:	2KOY
Title	:	Structure of the E1064A mutant of the N-domain of Wilson Disease Associated Protein
Authors	:	Dmitriev, O.Y.
Deposited on	:	2009-10-03

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

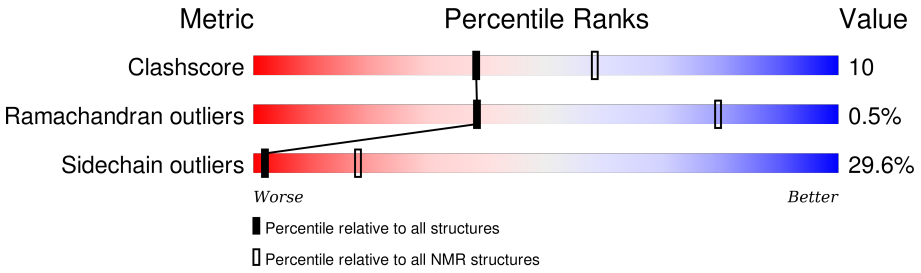
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 86%.

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	141	59% 34% • 6%

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 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:6-A:104, A:108-A:141 (133)	0.94	3

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2084 atoms, of which 1058 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-transporting ATPase 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	141	2084	645	1058	177	194	10	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	EXPRESSION TAG	UNP P35670
A	2	GLY	-	EXPRESSION TAG	UNP P35670
A	3	HIS	-	EXPRESSION TAG	UNP P35670
A	4	MET	-	EXPRESSION TAG	UNP P35670
A	33	ALA	GLU	ENGINEERED	UNP P35670
A	?	-	HIS	DELETION	UNP P35670
A	?	-	SER	DELETION	UNP P35670
A	?	-	GLU	DELETION	UNP P35670
A	?	-	ARG	DELETION	UNP P35670
A	?	-	PRO	DELETION	UNP P35670
A	?	-	LEU	DELETION	UNP P35670
A	?	-	SER	DELETION	UNP P35670
A	?	-	ALA	DELETION	UNP P35670
A	?	-	PRO	DELETION	UNP P35670
A	?	-	ALA	DELETION	UNP P35670
A	?	-	SER	DELETION	UNP P35670
A	?	-	HIS	DELETION	UNP P35670
A	?	-	LEU	DELETION	UNP P35670
A	?	-	ASN	DELETION	UNP P35670
A	?	-	GLU	DELETION	UNP P35670
A	?	-	ALA	DELETION	UNP P35670
A	?	-	GLY	DELETION	UNP P35670
A	?	-	SER	DELETION	UNP P35670
A	?	-	LEU	DELETION	UNP P35670
A	?	-	PRO	DELETION	UNP P35670
A	?	-	ALA	DELETION	UNP P35670
A	?	-	GLU	DELETION	UNP P35670
A	?	-	LYS	DELETION	UNP P35670
A	?	-	ASP	DELETION	UNP P35670

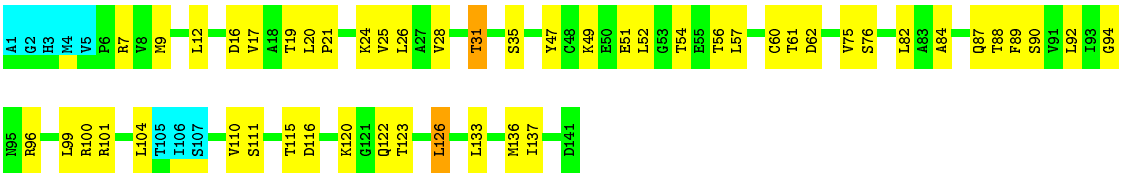
4 Residue-property plots

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: Copper-transporting ATPase 2

Chain A:



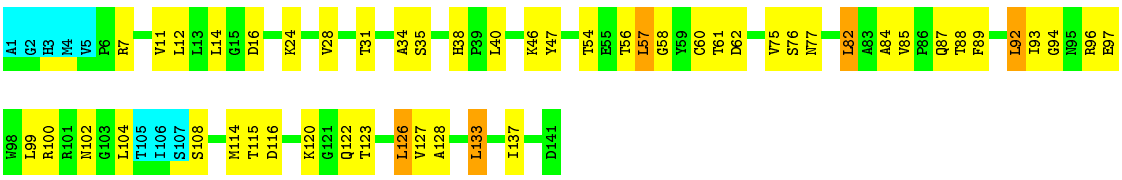
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Copper-transporting ATPase 2

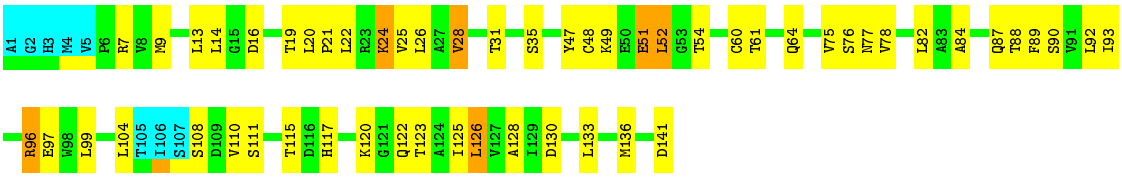
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Copper-transporting ATPase 2

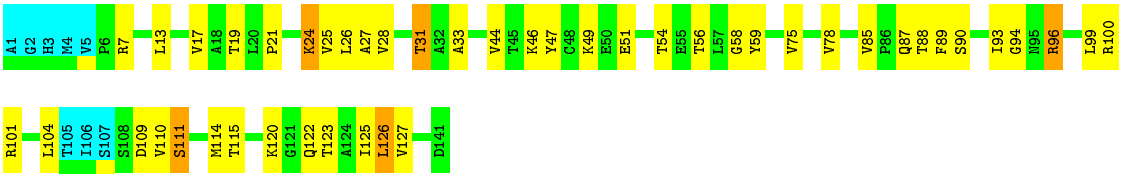
Chain A:



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Copper-transporting ATPase 2

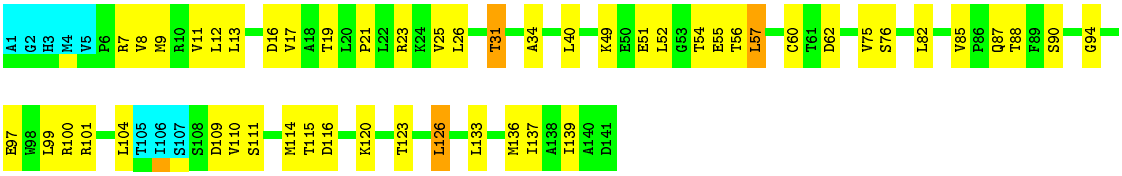
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Copper-transporting ATPase 2

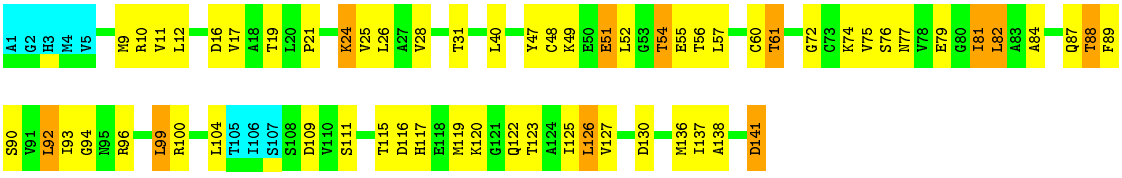
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Copper-transporting ATPase 2

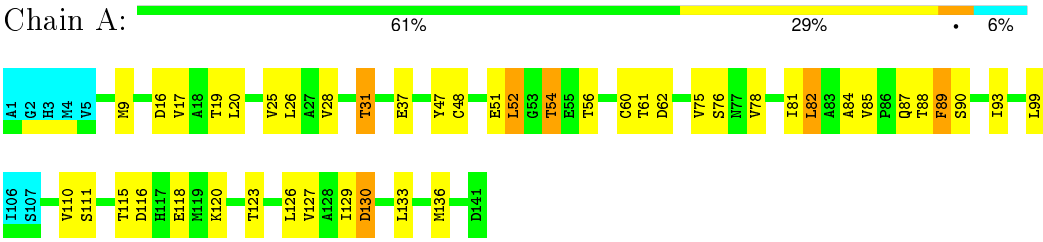
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Copper-transporting ATPase 2

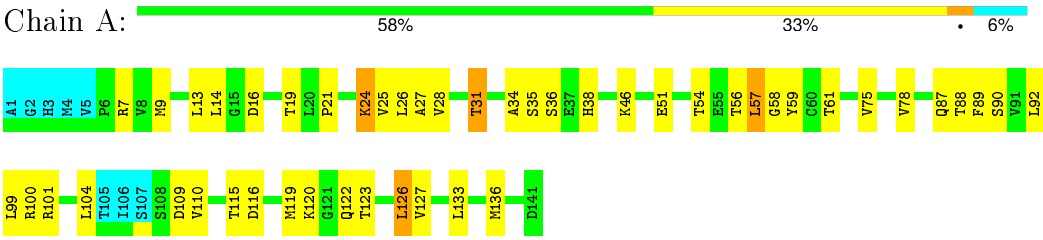
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Copper-transporting ATPase 2

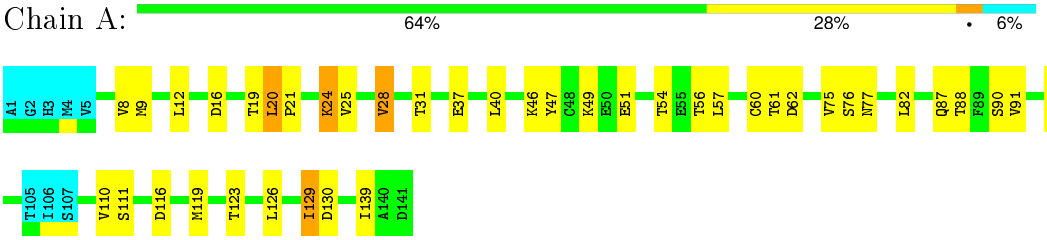
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Copper-transporting ATPase 2

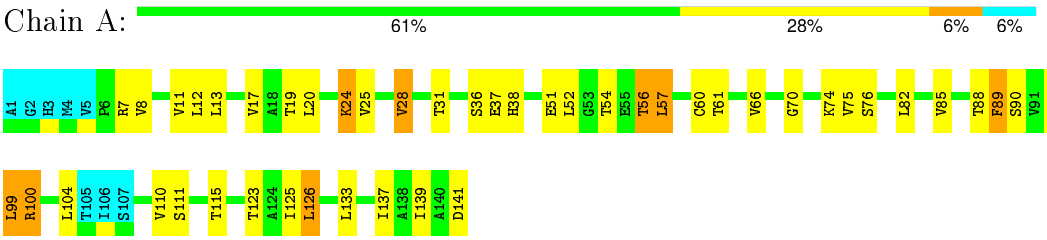
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Copper-transporting ATPase 2

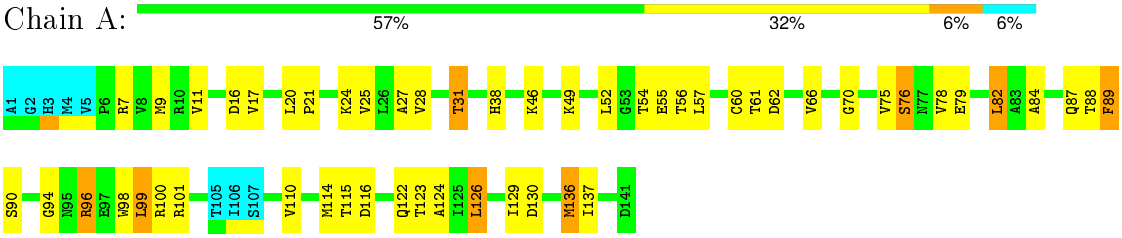
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Copper-transporting ATPase 2

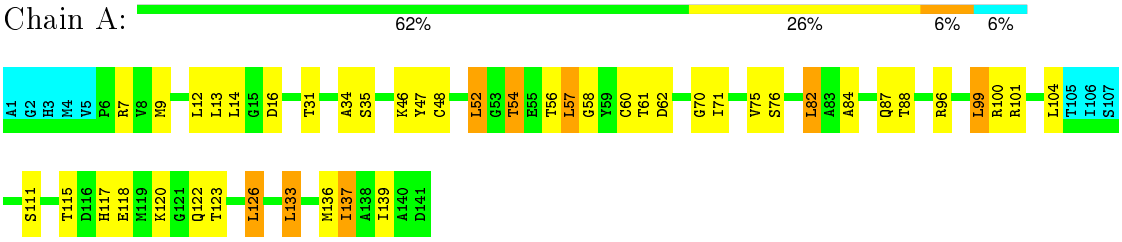
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Copper-transporting ATPase 2

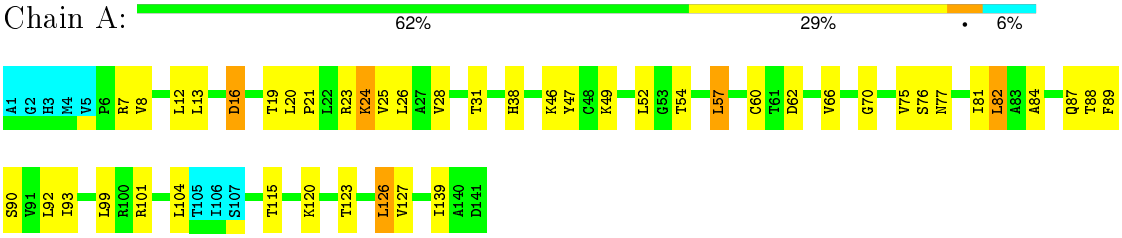
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Copper-transporting ATPase 2

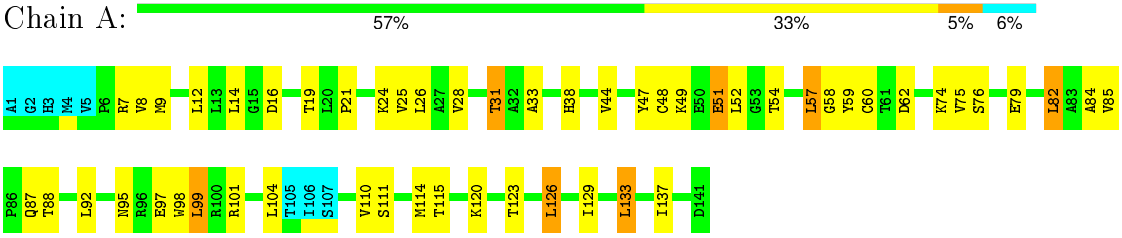
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Copper-transporting ATPase 2

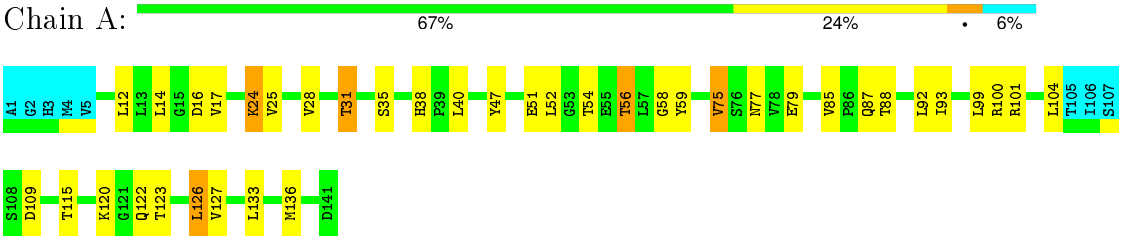
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Copper-transporting ATPase 2

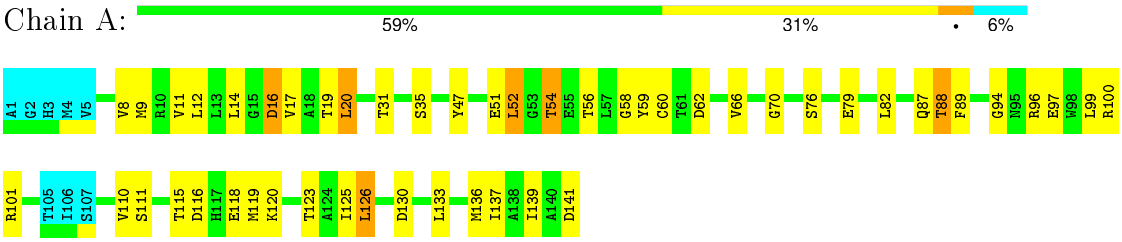
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Copper-transporting ATPase 2

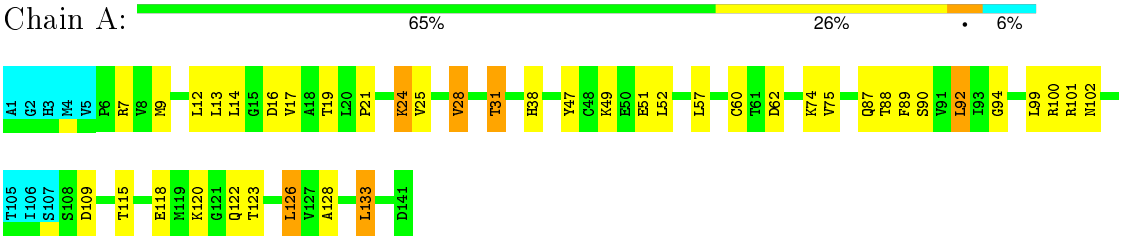
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Copper-transporting ATPase 2

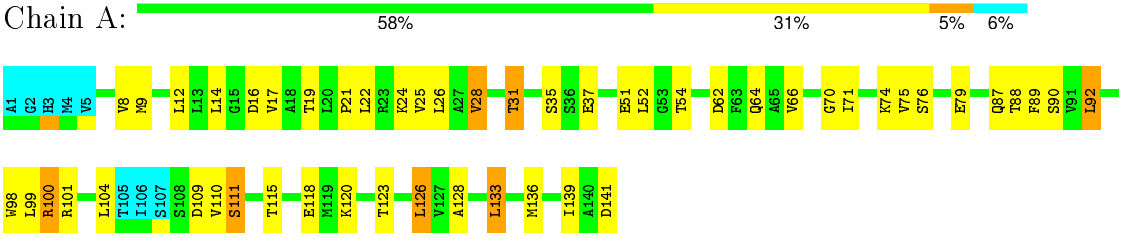
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Copper-transporting ATPase 2

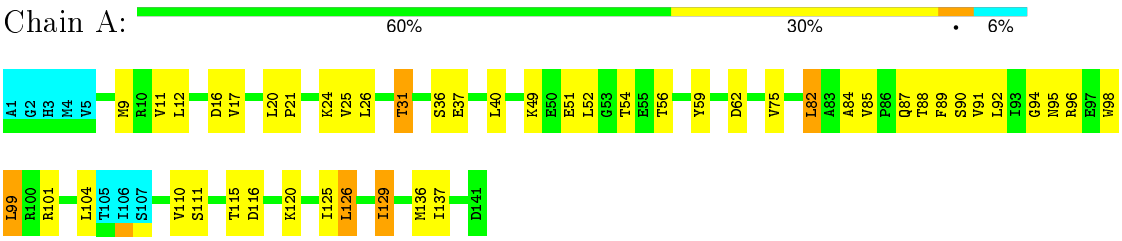
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Copper-transporting ATPase 2

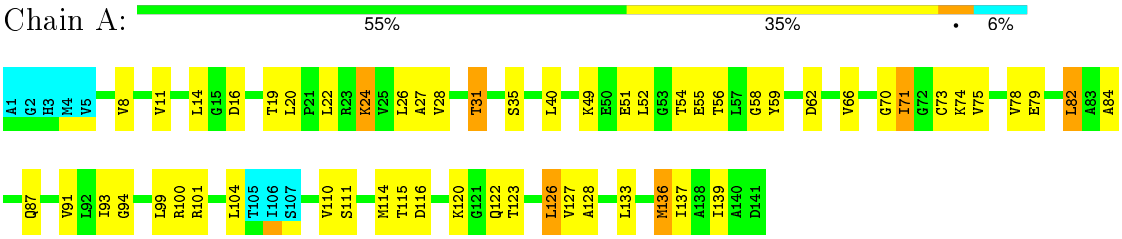
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Copper-transporting ATPase 2

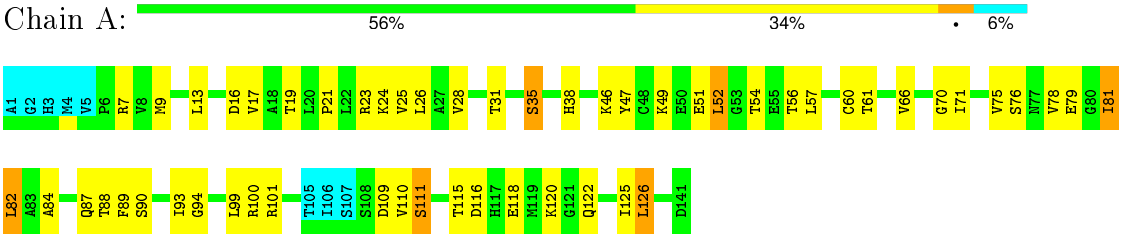
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Copper-transporting ATPase 2

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 1000 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
CYANA	structure solution	2.1
TALOS	refinement	

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

Chemical shift file(s)	BMRB entry 16536
Number of chemical shift lists	1
Total number of shifts	1529
Number of shifts mapped to atoms	1529
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	86%

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	971	1002	1002	19±4
All	All	19420	20040	20040	384

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 10.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:ALA:HB2	1:A:57:LEU:HD12	0.97	1.37	1	3
1:A:14:LEU:HD12	1:A:133:LEU:HD22	0.96	1.37	13	4
1:A:93:ILE:HD11	1:A:125:ILE:HD12	0.91	1.43	20	1
1:A:14:LEU:HD12	1:A:133:LEU:HD23	0.88	1.45	19	4
1:A:128:ALA:HB2	1:A:133:LEU:HD12	0.86	1.46	2	2
1:A:99:LEU:HD22	1:A:126:LEU:HD21	0.85	1.45	1	2
1:A:99:LEU:HD13	1:A:126:LEU:HD22	0.85	1.45	9	1
1:A:31:THR:HG22	1:A:75:VAL:HG12	0.85	1.44	19	3
1:A:99:LEU:HD21	1:A:133:LEU:HD11	0.83	1.49	11	1
1:A:31:THR:HG22	1:A:75:VAL:HG22	0.79	1.53	18	3
1:A:82:LEU:HD22	1:A:84:ALA:HB3	0.78	1.54	11	1
1:A:17:VAL:HG12	1:A:20:LEU:HD11	0.78	1.54	15	1
1:A:99:LEU:HD13	1:A:133:LEU:HD13	0.75	1.56	19	1
1:A:82:LEU:HD12	1:A:84:ALA:HB3	0.74	1.57	6	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:19:THR:HG23	1:A:20:LEU:HD22	0.74	1.59	6	2
1:A:11:VAL:HG12	1:A:137:ILE:HG23	0.73	1.59	5	2
1:A:99:LEU:HD22	1:A:126:LEU:HD22	0.70	1.60	16	4
1:A:11:VAL:HG22	1:A:137:ILE:HG23	0.70	1.62	15	1
1:A:14:LEU:HD12	1:A:133:LEU:HD11	0.69	1.62	7	1
1:A:99:LEU:HD12	1:A:126:LEU:HD13	0.68	1.65	10	1
1:A:17:VAL:HG22	1:A:25:VAL:HG22	0.68	1.64	16	2
1:A:93:ILE:HG22	1:A:125:ILE:HD11	0.67	1.66	2	2
1:A:82:LEU:HD13	1:A:85:VAL:CG2	0.65	2.22	1	1
1:A:93:ILE:HD13	1:A:127:VAL:HG22	0.65	1.69	19	1
1:A:99:LEU:HD12	1:A:126:LEU:HD21	0.64	1.70	18	1
1:A:11:VAL:HG13	1:A:137:ILE:HG13	0.64	1.68	15	1
1:A:14:LEU:HD12	1:A:133:LEU:CD1	0.64	2.23	7	2
1:A:92:LEU:HD13	1:A:98:TRP:CD1	0.63	2.29	13	2
1:A:111:SER:O	1:A:115:THR:HG22	0.63	1.94	20	3
1:A:28:VAL:HG22	1:A:89:PHE:CZ	0.63	2.29	9	3
1:A:31:THR:CG2	1:A:75:VAL:HG22	0.62	2.25	17	3
1:A:31:THR:CG2	1:A:75:VAL:HG12	0.61	2.21	19	4
1:A:99:LEU:HD11	1:A:133:LEU:HD12	0.61	1.72	13	1
1:A:14:LEU:CD1	1:A:133:LEU:HD23	0.61	2.23	19	3
1:A:126:LEU:N	1:A:126:LEU:HD13	0.60	2.12	12	2
1:A:35:SER:OG	1:A:75:VAL:HG11	0.60	1.96	20	2
1:A:8:VAL:HA	1:A:139:ILE:HG22	0.60	1.73	4	7
1:A:92:LEU:HD22	1:A:98:TRP:CZ3	0.60	2.32	17	1
1:A:31:THR:HG23	1:A:58:GLY:H	0.60	1.57	19	8
1:A:100:ARG:CB	1:A:110:VAL:HG11	0.60	2.27	17	1
1:A:52:LEU:HD22	1:A:54:THR:CG2	0.59	2.28	15	3
1:A:94:GLY:O	1:A:126:LEU:HD12	0.59	1.98	4	11
1:A:92:LEU:N	1:A:92:LEU:HD13	0.59	2.12	16	1
1:A:99:LEU:CB	1:A:126:LEU:HD13	0.59	2.28	14	2
1:A:14:LEU:HD12	1:A:133:LEU:CD2	0.58	2.28	17	3
1:A:100:ARG:HB2	1:A:110:VAL:HG11	0.58	1.73	17	2
1:A:93:ILE:HD12	1:A:127:VAL:HG22	0.58	1.72	6	2
1:A:92:LEU:HD13	1:A:98:TRP:CD2	0.58	2.34	17	1
1:A:31:THR:HG21	1:A:76:SER:N	0.58	2.13	9	13
1:A:60:CYS:HA	1:A:75:VAL:HG12	0.58	1.74	1	10
1:A:93:ILE:HG22	1:A:125:ILE:CD1	0.58	2.29	3	2
1:A:27:ALA:CB	1:A:78:VAL:HG11	0.57	2.29	3	1
1:A:26:LEU:HD12	1:A:52:LEU:CD2	0.57	2.29	2	1
1:A:99:LEU:CD2	1:A:133:LEU:HD11	0.57	2.26	11	1
1:A:100:ARG:NE	1:A:110:VAL:HG21	0.57	2.15	3	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:O	1:A:99:LEU:HD13	0.57	1.99	4	1
1:A:21:PRO:O	1:A:25:VAL:HG23	0.57	1.99	7	13
1:A:20:LEU:HD23	1:A:24:LYS:HB3	0.57	1.77	10	1
1:A:126:LEU:HD23	1:A:136:MET:HG2	0.56	1.76	4	1
1:A:20:LEU:HD12	1:A:25:VAL:HG22	0.56	1.75	8	1
1:A:54:THR:HG21	1:A:81:ILE:CD1	0.56	2.30	12	1
1:A:99:LEU:HD22	1:A:126:LEU:CD2	0.56	2.25	1	1
1:A:11:VAL:CG1	1:A:137:ILE:HG23	0.56	2.29	5	2
1:A:17:VAL:HB	1:A:25:VAL:HG22	0.56	1.77	5	8
1:A:28:VAL:HG13	1:A:89:PHE:CE2	0.56	2.35	10	2
1:A:28:VAL:HG22	1:A:89:PHE:CD1	0.56	2.35	20	6
1:A:82:LEU:CD2	1:A:84:ALA:HB3	0.56	2.30	11	1
1:A:74:LYS:HB3	1:A:88:THR:HG22	0.56	1.78	5	2
1:A:93:ILE:HG12	1:A:127:VAL:HG13	0.56	1.77	7	3
1:A:27:ALA:HB1	1:A:78:VAL:CG1	0.55	2.31	7	2
1:A:20:LEU:HD23	1:A:25:VAL:HG22	0.55	1.77	12	1
1:A:59:TYR:O	1:A:75:VAL:HG13	0.55	2.02	3	2
1:A:26:LEU:HD11	1:A:51:GLU:HB3	0.55	1.77	17	3
1:A:52:LEU:HD13	1:A:57:LEU:HD11	0.55	1.77	12	1
1:A:91:VAL:HG22	1:A:129:ILE:HD12	0.55	1.78	8	1
1:A:56:THR:C	1:A:57:LEU:HD13	0.55	2.23	9	1
1:A:126:LEU:HD12	1:A:126:LEU:O	0.55	2.02	6	1
1:A:33:ALA:HB1	1:A:44:VAL:HG21	0.54	1.79	13	1
1:A:82:LEU:HD23	1:A:85:VAL:HG22	0.54	1.78	4	1
1:A:66:VAL:HG23	1:A:70:GLY:O	0.53	2.02	10	2
1:A:31:THR:HG21	1:A:76:SER:CA	0.53	2.32	20	11
1:A:11:VAL:HG23	1:A:137:ILE:HG12	0.53	1.79	18	1
1:A:92:LEU:HD13	1:A:98:TRP:NE1	0.53	2.18	13	1
1:A:72:GLY:HA3	1:A:92:LEU:HD23	0.53	1.80	5	1
1:A:34:ALA:CB	1:A:57:LEU:HD12	0.53	2.33	7	1
1:A:11:VAL:HG23	1:A:137:ILE:HG13	0.53	1.78	9	1
1:A:100:ARG:CD	1:A:110:VAL:HG11	0.53	2.32	15	2
1:A:99:LEU:HD23	1:A:126:LEU:HB2	0.53	1.81	11	1
1:A:99:LEU:HD12	1:A:126:LEU:HD22	0.53	1.81	10	1
1:A:99:LEU:HB2	1:A:126:LEU:HD13	0.52	1.80	13	4
1:A:126:LEU:HD23	1:A:136:MET:CB	0.52	2.34	10	3
1:A:24:LYS:O	1:A:28:VAL:HG23	0.52	2.05	8	14
1:A:60:CYS:HB3	1:A:88:THR:HG23	0.52	1.82	15	1
1:A:137:ILE:CD1	1:A:139:ILE:HG23	0.52	2.34	11	1
1:A:57:LEU:HD13	1:A:57:LEU:N	0.52	2.20	9	1
1:A:93:ILE:HG13	1:A:127:VAL:HG13	0.52	1.81	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:LEU:HD13	1:A:133:LEU:HD11	0.51	1.81	1	1
1:A:99:LEU:CD2	1:A:133:LEU:HD13	0.51	2.35	14	1
1:A:99:LEU:CD2	1:A:126:LEU:HD22	0.51	2.35	19	1
1:A:100:ARG:CD	1:A:110:VAL:HG21	0.51	2.36	20	1
1:A:100:ARG:HD3	1:A:110:VAL:HG11	0.50	1.82	15	2
1:A:54:THR:HG21	1:A:81:ILE:HG21	0.50	1.83	20	1
1:A:92:LEU:HD13	1:A:98:TRP:CE3	0.50	2.42	17	1
1:A:35:SER:HB3	1:A:75:VAL:HG21	0.50	1.82	14	1
1:A:76:SER:OG	1:A:78:VAL:HG12	0.49	2.06	6	1
1:A:76:SER:OG	1:A:78:VAL:HG22	0.49	2.08	2	1
1:A:54:THR:CG2	1:A:81:ILE:HG21	0.49	2.37	20	1
1:A:14:LEU:HD12	1:A:133:LEU:HD12	0.49	1.83	15	1
1:A:92:LEU:CD2	1:A:128:ALA:HB3	0.49	2.37	16	2
1:A:126:LEU:HD23	1:A:136:MET:HB3	0.49	1.83	19	4
1:A:35:SER:CB	1:A:75:VAL:HG21	0.49	2.38	14	1
1:A:99:LEU:CD1	1:A:126:LEU:HD22	0.49	2.37	10	1
1:A:92:LEU:CD1	1:A:128:ALA:HB3	0.48	2.38	1	1
1:A:26:LEU:HD21	1:A:51:GLU:HB3	0.48	1.84	13	1
1:A:20:LEU:HD23	1:A:24:LYS:HG2	0.48	1.85	18	1
1:A:82:LEU:CD1	1:A:84:ALA:HB3	0.48	2.35	6	1
1:A:54:THR:HB	1:A:81:ILE:HD13	0.48	1.83	20	1
1:A:17:VAL:HG12	1:A:20:LEU:CD1	0.48	2.35	15	1
1:A:33:ALA:HB1	1:A:44:VAL:HG11	0.48	1.86	3	1
1:A:99:LEU:HD21	1:A:133:LEU:CD1	0.48	2.39	13	1
1:A:93:ILE:CD1	1:A:125:ILE:HD12	0.48	2.30	20	1
1:A:66:VAL:HG13	1:A:70:GLY:O	0.47	2.09	20	5
1:A:66:VAL:HG21	1:A:98:TRP:HE1	0.47	1.69	17	1
1:A:17:VAL:HG12	1:A:20:LEU:HD22	0.47	1.86	18	1
1:A:22:LEU:HD11	1:A:51:GLU:OE1	0.47	2.08	17	1
1:A:77:ASN:O	1:A:81:ILE:HG22	0.47	2.09	5	2
1:A:99:LEU:HD12	1:A:99:LEU:O	0.47	2.10	2	3
1:A:54:THR:HG21	1:A:81:ILE:HD13	0.46	1.87	5	1
1:A:93:ILE:HD11	1:A:125:ILE:CD1	0.46	2.31	20	1
1:A:93:ILE:HG12	1:A:127:VAL:HG22	0.46	1.87	12	1
1:A:92:LEU:HD21	1:A:128:ALA:HB3	0.46	1.88	16	1
1:A:28:VAL:HG22	1:A:89:PHE:CE1	0.46	2.46	3	1
1:A:20:LEU:CD1	1:A:25:VAL:HG22	0.46	2.39	8	1
1:A:91:VAL:HB	1:A:129:ILE:HD12	0.45	1.88	18	1
1:A:28:VAL:HG22	1:A:89:PHE:CE2	0.45	2.45	9	1
1:A:85:VAL:HG22	1:A:85:VAL:O	0.45	2.11	14	2
1:A:82:LEU:HD23	1:A:84:ALA:HB3	0.45	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:LYS:CB	1:A:88:THR:HG22	0.45	2.40	5	1
1:A:27:ALA:HB1	1:A:78:VAL:HG22	0.45	1.87	10	1
1:A:99:LEU:HD12	1:A:133:LEU:HD13	0.45	1.87	9	1
1:A:96:ARG:HG2	1:A:110:VAL:HG13	0.45	1.87	3	1
1:A:100:ARG:CZ	1:A:110:VAL:HG21	0.45	2.42	6	1
1:A:11:VAL:HG22	1:A:137:ILE:HD12	0.45	1.88	19	3
1:A:96:ARG:NH2	1:A:124:ALA:HB3	0.45	2.27	10	1
1:A:52:LEU:CD1	1:A:57:LEU:HD11	0.45	2.41	12	1
1:A:20:LEU:HD13	1:A:24:LYS:HG2	0.44	1.89	2	1
1:A:61:THR:HG21	1:A:88:THR:HG23	0.44	1.89	5	1
1:A:71:ILE:HG13	1:A:93:ILE:HG23	0.44	1.90	19	1
1:A:133:LEU:HD23	1:A:136:MET:SD	0.44	2.53	6	1
1:A:60:CYS:CA	1:A:75:VAL:HG12	0.44	2.42	5	2
1:A:85:VAL:O	1:A:85:VAL:HG13	0.44	2.13	13	2
1:A:22:LEU:O	1:A:26:LEU:HD23	0.44	2.12	2	1
1:A:70:GLY:O	1:A:71:ILE:HD13	0.44	2.13	11	1
1:A:20:LEU:HD12	1:A:25:VAL:CG2	0.44	2.40	8	1
1:A:92:LEU:HD22	1:A:98:TRP:HE1	0.43	1.73	7	1
1:A:26:LEU:HD22	1:A:52:LEU:HG	0.43	1.89	6	1
1:A:70:GLY:C	1:A:71:ILE:HD12	0.43	2.33	17	2
1:A:57:LEU:O	1:A:57:LEU:HD12	0.43	2.12	11	2
1:A:66:VAL:HG13	1:A:66:VAL:O	0.43	2.12	9	2
1:A:66:VAL:O	1:A:66:VAL:HG13	0.43	2.13	15	2
1:A:82:LEU:HD13	1:A:85:VAL:HB	0.43	1.89	18	1
1:A:26:LEU:O	1:A:52:LEU:HD11	0.43	2.13	20	1
1:A:70:GLY:O	1:A:71:ILE:HG23	0.43	2.14	19	1
1:A:99:LEU:HD23	1:A:126:LEU:CD2	0.43	2.43	5	1
1:A:129:ILE:C	1:A:130:ASP:CG	0.43	2.77	6	1
1:A:56:THR:HG22	1:A:77:ASN:HD21	0.43	1.73	14	1
1:A:126:LEU:O	1:A:126:LEU:HD22	0.43	2.14	5	2
1:A:99:LEU:HD23	1:A:133:LEU:HD13	0.43	1.89	14	1
1:A:100:ARG:HE	1:A:110:VAL:HG21	0.42	1.73	7	1
1:A:126:LEU:N	1:A:126:LEU:CD1	0.42	2.82	5	1
1:A:85:VAL:HG13	1:A:85:VAL:O	0.42	2.14	3	3
1:A:99:LEU:HD13	1:A:133:LEU:CD1	0.42	2.44	1	1
1:A:26:LEU:HD11	1:A:51:GLU:CG	0.42	2.44	2	1
1:A:99:LEU:HD12	1:A:126:LEU:CD1	0.42	2.40	10	1
1:A:8:VAL:HG13	1:A:137:ILE:HD11	0.42	1.90	13	1
1:A:100:ARG:NH2	1:A:104:LEU:HD22	0.42	2.29	9	1
1:A:73:CYS:O	1:A:91:VAL:HG12	0.42	2.14	19	1
1:A:11:VAL:HG22	1:A:137:ILE:CD1	0.42	2.44	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:ILE:O	1:A:130:ASP:CG	0.41	2.58	10	1
1:A:138:ALA:HB1	1:A:141:ASP:OD2	0.41	2.15	5	1
1:A:26:LEU:HD21	1:A:51:GLU:CG	0.41	2.45	18	1
1:A:94:GLY:O	1:A:125:ILE:HG23	0.41	2.16	5	1
1:A:92:LEU:HD22	1:A:98:TRP:CH2	0.41	2.50	17	1
1:A:99:LEU:HD13	1:A:99:LEU:C	0.41	2.36	20	2
1:A:11:VAL:CG2	1:A:137:ILE:HD12	0.41	2.45	10	1
1:A:100:ARG:CG	1:A:110:VAL:HG11	0.41	2.46	15	1
1:A:34:ALA:CB	1:A:57:LEU:HD13	0.41	2.45	11	1
1:A:11:VAL:HG23	1:A:137:ILE:CG1	0.41	2.45	9	1
1:A:96:ARG:CG	1:A:110:VAL:HG13	0.41	2.46	3	1
1:A:93:ILE:CD1	1:A:127:VAL:HG22	0.41	2.44	6	1
1:A:75:VAL:O	1:A:75:VAL:HG23	0.41	2.15	13	1
1:A:99:LEU:C	1:A:99:LEU:HD13	0.41	2.35	14	1
1:A:35:SER:CB	1:A:75:VAL:HG11	0.41	2.46	14	1
1:A:99:LEU:HD12	1:A:126:LEU:CD2	0.40	2.45	18	1
1:A:99:LEU:HD13	1:A:126:LEU:CD2	0.40	2.45	6	1
1:A:20:LEU:CD2	1:A:25:VAL:HG22	0.40	2.45	12	1
1:A:31:THR:HG22	1:A:75:VAL:CG1	0.40	2.46	3	1
1:A:93:ILE:HD12	1:A:126:LEU:O	0.40	2.17	19	1
1:A:95:ASN:HB3	1:A:125:ILE:HG22	0.40	1.93	18	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	132/141 (94%)	117±3 (88±2%)	15±3 (11±2%)	1±1 (0±0%)	38	79
All	All	2640/2820 (94%)	2334 (88%)	294 (11%)	12 (0%)	38	79

All 5 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	28	VAL	5

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Mol	Chain	Res	Type	Models (Total)
1	A	84	ALA	3
1	A	16	ASP	2
1	A	61	THR	1
1	A	78	VAL	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	105/111 (95%)	74±4 (70±4%)	31±4 (30±4%)	2 18
All	All	2100/2220 (95%)	1478 (70%)	622 (30%)	2 18

All 75 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	126	LEU	19
1	A	87	GLN	19
1	A	16	ASP	18
1	A	88	THR	18
1	A	123	THR	18
1	A	120	LYS	17
1	A	54	THR	17
1	A	115	THR	16
1	A	52	LEU	15
1	A	56	THR	15
1	A	111	SER	14
1	A	9	MET	14
1	A	104	LEU	14
1	A	82	LEU	14
1	A	101	ARG	14
1	A	90	SER	14
1	A	51	GLU	13
1	A	12	LEU	13
1	A	62	ASP	13
1	A	19	THR	13
1	A	47	TYR	13

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Mol	Chain	Res	Type	Models (Total)
1	A	7	ARG	12
1	A	49	LYS	12
1	A	57	LEU	12
1	A	100	ARG	11
1	A	31	THR	11
1	A	116	ASP	11
1	A	122	GLN	11
1	A	24	LYS	10
1	A	96	ARG	9
1	A	13	LEU	9
1	A	61	THR	9
1	A	38	HIS	9
1	A	92	LEU	8
1	A	99	LEU	8
1	A	46	LYS	8
1	A	136	MET	8
1	A	79	GLU	8
1	A	35	SER	8
1	A	109	ASP	8
1	A	40	LEU	7
1	A	118	GLU	6
1	A	133	LEU	6
1	A	89	PHE	6
1	A	114	MET	6
1	A	97	GLU	6
1	A	48	CYS	5
1	A	37	GLU	5
1	A	130	ASP	5
1	A	141	ASP	5
1	A	59	TYR	5
1	A	26	LEU	4
1	A	74	LYS	4
1	A	55	GLU	4
1	A	119	MET	4
1	A	23	ARG	3
1	A	60	CYS	3
1	A	77	ASN	3
1	A	81	ILE	3
1	A	129	ILE	3
1	A	36	SER	3
1	A	20	LEU	3
1	A	117	HIS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	64	GLN	2
1	A	125	ILE	2
1	A	108	SER	2
1	A	102	ASN	2
1	A	76	SER	2
1	A	137	ILE	1
1	A	95	ASN	1
1	A	98	TRP	1
1	A	10	ARG	1
1	A	71	ILE	1
1	A	22	LEU	1
1	A	75	VAL	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 86% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16536

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	1529
Number of shifts mapped to atoms	1529
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 ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	138	-0.51 ± 0.15	Should be applied
$^{13}C_{\beta}$	119	-0.22 ± 0.18	None needed (< 0.5 ppm)
$^{13}C'$	133	-0.20 ± 0.12	None needed (< 0.5 ppm)
^{15}N	134	0.14 ± 0.31	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 86%, i.e. 1287 atoms were assigned a chemical shift out of a possible 1505. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	642/655 (98%)	259/261 (99%)	256/266 (96%)	127/128 (99%)
Sidechain	626/790 (79%)	382/454 (84%)	238/307 (78%)	6/29 (21%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	19/60 (32%)	18/32 (56%)	0/25 (0%)	1/3 (33%)
Overall	1287/1505 (86%)	659/747 (88%)	494/598 (83%)	134/160 (84%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1353 atoms were assigned a chemical shift out of a possible 1587. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	678/695 (98%)	273/277 (99%)	271/282 (96%)	134/136 (99%)
Sidechain	656/825 (80%)	400/474 (84%)	250/322 (78%)	6/29 (21%)
Aromatic	19/67 (28%)	18/36 (50%)	0/27 (0%)	1/4 (25%)
Overall	1353/1587 (85%)	691/787 (88%)	521/631 (83%)	141/169 (83%)

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: