Full wwPDB NMR Structure Validation Report (i)

May 29, 2020 – 07:36 am BST

PDB ID	:	5LVY
Title	:	Structural studies of the Aggregative Adherence Fimbriae of Enteroaggregative Escherichia coli
Authors	:	Liu, B.; Matthews, S.
Deposited on	:	2016-09-14

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
https://www.wwpdb.org/validation/2017/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:

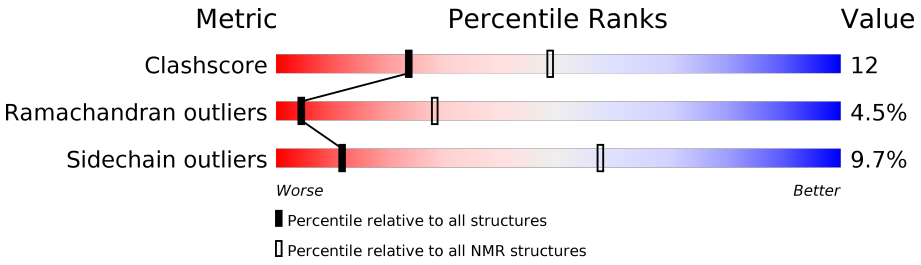
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 85%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	154	58% 27% • 11%

2 Ensemble composition and analysis

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:79, A:89-A:144, A:151-A:162 (137)	0.29	6

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2311 atoms, of which 1151 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adhesin protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2311	732	1151	192	232	4	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	VAL	ALA	conflict	UNP C9K5V2
A	132	ASP	-	expression tag	UNP C9K5V2
A	133	ASN	-	expression tag	UNP C9K5V2
A	134	LYS	-	expression tag	UNP C9K5V2
A	135	GLN	-	expression tag	UNP C9K5V2
A	136	ALA	-	expression tag	UNP C9K5V2
A	137	ASN	-	expression tag	UNP C9K5V2
A	138	PRO	-	expression tag	UNP C9K5V2
A	139	THR	-	expression tag	UNP C9K5V2
A	140	PRO	-	expression tag	UNP C9K5V2
A	141	SER	-	expression tag	UNP C9K5V2
A	142	SER	-	expression tag	UNP C9K5V2
A	143	LEU	-	expression tag	UNP C9K5V2
A	144	THR	-	expression tag	UNP C9K5V2
A	145	SER	-	expression tag	UNP C9K5V2
A	146	LYS	-	expression tag	UNP C9K5V2
A	147	ALA	-	expression tag	UNP C9K5V2
A	148	ALA	-	expression tag	UNP C9K5V2
A	149	GLY	-	expression tag	UNP C9K5V2
A	150	LYS	-	expression tag	UNP C9K5V2
A	151	ASN	-	expression tag	UNP C9K5V2
A	152	ILE	-	expression tag	UNP C9K5V2
A	153	VAL	-	expression tag	UNP C9K5V2
A	154	SER	-	expression tag	UNP C9K5V2
A	155	SER	-	expression tag	UNP C9K5V2
A	156	THR	-	expression tag	UNP C9K5V2
A	157	GLY	-	expression tag	UNP C9K5V2
A	158	THR	-	expression tag	UNP C9K5V2
A	159	ILE	-	expression tag	UNP C9K5V2
A	160	THR	-	expression tag	UNP C9K5V2
A	161	ILE	-	expression tag	UNP C9K5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP C9K5V2

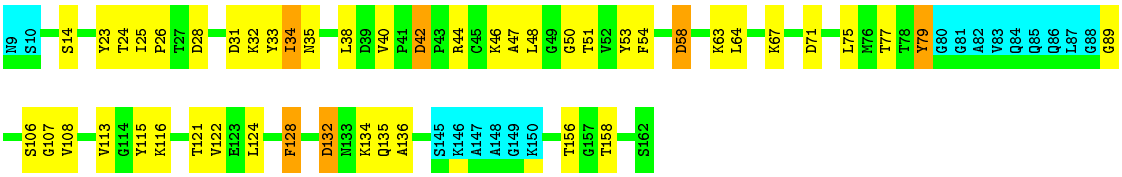
4 Residue-property plots (i)

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: Adhesin protein

Chain A:



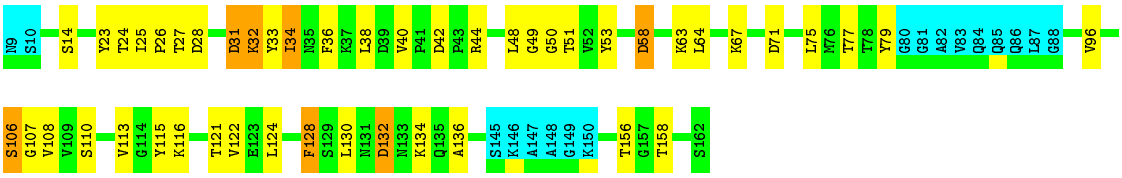
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Adhesin protein

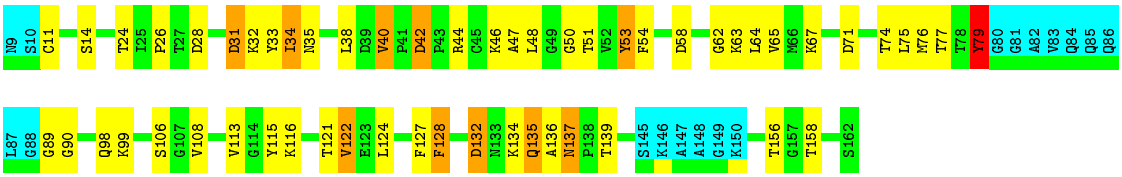
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: Adhesin protein

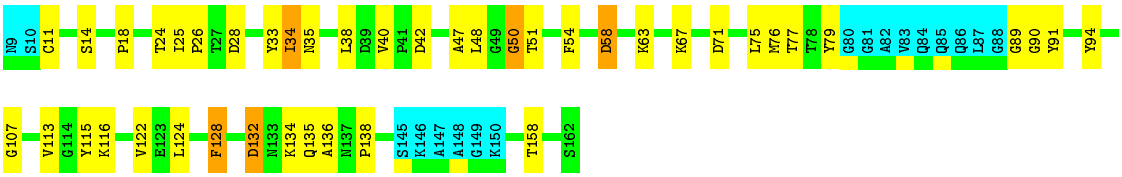
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: Adhesin protein

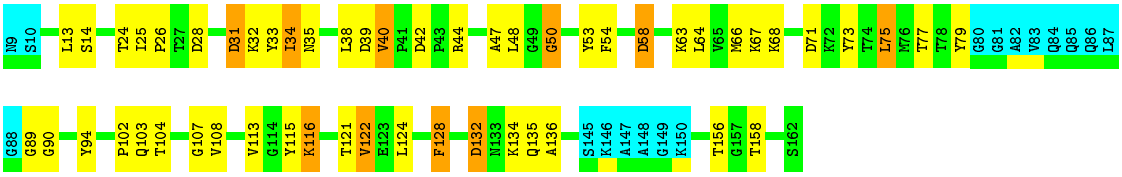
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Adhesin protein

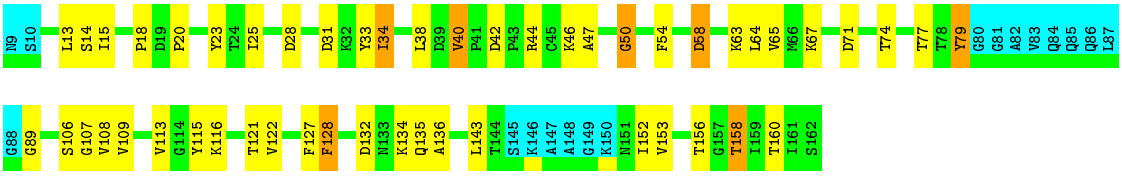
Chain A:



4.2.5 Score per residue for model 5

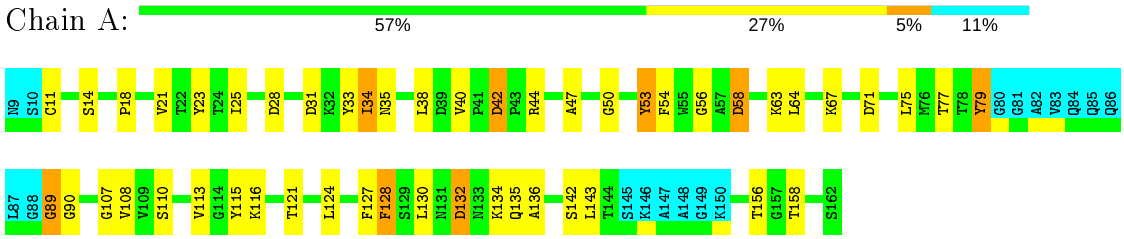
- Molecule 1: Adhesin protein

Chain A:



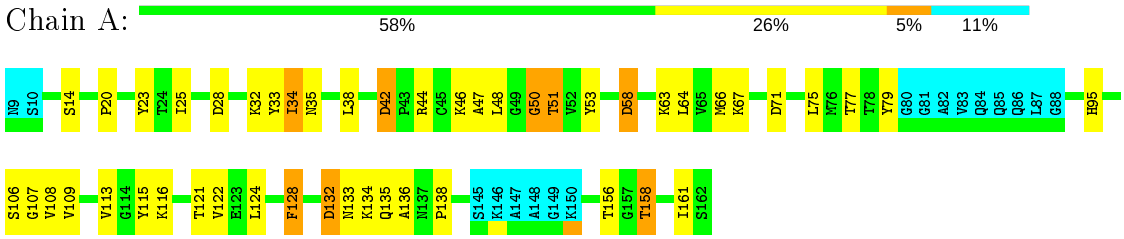
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Adhesin protein



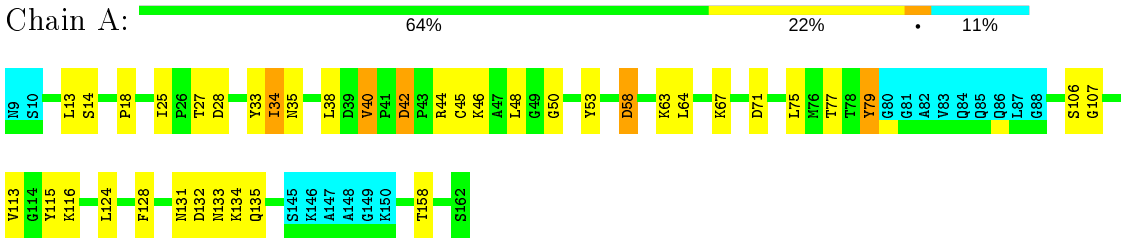
4.2.7 Score per residue for model 7

- Molecule 1: Adhesin protein



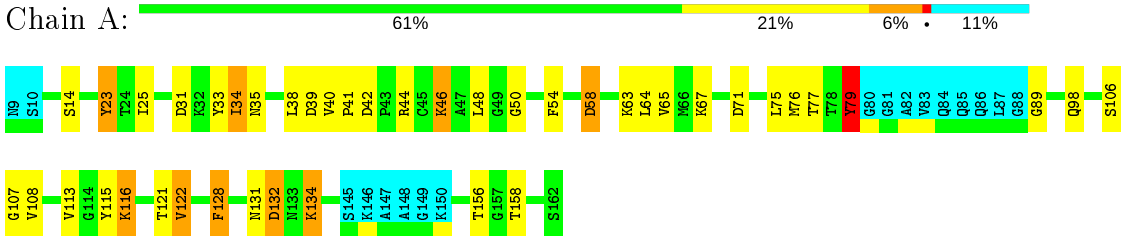
4.2.8 Score per residue for model 8

- Molecule 1: Adhesin protein



4.2.9 Score per residue for model 9

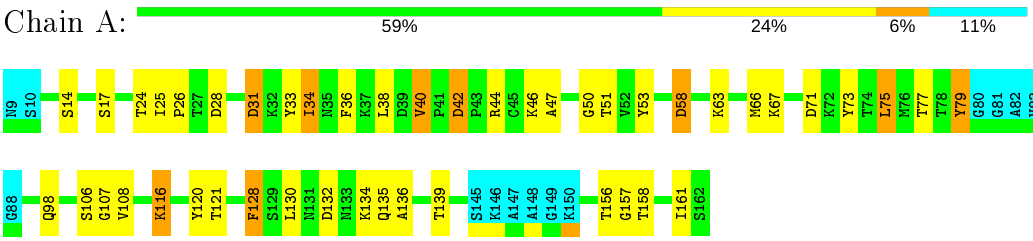
- Molecule 1: Adhesin protein



4.2.10 Score per residue for model 10

- Molecule 1: Adhesin protein

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 10 calculated structures, 10 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
ARIA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1049	1036	1035	26±4
All	All	10490	10360	10350	255

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:PHE:CZ	1:A:130:LEU:HG	0.71	2.19	10	2
1:A:14:SER:O	1:A:38:LEU:HA	0.70	1.87	1	10
1:A:50:GLY:HA2	1:A:128:PHE:CD2	0.62	2.30	10	9
1:A:67:LYS:HA	1:A:71:ASP:O	0.61	1.95	10	10
1:A:58:ASP:HB3	1:A:63:LYS:H	0.61	1.56	4	10
1:A:33:TYR:HA	1:A:107:GLY:O	0.60	1.96	3	9
1:A:47:ALA:O	1:A:135:GLN:HA	0.60	1.97	7	7
1:A:58:ASP:OD1	1:A:63:LYS:HG2	0.59	1.97	10	7
1:A:63:LYS:CB	1:A:77:THR:HB	0.58	2.29	10	9
1:A:42:ASP:O	1:A:46:LYS:HG3	0.57	1.98	5	3
1:A:24:THR:O	1:A:26:PRO:HD3	0.57	1.98	4	5
1:A:113:VAL:HG11	1:A:115:TYR:CE1	0.57	2.34	7	9
1:A:58:ASP:HB3	1:A:63:LYS:N	0.57	2.15	5	7
1:A:54:PHE:CZ	1:A:89:GLY:HA2	0.56	2.35	4	4
1:A:48:LEU:HG	1:A:132:ASP:H	0.54	1.63	9	7
1:A:20:PRO:CB	1:A:158:THR:HB	0.53	2.33	7	1
1:A:76:MET:O	1:A:108:VAL:HB	0.53	2.03	9	1
1:A:33:TYR:CE2	1:A:108:VAL:HG22	0.53	2.38	6	6
1:A:34:ILE:HD13	1:A:35:ASN:N	0.53	2.19	6	7
1:A:56:GLY:HA3	1:A:63:LYS:O	0.52	2.05	6	1
1:A:121:THR:CG2	1:A:156:THR:HB	0.52	2.34	4	8
1:A:34:ILE:O	1:A:106:SER:HA	0.52	2.05	5	7
1:A:25:ILE:CG2	1:A:28:ASP:HA	0.51	2.36	10	7
1:A:11:CYS:SG	1:A:42:ASP:HB2	0.51	2.46	3	2
1:A:42:ASP:OD1	1:A:44:ARG:HB3	0.51	2.05	8	2
1:A:127:PHE:CD1	1:A:152:ILE:HG13	0.50	2.41	5	1
1:A:46:LYS:HD3	1:A:98:GLN:O	0.49	2.08	10	2
1:A:64:LEU:HD21	1:A:124:LEU:HB2	0.49	1.83	6	6
1:A:46:LYS:CB	1:A:98:GLN:HA	0.48	2.38	2	1
1:A:33:TYR:CE1	1:A:108:VAL:HG22	0.48	2.43	4	1
1:A:17:SER:OG	1:A:157:GLY:HA2	0.48	2.08	10	1
1:A:63:LYS:HB3	1:A:77:THR:HB	0.48	1.84	4	8
1:A:54:PHE:CE1	1:A:89:GLY:HA2	0.48	2.43	2	5
1:A:128:PHE:CZ	1:A:130:LEU:HD23	0.48	2.43	1	1
1:A:51:THR:O	1:A:128:PHE:HA	0.48	2.09	3	5
1:A:45:CYS:O	1:A:48:LEU:HD23	0.47	2.09	8	1
1:A:65:VAL:HG22	1:A:74:THR:HA	0.47	1.84	5	2
1:A:58:ASP:HB3	1:A:64:LEU:H	0.47	1.70	4	2
1:A:128:PHE:CE2	1:A:130:LEU:HG	0.47	2.45	10	2
1:A:20:PRO:HB2	1:A:160:THR:OG1	0.47	2.10	5	1
1:A:63:LYS:HB2	1:A:77:THR:HB	0.46	1.87	10	2
1:A:46:LYS:HB3	1:A:46:LYS:NZ	0.46	2.26	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:VAL:HG21	1:A:33:TYR:O	0.46	2.11	6	1
1:A:23:TYR:CE2	1:A:109:VAL:HG11	0.45	2.46	5	2
1:A:64:LEU:HB2	1:A:77:THR:OG1	0.45	2.12	5	2
1:A:48:LEU:HG	1:A:132:ASP:N	0.45	2.26	9	1
1:A:40:VAL:HG21	1:A:128:PHE:CE1	0.45	2.46	10	2
1:A:33:TYR:CD1	1:A:108:VAL:HG22	0.45	2.46	4	1
1:A:23:TYR:CZ	1:A:25:ILE:HG12	0.45	2.47	6	3
1:A:23:TYR:CD1	1:A:32:LYS:HD2	0.45	2.47	1	1
1:A:11:CYS:SG	1:A:42:ASP:HB3	0.45	2.51	6	1
1:A:51:THR:HA	1:A:94:TYR:O	0.44	2.13	3	1
1:A:54:PHE:CD1	1:A:124:LEU:HD11	0.44	2.47	3	1
1:A:58:ASP:CB	1:A:63:LYS:H	0.44	2.24	4	2
1:A:131:ASN:OD1	1:A:134:LYS:HD2	0.43	2.13	9	1
1:A:48:LEU:HD11	1:A:133:ASN:N	0.43	2.28	7	1
1:A:39:ASP:O	1:A:41:PRO:HD3	0.43	2.12	9	1
1:A:66:MET:HB2	1:A:120:TYR:CB	0.43	2.44	10	1
1:A:64:LEU:HD22	1:A:122:VAL:HB	0.43	1.91	4	1
1:A:48:LEU:HD13	1:A:135:GLN:H	0.43	1.73	3	1
1:A:79:TYR:HA	1:A:106:SER:OG	0.42	2.13	2	1
1:A:20:PRO:HA	1:A:158:THR:O	0.42	2.14	7	2
1:A:51:THR:HG23	1:A:138:PRO:HD2	0.42	1.91	7	2
1:A:66:MET:HG2	1:A:75:LEU:HD21	0.42	1.90	4	2
1:A:32:LYS:C	1:A:33:TYR:HD2	0.42	2.18	7	1
1:A:33:TYR:HB3	1:A:106:SER:HB3	0.42	1.91	8	1
1:A:34:ILE:HD12	1:A:36:PHE:CE1	0.42	2.49	1	2
1:A:73:TYR:OH	1:A:116:LYS:HD2	0.42	2.15	10	2
1:A:67:LYS:HG2	1:A:121:THR:O	0.42	2.14	5	1
1:A:25:ILE:HG23	1:A:28:ASP:HA	0.42	1.92	6	1
1:A:131:ASN:OD1	1:A:134:LYS:HB2	0.42	2.15	8	1
1:A:40:VAL:O	1:A:46:LYS:HE2	0.41	2.15	2	1
1:A:32:LYS:C	1:A:33:TYR:HD1	0.41	2.19	4	1
1:A:15:ILE:HD11	1:A:153:VAL:HG23	0.41	1.93	5	1
1:A:20:PRO:HB3	1:A:158:THR:HB	0.41	1.91	7	1
1:A:27:THR:O	1:A:28:ASP:HB2	0.41	2.16	1	2
1:A:33:TYR:N	1:A:33:TYR:CD1	0.41	2.86	4	1
1:A:65:VAL:O	1:A:122:VAL:HA	0.41	2.16	2	2
1:A:33:TYR:CD2	1:A:33:TYR:N	0.41	2.89	10	1
1:A:53:TYR:HB2	1:A:127:PHE:CE1	0.41	2.50	2	2
1:A:13:LEU:HD23	1:A:40:VAL:N	0.41	2.31	4	3
1:A:66:MET:SD	1:A:161:ILE:HD11	0.41	2.56	10	2
1:A:49:GLY:HA2	1:A:96:VAL:O	0.40	2.16	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:137:ASN:N	1:A:137:ASN:HD22	0.40	2.14	2	1
1:A:46:LYS:HB2	1:A:98:GLN:HA	0.40	1.93	2	1
1:A:68:LYS:O	1:A:68:LYS:HG3	0.40	2.16	4	1
1:A:116:LYS:H	1:A:116:LYS:HD2	0.40	1.77	9	1
1:A:13:LEU:HD23	1:A:39:ASP:C	0.40	2.36	4	1

5.2 Torsion angles (i)

5.2.1 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	136/154 (88%)	112±2 (82±2%)	18±2 (13±1%)	6±1 (4±1%)	4	28
All	All	1360/1540 (88%)	1118 (82%)	181 (13%)	61 (4%)	4	28

All 15 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	132	ASP	9
1	A	134	LYS	9
1	A	136	ALA	8
1	A	42	ASP	8
1	A	50	GLY	5
1	A	31	ASP	5
1	A	18	PRO	4
1	A	90	GLY	4
1	A	110	SER	2
1	A	28	ASP	2
1	A	89	GLY	1
1	A	135	GLN	1
1	A	133	ASN	1
1	A	139	THR	1
1	A	62	GLY	1

5.2.2 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	120/130 (92%)	108±2 (90±2%)	12±2 (10±2%)	12	57
All	All	1200/1300 (92%)	1084 (90%)	116 (10%)	12	57

All 27 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	79	TYR	10
1	A	128	PHE	10
1	A	158	THR	10
1	A	116	LYS	10
1	A	34	ILE	10
1	A	75	LEU	9
1	A	58	ASP	9
1	A	40	VAL	8
1	A	122	VAL	7
1	A	44	ARG	7
1	A	31	ASP	6
1	A	76	MET	2
1	A	143	LEU	2
1	A	32	LYS	2
1	A	46	LYS	2
1	A	102	PRO	1
1	A	99	LYS	1
1	A	137	ASN	1
1	A	91	TYR	1
1	A	95	HIS	1
1	A	135	GLN	1
1	A	42	ASP	1
1	A	132	ASP	1
1	A	103	GLN	1
1	A	51	THR	1
1	A	106	SER	1
1	A	139	THR	1

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

There are no ligands in this entry.

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 85% for the well-defined parts and 83% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *agg3.str*

6.1.1 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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	134

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	144	0.11 ± 0.14	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	127	-0.12 ± 0.10	None needed (< 0.5 ppm)
$^{13}C'$	139	0.29 ± 0.06	None needed (< 0.5 ppm)
^{15}N	129	-0.53 ± 0.38	None needed (imprecise)

6.1.3 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 85%, i.e. 1364 atoms were assigned a chemical shift out of a possible 1596. 18 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	628/665 (94%)	250/264 (95%)	259/274 (95%)	119/127 (94%)
Sidechain	625/795 (79%)	383/468 (82%)	242/298 (81%)	0/29 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	111/136 (82%)	56/70 (80%)	54/63 (86%)	1/3 (33%)
Overall	1364/1596 (85%)	689/802 (86%)	555/635 (87%)	120/159 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 1462 atoms were assigned a chemical shift out of a possible 1771. 19 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	683/750 (91%)	271/298 (91%)	283/308 (92%)	129/144 (90%)
Sidechain	668/885 (75%)	409/521 (79%)	259/329 (79%)	0/35 (0%)
Aromatic	111/136 (82%)	56/70 (80%)	54/63 (86%)	1/3 (33%)
Overall	1462/1771 (83%)	736/889 (83%)	596/700 (85%)	130/182 (71%)

6.1.4 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	128	PHE	CD2	91.39	137.34 – 125.84	-35.0
1	A	127	PHE	CD2	91.57	137.34 – 125.84	-34.8
1	A	54	PHE	CD2	91.66	137.34 – 125.84	-34.7
1	A	36	PHE	CD2	91.83	137.34 – 125.84	-34.6
1	A	53	TYR	CE1	75.75	124.14 – 111.74	-34.0
1	A	128	PHE	CE2	89.97	136.81 – 124.71	-33.7
1	A	127	PHE	CE2	90.47	136.81 – 124.71	-33.3
1	A	36	PHE	CE2	90.58	136.81 – 124.71	-33.2
1	A	93	TYR	CE1	76.92	124.14 – 111.74	-33.1
1	A	120	TYR	CE1	76.93	124.14 – 111.74	-33.1
1	A	23	TYR	CD1	90.78	139.11 – 126.41	-33.1
1	A	128	PHE	CD1	91.39	137.63 – 125.43	-32.9
1	A	127	PHE	CD1	91.57	137.63 – 125.43	-32.8
1	A	33	TYR	CE1	77.38	124.14 – 111.74	-32.7
1	A	54	PHE	CD1	91.66	137.63 – 125.43	-32.7
1	A	79	TYR	CE1	77.47	124.14 – 111.74	-32.6
1	A	23	TYR	CE1	77.56	124.14 – 111.74	-32.6
1	A	36	PHE	CD1	91.83	137.63 – 125.43	-32.5
1	A	115	TYR	CD1	91.67	139.11 – 126.41	-32.4
1	A	73	TYR	CE1	77.92	124.14 – 111.74	-32.3
1	A	115	TYR	CE1	78.19	124.14 – 111.74	-32.1
1	A	93	TYR	CD1	92.29	139.11 – 126.41	-31.9

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	33	TYR	CD1	92.47	139.11 – 126.41	-31.7
1	A	94	TYR	CD1	92.97	139.11 – 126.41	-31.3
1	A	79	TYR	CD1	93.01	139.11 – 126.41	-31.3
1	A	53	TYR	CE2	75.75	124.68 – 111.18	-31.2
1	A	91	TYR	CD1	93.58	139.11 – 126.41	-30.9
1	A	73	TYR	CD1	93.64	139.11 – 126.41	-30.8
1	A	53	TYR	CD1	93.72	139.11 – 126.41	-30.7
1	A	120	TYR	CD1	93.88	139.11 – 126.41	-30.6
1	A	93	TYR	CE2	76.92	124.68 – 111.18	-30.4
1	A	120	TYR	CE2	76.93	124.68 – 111.18	-30.4
1	A	33	TYR	CE2	77.38	124.68 – 111.18	-30.0
1	A	79	TYR	CE2	77.47	124.68 – 111.18	-30.0
1	A	23	TYR	CE2	77.56	124.68 – 111.18	-29.9
1	A	15	ILE	CG2	59.91	24.63 – 10.43	29.8
1	A	105	ILE	CG2	59.80	24.63 – 10.43	29.8
1	A	73	TYR	CE2	77.92	124.68 – 111.18	-29.6
1	A	152	ILE	CG2	59.58	24.63 – 10.43	29.6
1	A	115	TYR	CE2	78.19	124.68 – 111.18	-29.4
1	A	159	ILE	CG2	58.17	24.63 – 10.43	28.6
1	A	161	ILE	CG2	57.92	24.63 – 10.43	28.4
1	A	25	ILE	CG2	57.84	24.63 – 10.43	28.4
1	A	23	TYR	CD2	90.78	140.11 – 125.31	-28.3
1	A	153	VAL	CG1	60.57	28.40 – 14.60	28.3
1	A	128	PHE	CE1	89.97	137.92 – 123.42	-28.1
1	A	145	SER	CB	22.21	71.24 – 56.34	-27.9
1	A	141	SER	CB	22.21	71.24 – 56.34	-27.9
1	A	16	SER	CB	22.39	71.24 – 56.34	-27.8
1	A	17	SER	CB	22.47	71.24 – 56.34	-27.7
1	A	115	TYR	CD2	91.67	140.11 – 125.31	-27.7
1	A	127	PHE	CE1	90.47	137.92 – 123.42	-27.7
1	A	36	PHE	CE1	90.58	137.92 – 123.42	-27.7
1	A	10	SER	CB	22.68	71.24 – 56.34	-27.6
1	A	142	SER	CB	22.73	71.24 – 56.34	-27.6
1	A	34	ILE	CG2	56.34	24.63 – 10.43	27.3
1	A	93	TYR	CD2	92.29	140.11 – 125.31	-27.3
1	A	33	TYR	CD2	92.47	140.11 – 125.31	-27.2
1	A	110	SER	CB	23.76	71.24 – 56.34	-26.9
1	A	94	TYR	CD2	92.97	140.11 – 125.31	-26.8
1	A	79	TYR	CD2	93.01	140.11 – 125.31	-26.8
1	A	129	SER	CB	23.84	71.24 – 56.34	-26.8
1	A	14	SER	CB	24.00	71.24 – 56.34	-26.7
1	A	12	SER	CB	24.18	71.24 – 56.34	-26.6

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	138	PRO	CA	21.88	71.13 – 55.53	-26.6
1	A	106	SER	CB	24.21	71.24 – 56.34	-26.6
1	A	162	SER	CB	24.34	71.24 – 56.34	-26.5
1	A	91	TYR	CD2	93.58	140.11 – 125.31	-26.4
1	A	102	PRO	CA	22.11	71.13 – 55.53	-26.4
1	A	73	TYR	CD2	93.64	140.11 – 125.31	-26.4
1	A	53	TYR	CD2	93.72	140.11 – 125.31	-26.3
1	A	97	SER	CB	24.55	71.24 – 56.34	-26.3
1	A	20	PRO	CA	22.29	71.13 – 55.53	-26.3
1	A	120	TYR	CD2	93.88	140.11 – 125.31	-26.2
1	A	55	TRP	CZ2	74.59	121.76 – 106.66	-26.2
1	A	117	PRO	CA	22.64	71.13 – 55.53	-26.1
1	A	127	PHE	CZ	89.23	137.04 – 121.44	-25.6
1	A	155	SER	CB	25.62	71.24 – 56.34	-25.6
1	A	159	ILE	CD1	56.60	21.91 – 5.01	25.5
1	A	154	SER	CB	25.77	71.24 – 56.34	-25.5
1	A	140	PRO	CA	23.65	71.13 – 55.53	-25.4
1	A	43	PRO	CA	23.88	71.13 – 55.53	-25.3
1	A	26	PRO	CA	24.18	71.13 – 55.53	-25.1
1	A	74	THR	CB	27.77	78.10 – 61.30	-25.0
1	A	144	THR	CB	27.88	78.10 – 61.30	-24.9
1	A	59	THR	CB	27.88	78.10 – 61.30	-24.9
1	A	153	VAL	CG2	60.57	29.20 – 13.40	24.9
1	A	34	ILE	CD1	55.33	21.91 – 5.01	24.8
1	A	139	THR	CB	28.26	78.10 – 61.30	-24.7
1	A	25	ILE	CD1	54.95	21.91 – 5.01	24.5
1	A	104	THR	CB	28.48	78.10 – 61.30	-24.5
1	A	160	THR	CB	28.67	78.10 – 61.30	-24.4
1	A	15	ILE	CD1	54.58	21.91 – 5.01	24.3
1	A	24	THR	CB	29.00	78.10 – 61.30	-24.2
1	A	100	THR	CB	29.14	78.10 – 61.30	-24.1
1	A	27	THR	CB	29.22	78.10 – 61.30	-24.1
1	A	152	ILE	CD1	53.83	21.91 – 5.01	23.9
1	A	22	THR	CB	29.63	78.10 – 61.30	-23.9
1	A	105	ILE	CD1	53.63	21.91 – 5.01	23.8
1	A	125	THR	CB	29.84	78.10 – 61.30	-23.7
1	A	121	THR	CB	30.45	78.10 – 61.30	-23.4
1	A	77	THR	CB	30.64	78.10 – 61.30	-23.3
1	A	147	ALA	CB	61.02	28.03 – 9.93	23.2
1	A	55	TRP	CH2	80.97	133.06 – 114.56	-23.2
1	A	78	THR	CB	30.89	78.10 – 61.30	-23.1
1	A	156	THR	CB	30.94	78.10 – 61.30	-23.1

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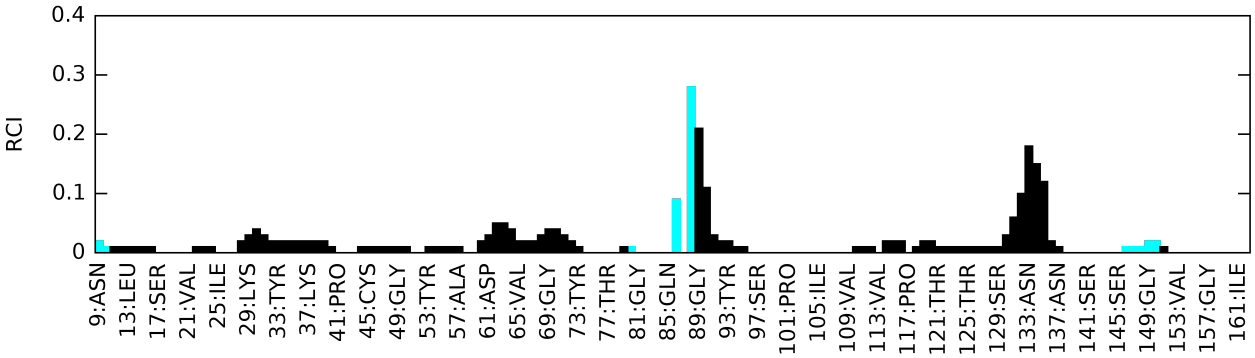
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	158	THR	CB	30.97	78.10 – 61.30	-23.1
1	A	51	THR	CB	31.07	78.10 – 61.30	-23.0
1	A	57	ALA	CB	60.55	28.03 – 9.93	23.0
1	A	136	ALA	CB	60.44	28.03 – 9.93	22.9
1	A	161	ILE	CD1	51.73	21.91 – 5.01	22.6
1	A	82	ALA	CB	59.60	28.03 – 9.93	22.4
1	A	148	ALA	CB	59.16	28.03 – 9.93	22.2
1	A	47	ALA	CB	59.08	28.03 – 9.93	22.2
1	A	55	TRP	CD1	88.08	136.18 – 116.78	-19.8
1	A	158	THR	CA	20.30	75.37 – 49.07	-15.9
1	A	77	THR	CA	20.77	75.37 – 49.07	-15.8
1	A	104	THR	CA	20.98	75.37 – 49.07	-15.7
1	A	51	THR	CA	20.98	75.37 – 49.07	-15.7
1	A	27	THR	CA	21.02	75.37 – 49.07	-15.7
1	A	160	THR	CA	21.30	75.37 – 49.07	-15.6
1	A	100	THR	CA	21.87	75.37 – 49.07	-15.3
1	A	59	THR	CA	22.28	75.37 – 49.07	-15.2
1	A	144	THR	CA	22.29	75.37 – 49.07	-15.2
1	A	152	ILE	CA	20.88	75.08 – 48.18	-15.1
1	A	74	THR	CA	22.65	75.37 – 49.07	-15.0
1	A	96	VAL	CA	20.67	76.93 – 48.03	-14.5
1	A	52	VAL	CA	20.80	76.93 – 48.03	-14.4
1	A	109	VAL	CA	20.98	76.93 – 48.03	-14.4
1	A	83	VAL	CA	21.16	76.93 – 48.03	-14.3
1	A	113	VAL	CA	21.37	76.93 – 48.03	-14.2
1	A	108	VAL	CA	21.44	76.93 – 48.03	-14.2
1	A	95	HIS	CD2	79.80	137.40 – 103.40	-11.9
1	A	125	THR	HB	2.51	5.82 – 2.52	-5.0

6.1.5 Random Coil Index (RCI) plots

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:


RCI
0.4
0.3
0.2
0.1
0
9:ASN
13:LEU
17:SER
21:VAL
25:ILE
29:LYS
33:TYR
37:LYS
41:PRO
45:CYS
49:GLY
53:TYR
57:ALA
61:ASP
65:VAL
69:GLY
73:TYR
77:THR
81:GLY
85:GLN
89:GLY
93:TYR
97:SER
101:PRO
105:ILE
109:VAL
113:VAL
117:PRO
121:THR
125:THR
129:SER
133:ASN
137:ASN
141:SER
145:SER
149:GLY
153:VAL
157:GLY
161:ILE