Full wwPDB NMR Structure Validation Report (i)

Apr 16, 2023 – 07:48 AM EDT

PDB ID	:	7Z3C
BMRB ID	:	51096
Title	:	A novel molecular switch controls assembly of bacterial focal adhesions in response to changes in surface structure.
Authors	:	Attia, B.; My, L.; Castaing, J.P.; Le Guenno, H.; Espinosa, L.; Schmidt, V.; Nouailler, M.; Bornet, O.; Elantak, L.; Mignot, T.
Deposited on	:	2022-03-02

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

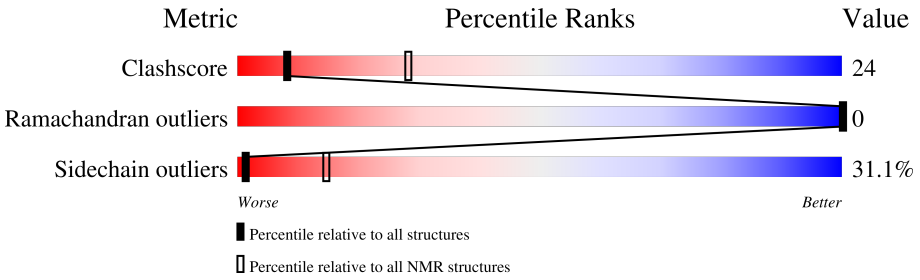
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance

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

The overall completeness of chemical shifts assignment is 88%.

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	85	35% 27% 6% 32%

2 Ensemble composition and analysis (i)

This entry contains 19 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:149-A:206 (58)	0.20	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1292 atoms, of which 635 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adventurous gliding motility protein GltJ.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	85	1292	419	635	109	127	2	0

There is a discrepancy between the modelled and reference sequences:

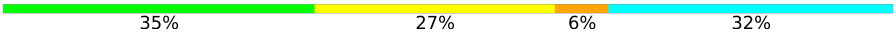
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP A0A7Y4JDV0

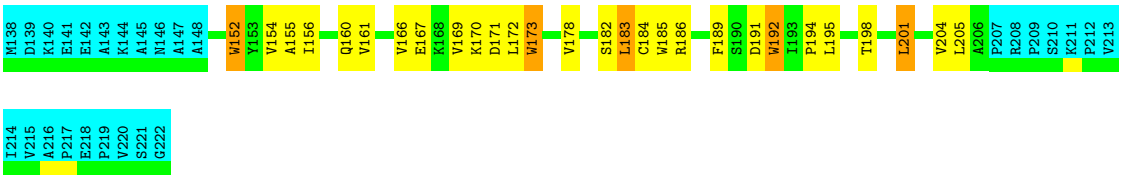
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Adventurous gliding motility protein GltJ

Chain A: 

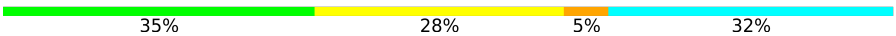


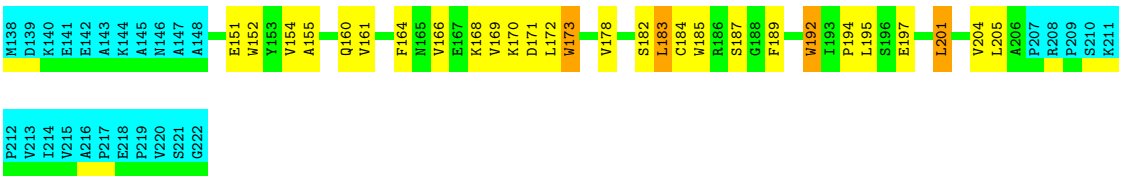
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

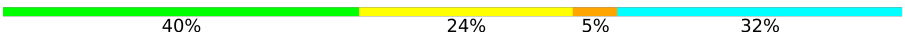
• Molecule 1: Adventurous gliding motility protein GltJ

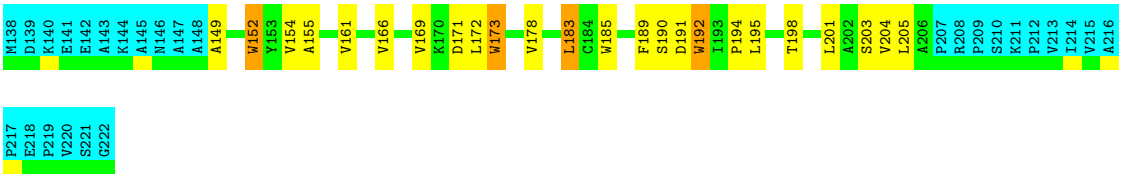
Chain A: 



4.2.2 Score per residue for model 2

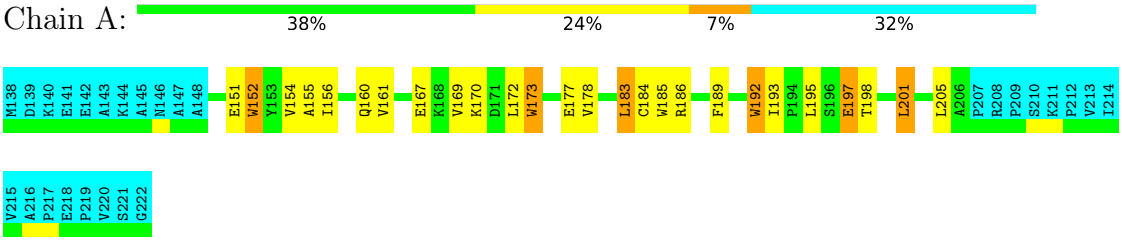
• Molecule 1: Adventurous gliding motility protein GltJ

Chain A: 



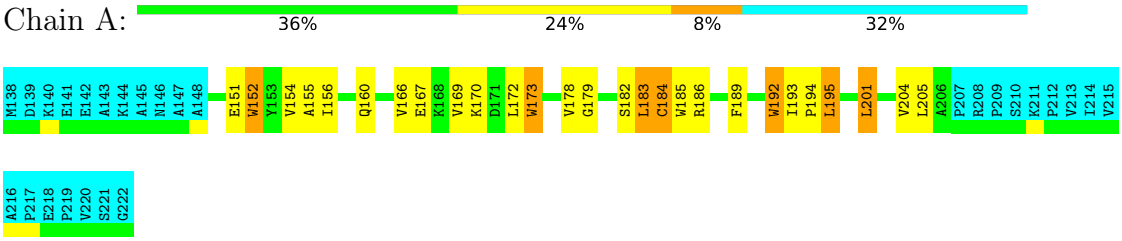
4.2.3 Score per residue for model 3

• Molecule 1: Adventurous gliding motility protein GltJ



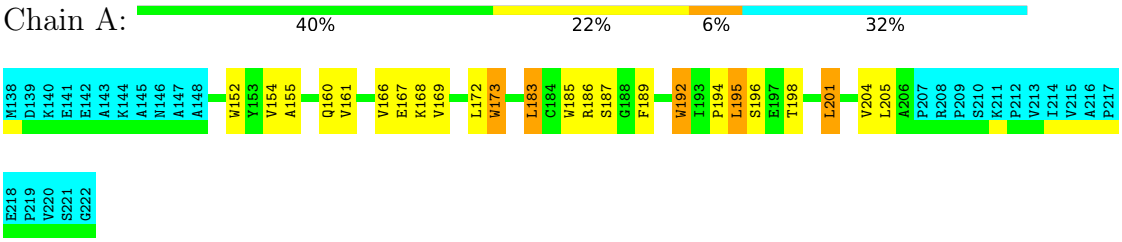
4.2.4 Score per residue for model 4

• Molecule 1: Adventurous gliding motility protein GltJ



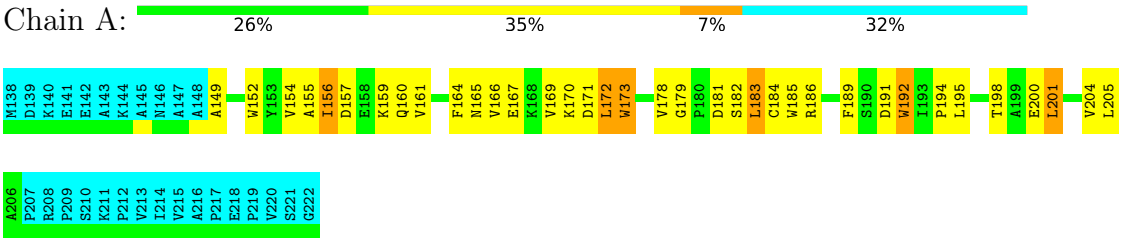
4.2.5 Score per residue for model 5

• Molecule 1: Adventurous gliding motility protein GltJ



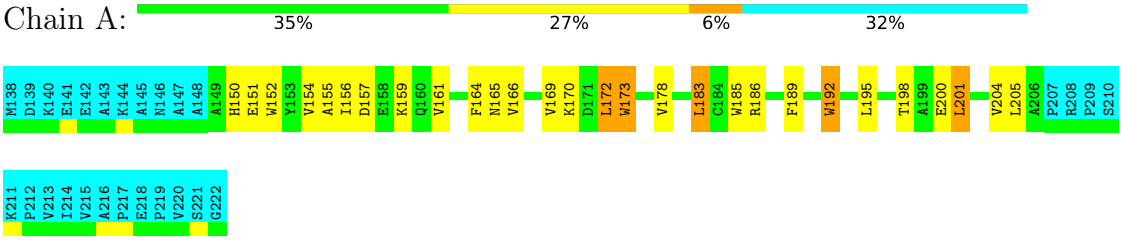
4.2.6 Score per residue for model 6

• Molecule 1: Adventurous gliding motility protein GltJ



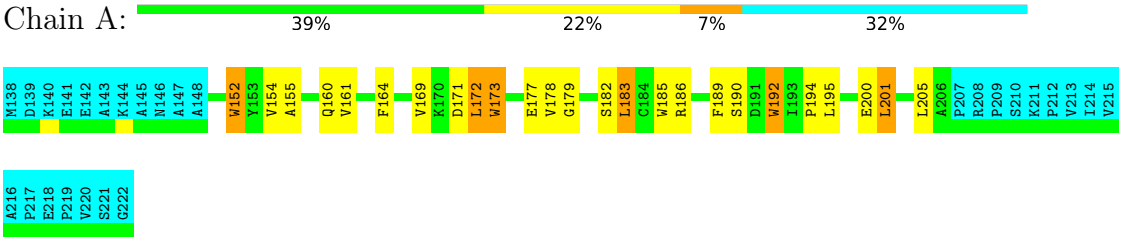
4.2.7 Score per residue for model 7

• Molecule 1: Adventurous gliding motility protein GltJ



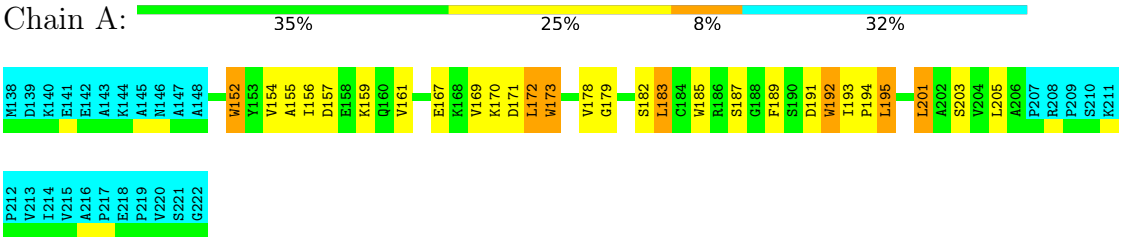
4.2.8 Score per residue for model 8

• Molecule 1: Adventurous gliding motility protein GltJ



4.2.9 Score per residue for model 9

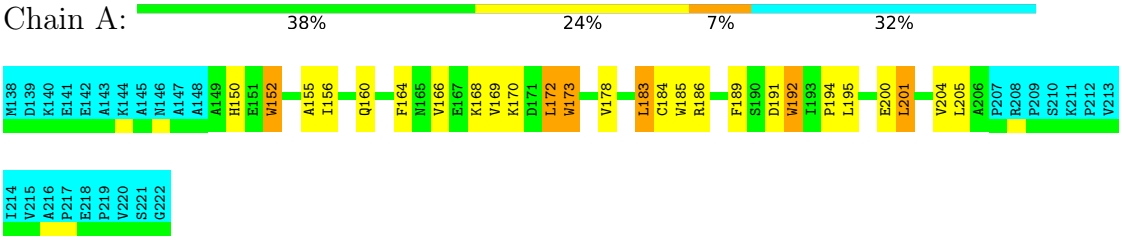
• Molecule 1: Adventurous gliding motility protein GltJ



4.2.10 Score per residue for model 10

• Molecule 1: Adventurous gliding motility protein GltJ

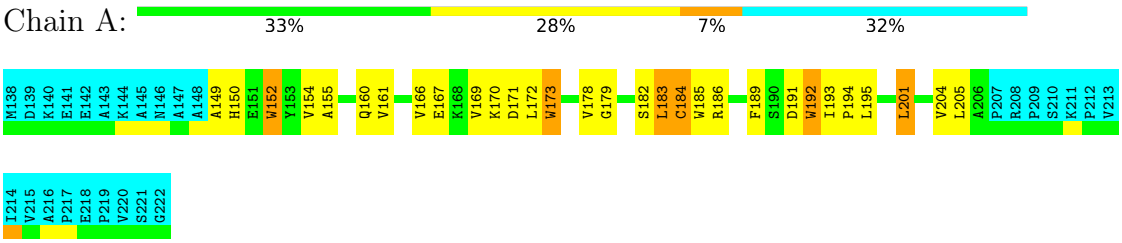
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Adventurous gliding motility protein GltJ

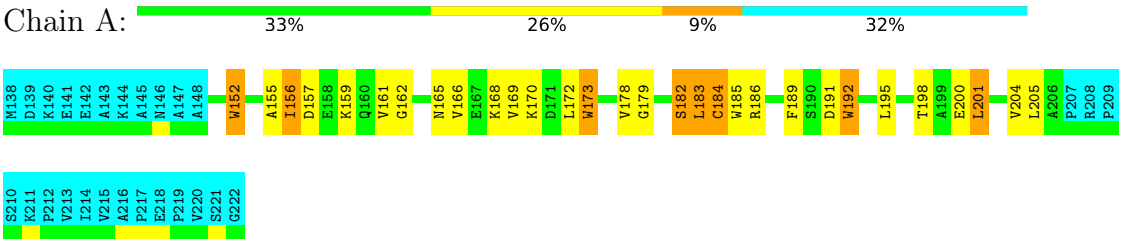
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Adventurous gliding motility protein GltJ

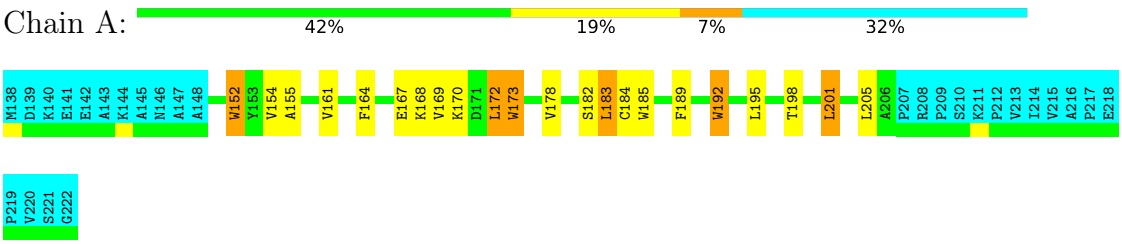
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Adventurous gliding motility protein GltJ

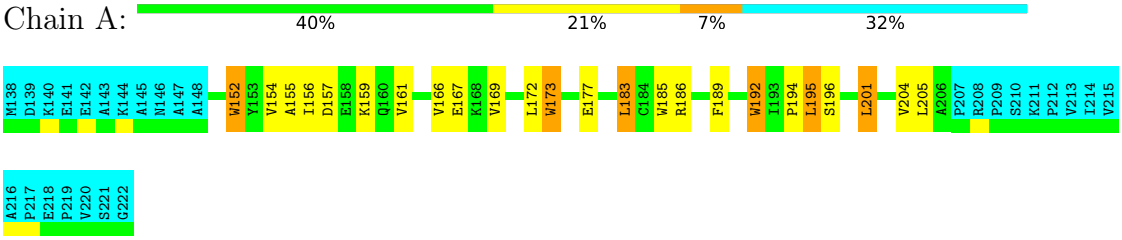
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Adventurous gliding motility protein GltJ

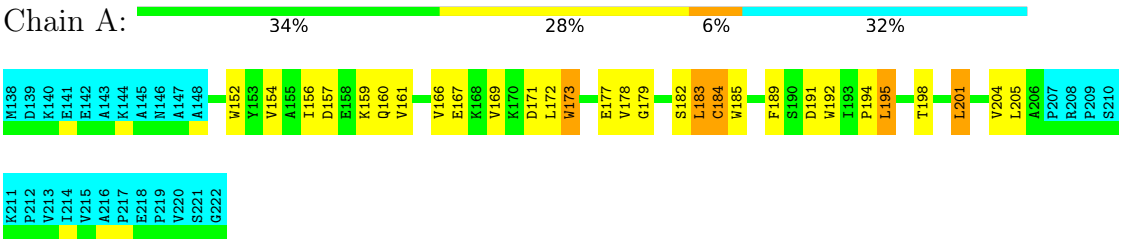
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Adventurous gliding motility protein GltJ

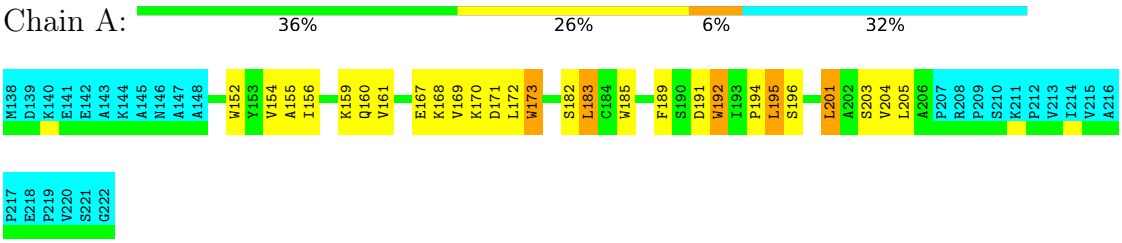
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Adventurous gliding motility protein GltJ

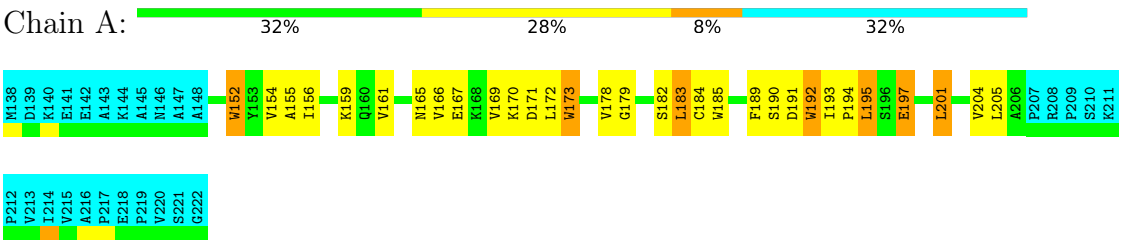
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Adventurous gliding motility protein GltJ

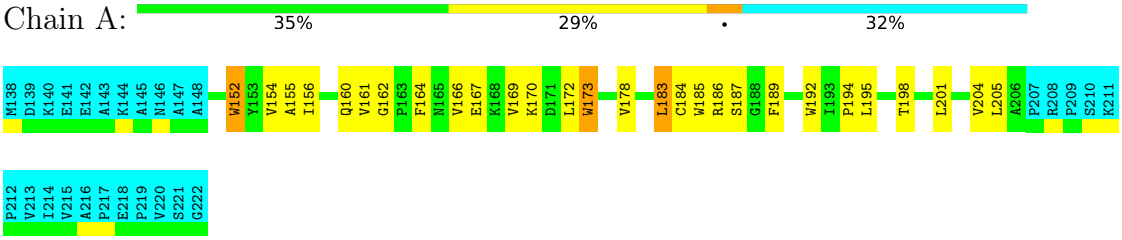
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Adventurous gliding motility protein GltJ

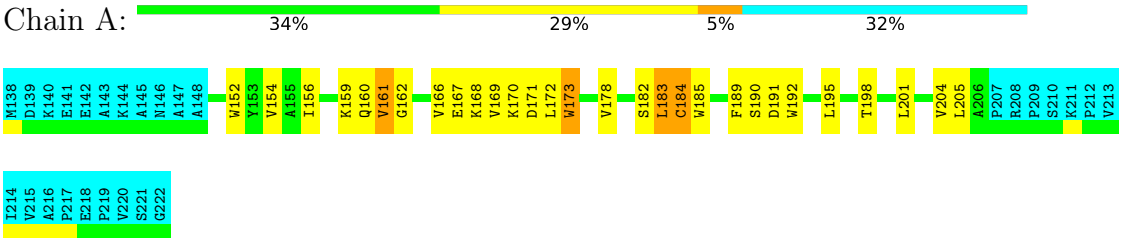
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Adventurous gliding motility protein GltJ

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 19 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
Amber	refinement	
CYANA	structure calculation	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	947
Number of shifts mapped to atoms	947
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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	463	435	435	22±3
All	All	8797	8265	8265	418

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:LEU:HD11	1:A:205:LEU:HD22	0.99	1.33	2	4
1:A:195:LEU:HD22	1:A:195:LEU:O	0.82	1.75	14	2
1:A:201:LEU:HD12	1:A:205:LEU:HD22	0.81	1.50	13	12
1:A:195:LEU:HD23	1:A:201:LEU:HB3	0.80	1.50	14	2
1:A:152:TRP:CZ2	1:A:169:VAL:HG21	0.74	2.18	17	19
1:A:201:LEU:HD12	1:A:205:LEU:HD23	0.72	1.61	17	2
1:A:169:VAL:HG12	1:A:205:LEU:HD11	0.69	1.65	19	3
1:A:195:LEU:C	1:A:195:LEU:HD13	0.68	2.08	16	2
1:A:195:LEU:HD13	1:A:196:SER:N	0.68	2.03	14	2
1:A:154:VAL:O	1:A:161:VAL:HG23	0.66	1.90	18	1
1:A:201:LEU:CD1	1:A:205:LEU:HD22	0.66	2.19	9	13
1:A:172:LEU:HB3	1:A:178:VAL:HG13	0.65	1.68	9	13
1:A:201:LEU:CD1	1:A:205:LEU:HD23	0.65	2.22	15	3
1:A:155:ALA:HB2	1:A:192:TRP:CZ2	0.64	2.27	3	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:LEU:HD23	1:A:201:LEU:HG	0.64	1.68	12	6
1:A:183:LEU:HD13	1:A:183:LEU:N	0.63	2.09	14	17
1:A:201:LEU:O	1:A:201:LEU:HD13	0.62	1.95	2	3
1:A:173:TRP:C	1:A:173:TRP:CD1	0.61	2.74	9	16
1:A:173:TRP:CD1	1:A:173:TRP:C	0.60	2.75	8	3
1:A:169:VAL:HA	1:A:172:LEU:HD12	0.60	1.74	15	13
1:A:169:VAL:CG1	1:A:205:LEU:HD21	0.59	2.27	5	16
1:A:154:VAL:O	1:A:161:VAL:HG13	0.59	1.97	9	10
1:A:183:LEU:HD12	1:A:194:PRO:HD3	0.59	1.72	16	14
1:A:193:ILE:HD11	1:A:197:GLU:CD	0.59	2.18	17	2
1:A:154:VAL:H	1:A:161:VAL:HG22	0.58	1.59	17	14
1:A:195:LEU:HD12	1:A:201:LEU:CD2	0.57	2.30	17	3
1:A:152:TRP:CD1	1:A:152:TRP:N	0.56	2.74	4	3
1:A:172:LEU:CB	1:A:178:VAL:HG13	0.56	2.31	3	14
1:A:154:VAL:H	1:A:161:VAL:HG12	0.55	1.61	19	1
1:A:198:THR:HG21	1:A:201:LEU:HD23	0.55	1.77	13	1
1:A:155:ALA:HB2	1:A:192:TRP:CE2	0.55	2.37	2	9
1:A:183:LEU:CD1	1:A:183:LEU:N	0.54	2.71	7	2
1:A:168:LYS:HD2	1:A:172:LEU:HD11	0.54	1.79	16	1
1:A:184:CYS:HB3	1:A:195:LEU:HD11	0.54	1.78	13	3
1:A:183:LEU:HD12	1:A:194:PRO:CD	0.54	2.33	14	3
1:A:184:CYS:SG	1:A:195:LEU:HD21	0.53	2.43	15	3
1:A:201:LEU:CD1	1:A:205:LEU:HD13	0.53	2.34	7	3
1:A:195:LEU:HD23	1:A:196:SER:N	0.53	2.19	5	1
1:A:195:LEU:HD23	1:A:195:LEU:C	0.52	2.24	5	1
1:A:161:VAL:CG1	1:A:162:GLY:N	0.52	2.72	12	1
1:A:173:TRP:CG	1:A:205:LEU:HD23	0.52	2.39	9	5
1:A:156:ILE:HD11	1:A:179:GLY:N	0.52	2.19	6	2
1:A:183:LEU:HD23	1:A:192:TRP:HB3	0.52	1.81	7	2
1:A:152:TRP:N	1:A:152:TRP:CD1	0.51	2.78	11	16
1:A:169:VAL:HG12	1:A:205:LEU:HD21	0.50	1.83	10	6
1:A:201:LEU:HD21	1:A:205:LEU:HD23	0.50	1.84	19	1
1:A:195:LEU:HD22	1:A:201:LEU:CD2	0.50	2.37	6	1
1:A:195:LEU:HA	1:A:198:THR:HG22	0.49	1.84	6	9
1:A:166:VAL:HG13	1:A:204:VAL:CG1	0.49	2.37	7	14
1:A:173:TRP:CB	1:A:205:LEU:HD23	0.49	2.37	10	3
1:A:195:LEU:HD12	1:A:195:LEU:H	0.49	1.67	12	3
1:A:195:LEU:HD12	1:A:201:LEU:HD23	0.49	1.84	7	2
1:A:195:LEU:HD22	1:A:195:LEU:C	0.49	2.27	14	2
1:A:179:GLY:O	1:A:195:LEU:HD13	0.48	2.07	11	3
1:A:161:VAL:HG12	1:A:162:GLY:N	0.48	2.23	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:HIS:CG	1:A:166:VAL:HG23	0.48	2.44	10	2
1:A:183:LEU:H	1:A:183:LEU:HD22	0.47	1.69	3	17
1:A:154:VAL:HG13	1:A:184:CYS:SG	0.47	2.49	4	4
1:A:184:CYS:CB	1:A:195:LEU:HD11	0.47	2.39	19	1
1:A:195:LEU:C	1:A:195:LEU:CD1	0.47	2.79	14	2
1:A:184:CYS:HB2	1:A:195:LEU:HD11	0.47	1.87	15	2
1:A:184:CYS:SG	1:A:195:LEU:HD11	0.47	2.49	11	4
1:A:164:PHE:HB3	1:A:169:VAL:HG23	0.47	1.85	7	7
1:A:173:TRP:CE2	1:A:205:LEU:HB3	0.47	2.45	15	3
1:A:201:LEU:HD11	1:A:205:LEU:HD23	0.47	1.85	19	1
1:A:182:SER:O	1:A:195:LEU:HD12	0.47	2.10	8	2
1:A:201:LEU:CD2	1:A:205:LEU:HD23	0.46	2.40	19	1
1:A:198:THR:O	1:A:198:THR:HG23	0.46	2.11	19	3
1:A:195:LEU:HD12	1:A:195:LEU:N	0.46	2.26	19	2
1:A:154:VAL:N	1:A:161:VAL:HG22	0.46	2.26	17	7
1:A:195:LEU:HD22	1:A:201:LEU:HG	0.45	1.87	6	2
1:A:179:GLY:O	1:A:195:LEU:HD23	0.45	2.10	4	4
1:A:152:TRP:CH2	1:A:169:VAL:HG11	0.45	2.46	18	2
1:A:198:THR:HG23	1:A:201:LEU:HB2	0.45	1.89	3	1
1:A:183:LEU:HB3	1:A:192:TRP:CD1	0.45	2.47	7	2
1:A:195:LEU:HD13	1:A:201:LEU:HG	0.44	1.89	18	2
1:A:183:LEU:N	1:A:183:LEU:HD13	0.44	2.28	13	2
1:A:184:CYS:HB2	1:A:195:LEU:HD21	0.44	1.88	18	1
1:A:161:VAL:HG13	1:A:162:GLY:O	0.43	2.14	19	1
1:A:168:LYS:CD	1:A:172:LEU:HD11	0.42	2.44	1	2
1:A:169:VAL:HG11	1:A:205:LEU:HD21	0.42	1.92	4	4
1:A:161:VAL:HG13	1:A:162:GLY:N	0.42	2.29	19	1
1:A:183:LEU:N	1:A:183:LEU:CD1	0.42	2.80	14	1
1:A:198:THR:HG23	1:A:198:THR:O	0.41	2.15	5	1
1:A:195:LEU:HD22	1:A:201:LEU:CG	0.41	2.45	6	1
1:A:154:VAL:HG12	1:A:155:ALA:N	0.41	2.31	18	1
1:A:168:LYS:CE	1:A:172:LEU:HD11	0.41	2.46	1	1
1:A:152:TRP:CZ3	1:A:195:LEU:HD21	0.40	2.50	3	1
1:A:155:ALA:HB2	1:A:192:TRP:CH2	0.40	2.51	14	1
1:A:173:TRP:CZ3	1:A:195:LEU:CD1	0.40	3.05	5	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	58/85 (68%)	54±1 (93±2%)	4±1 (7±2%)	0±0 (0±0%)	100	100
All	All	1102/1615 (68%)	1030 (93%)	72 (7%)	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	49/70 (70%)	34±3 (69±5%)	15±3 (31±5%)	1	15
All	All	931/1330 (70%)	641 (69%)	290 (31%)	1	15

All 33 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	173	TRP	19
1	A	183	LEU	19
1	A	185	TRP	19
1	A	189	PHE	19
1	A	192	TRP	19
1	A	201	LEU	16
1	A	170	LYS	14
1	A	156	ILE	13
1	A	160	GLN	12
1	A	152	TRP	12
1	A	182	SER	11
1	A	186	ARG	11
1	A	171	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	191	ASP	10
1	A	167	GLU	9
1	A	159	LYS	9
1	A	184	CYS	7
1	A	195	LEU	7
1	A	157	ASP	6
1	A	172	LEU	6
1	A	168	LYS	5
1	A	200	GLU	5
1	A	151	GLU	4
1	A	187	SER	4
1	A	190	SER	4
1	A	177	GLU	4
1	A	165	ASN	4
1	A	197	GLU	3
1	A	203	SER	3
1	A	193	ILE	3
1	A	181	ASP	1
1	A	204	VAL	1
1	A	161	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	947
Number of shifts mapped to atoms	947
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	85	-1.33 ± 0.17	Should be applied
$^{13}C_{\beta}$	80	-1.21 ± 0.09	Should be applied
$^{13}C'$	77	0.01 ± 0.15	None needed (< 0.5 ppm)
^{15}N	75	-0.16 ± 0.32	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 88%, i.e. 678 atoms were assigned a chemical shift out of a possible 772. 0 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	281/288 (98%)	116/117 (99%)	111/116 (96%)	54/55 (98%)
Sidechain	339/400 (85%)	229/260 (88%)	106/129 (82%)	4/11 (36%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	58/84 (69%)	29/42 (69%)	25/37 (68%)	4/5 (80%)
Overall	678/772 (88%)	374/419 (89%)	242/282 (86%)	62/71 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 947 atoms were assigned a chemical shift out of a possible 1111. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	399/414 (96%)	162/167 (97%)	162/170 (95%)	75/77 (97%)
Sidechain	490/613 (80%)	330/399 (83%)	154/196 (79%)	6/18 (33%)
Aromatic	58/84 (69%)	29/42 (69%)	25/37 (68%)	4/5 (80%)
Overall	947/1111 (85%)	521/608 (86%)	341/403 (85%)	85/100 (85%)

7.1.4 Statistically unusual chemical shifts (i)

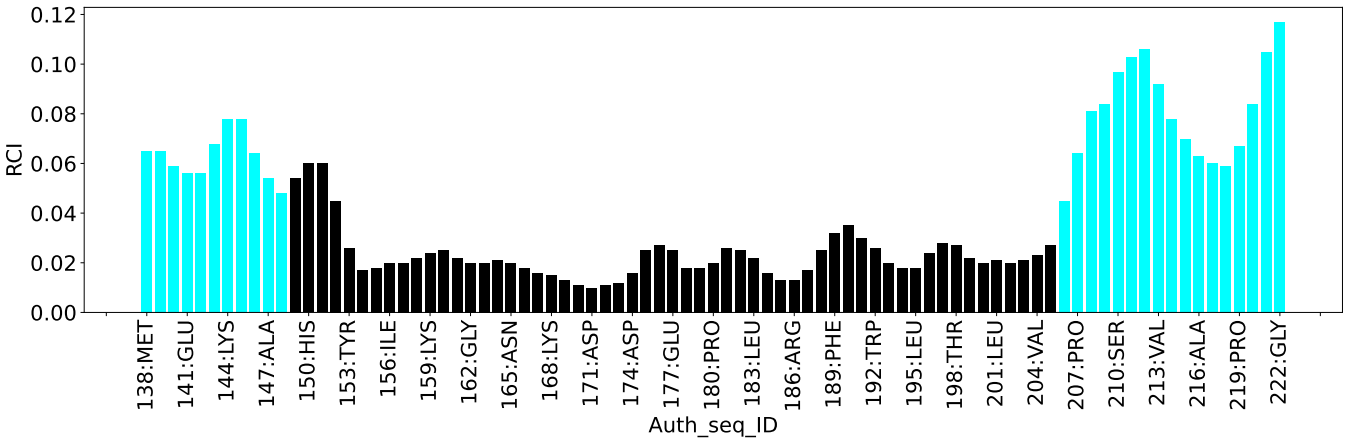
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	186	ARG	NE	115.25	76.53 – 92.65	19.0
1	A	208	ARG	NE	115.04	76.53 – 92.65	18.9
1	A	175	ARG	NE	114.99	76.53 – 92.65	18.9
1	A	186	ARG	HD2	0.55	1.97 – 4.26	-11.2
1	A	186	ARG	HD3	0.55	1.81 – 4.39	-9.9
1	A	186	ARG	HG2	-0.99	0.26 – 2.87	-9.8
1	A	186	ARG	HG3	-0.54	0.15 – 2.94	-7.5
1	A	186	ARG	HB2	0.01	0.52 – 3.08	-7.0
1	A	186	ARG	HB3	0.01	0.43 – 3.11	-6.6
1	A	209	PRO	CG	20.74	21.69 – 32.72	-5.9

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
138:MET
141:GLU
144:LYS
147:ALA
150:HIS
153:TYR
156:ILE
159:LYS
162:GLY
165:ASN
168:LYS
171:ASP
174:ASP
177:GLU
180:PRO
183:LEU
186:ARG
189:PHE
192:TRP
195:LEU
198:THR
201:LEU
204:VAL
207:PRO
210:SER
213:VAL
216:ALA
219:PRO
222:GLY
Auth_seq_ID