



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:48 pm BST

PDB ID : 2KV7  
Title : NMR solution structure of a soluble PrgI mutant from Salmonella Typhimurium  
Authors : Schmidt, H.; Poyraz, O.; Seidel, K.; Delissen, F.; Ader, C.; Tenenboim, H.; Goosmann, C.; Laube, B.; Thuenemann, A.F.; Zychlinski, A.; Baldus, M.; Lange, A.; Griesinger, C.; Kolbe, M.  
Deposited on : 2010-03-09

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 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

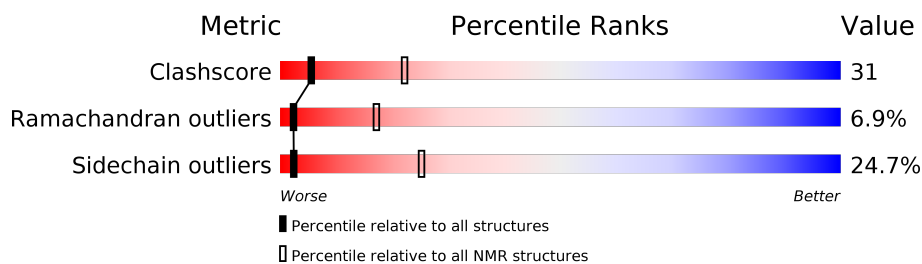
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	83	

## 2 Ensemble composition and analysis

This entry contains 25 models. Model 7 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:8-A:83 (76)	0.18	7

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	1, 5, 6, 7, 8, 9, 10, 14, 15, 18, 19, 22, 24
2	2, 12, 13
3	20, 21, 25
4	11, 16, 23
5	3, 4
Single-model clusters	17

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1263 atoms, of which 622 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein prgI.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	83	1263	402	622	108	130	1	0

There are 5 discrepancies between the modelled and reference sequences:

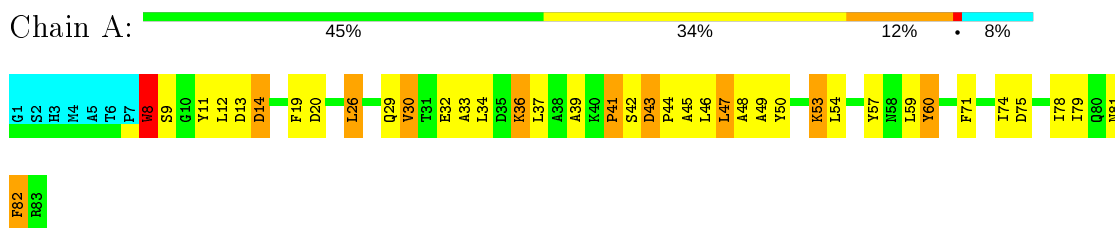
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P41784
A	2	SER	-	expression tag	UNP P41784
A	3	HIS	-	expression tag	UNP P41784
A	68	ALA	VAL	engineered mutation	UNP P41784
A	70	ALA	VAL	engineered mutation	UNP P41784

## 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: Protein prgI

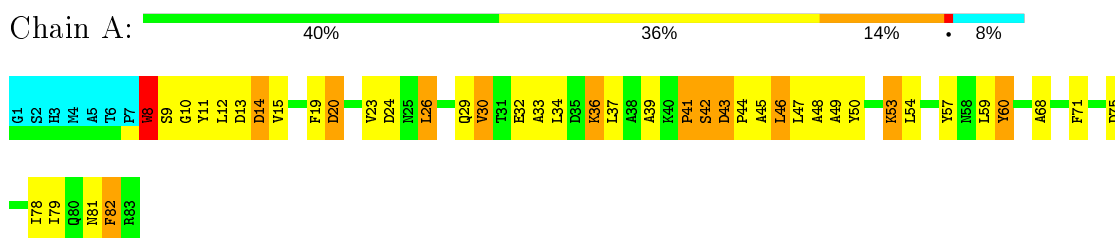


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

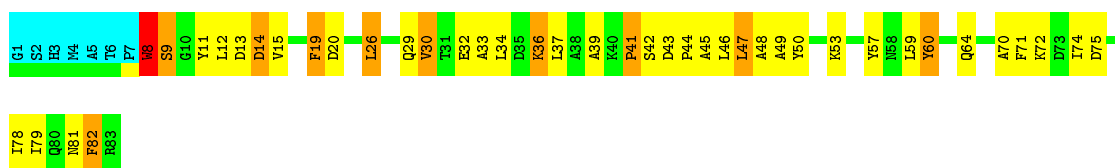
- Molecule 1: Protein prgI



#### 4.2.2 Score per residue for model 2

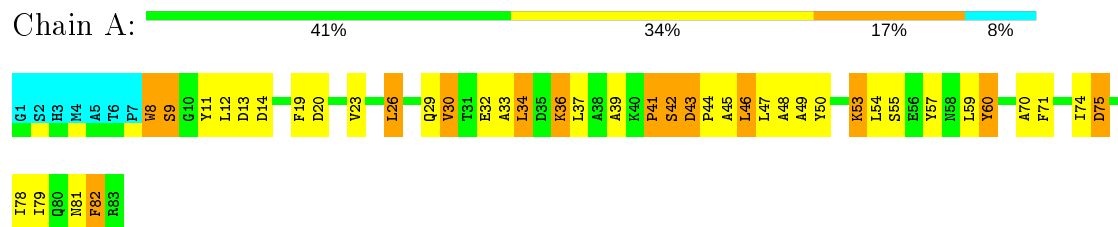
- Molecule 1: Protein prgI





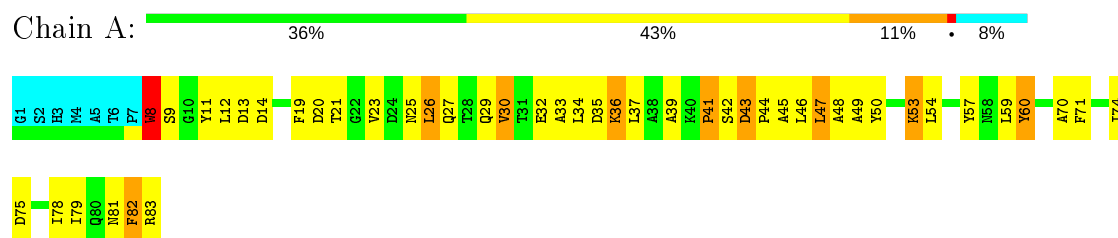
#### 4.2.3 Score per residue for model 3

- Molecule 1: Protein prgI



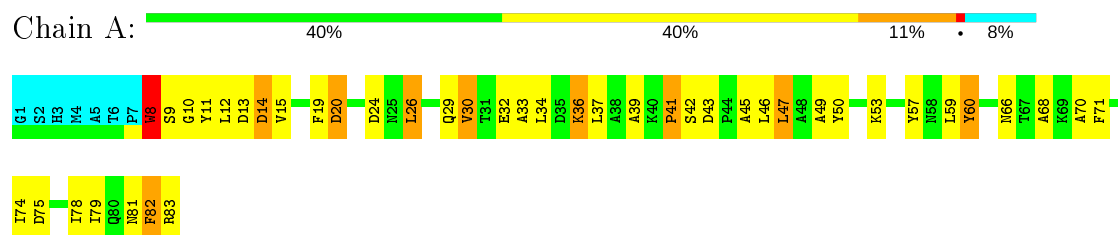
#### 4.2.4 Score per residue for model 4

- Molecule 1: Protein prgI



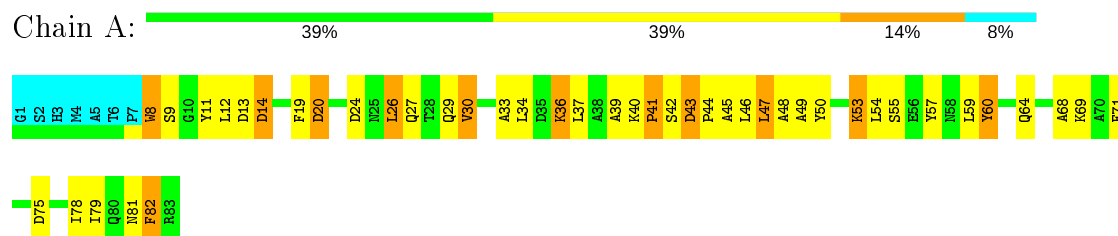
#### 4.2.5 Score per residue for model 5

- Molecule 1: Protein prgI



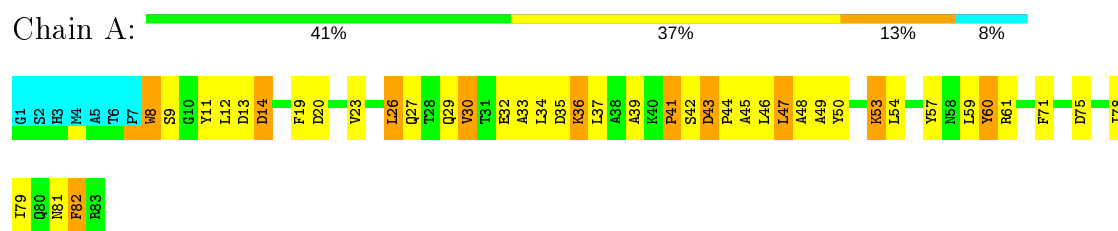
#### 4.2.6 Score per residue for model 6

- Molecule 1: Protein prgI



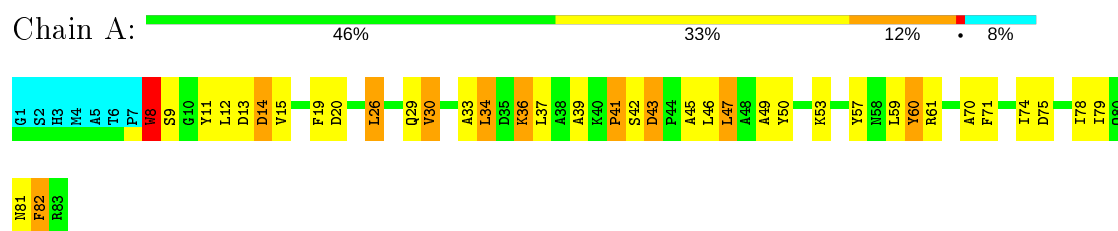
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Protein prgI



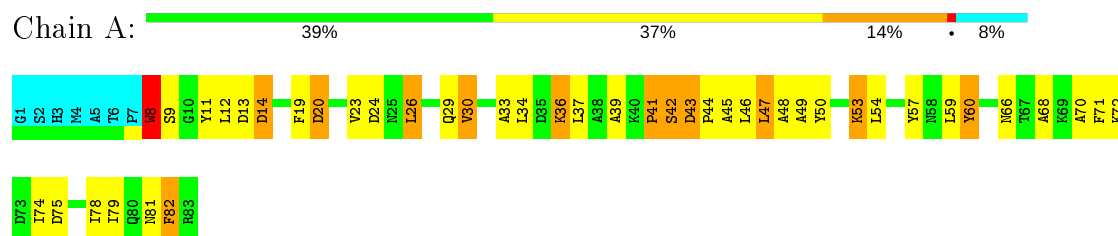
#### 4.2.8 Score per residue for model 8

- Molecule 1: Protein prgI



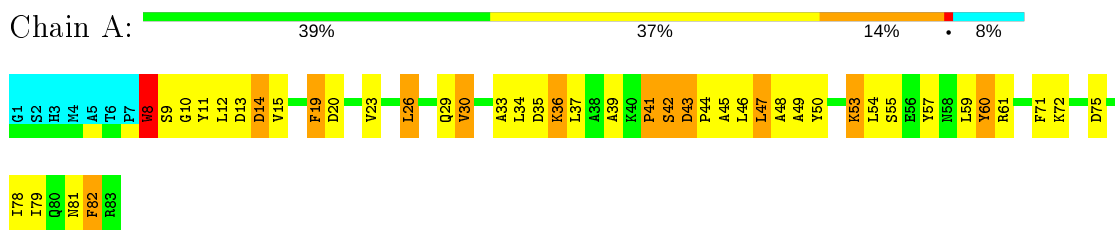
#### 4.2.9 Score per residue for model 9

- Molecule 1: Protein prgI



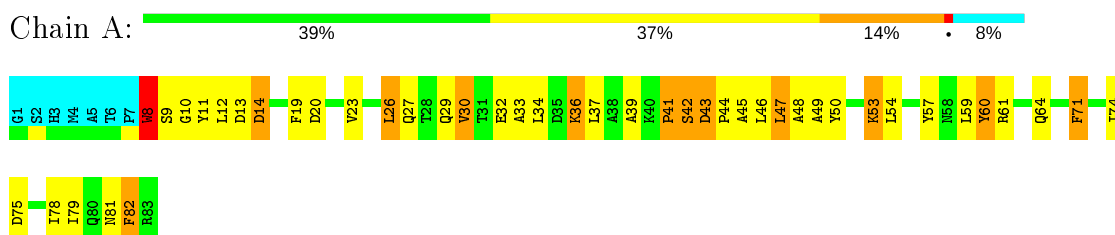
#### 4.2.10 Score per residue for model 10

- Molecule 1: Protein prgI



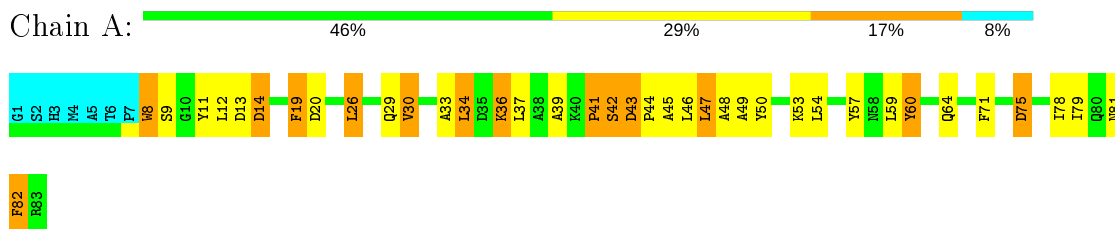
#### 4.2.11 Score per residue for model 11

- Molecule 1: Protein prgI



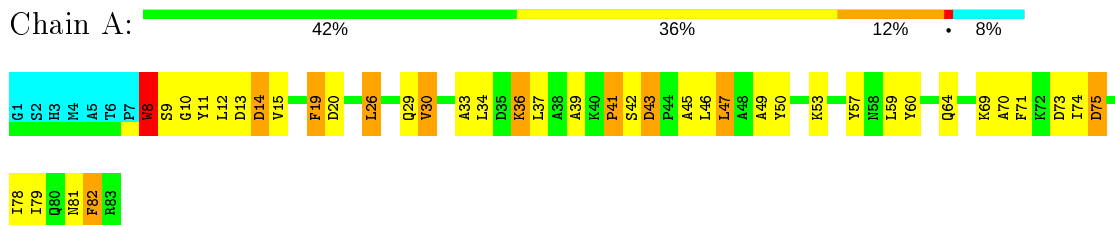
#### 4.2.12 Score per residue for model 12

- Molecule 1: Protein prgI



#### 4.2.13 Score per residue for model 13

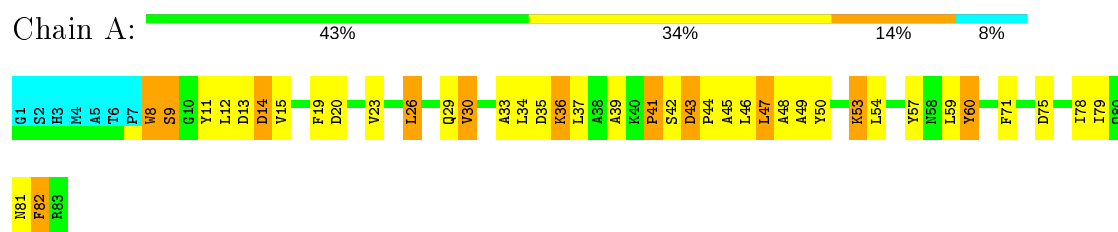
- Molecule 1: Protein prgI





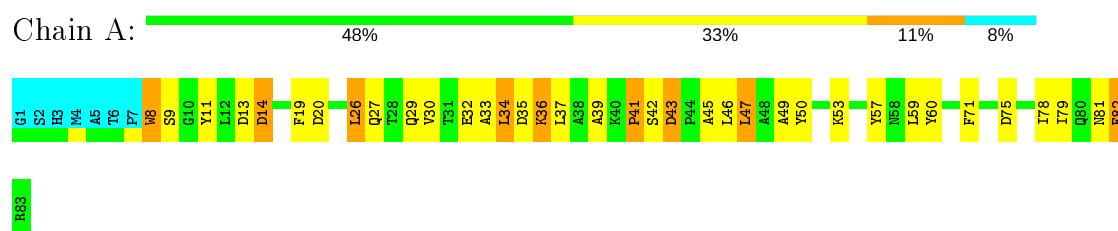
#### 4.2.14 Score per residue for model 14

- Molecule 1: Protein prgI



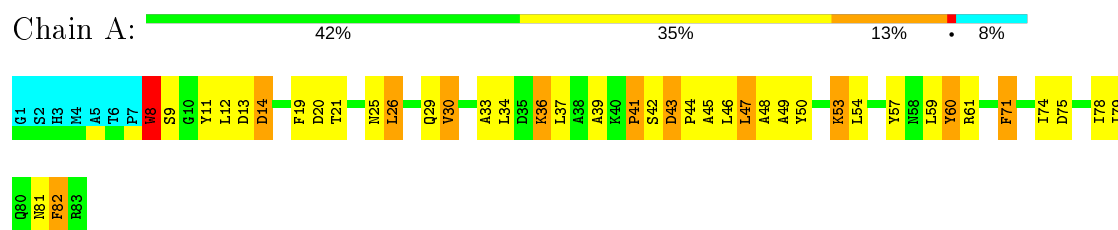
#### 4.2.15 Score per residue for model 15

- Molecule 1: Protein prgI



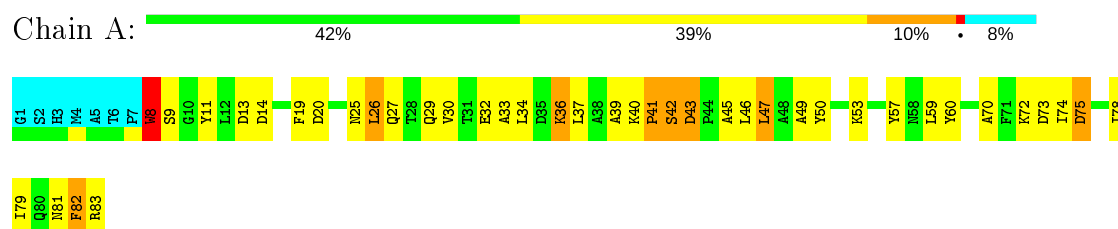
#### 4.2.16 Score per residue for model 16

- Molecule 1: Protein prgI



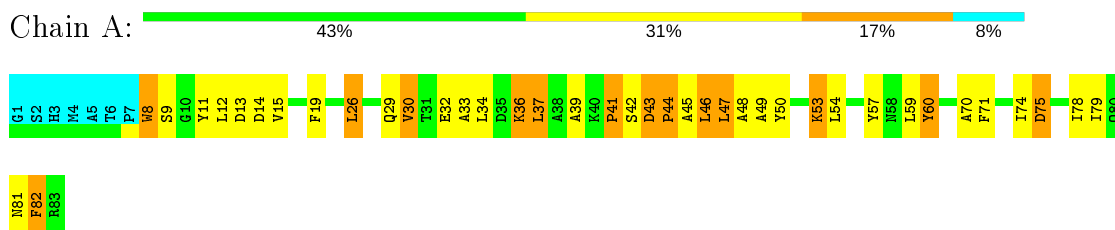
#### 4.2.17 Score per residue for model 17

- Molecule 1: Protein prgI



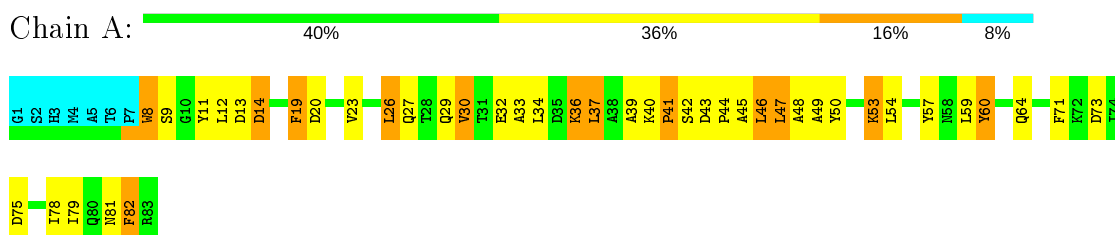
#### 4.2.18 Score per residue for model 18

- Molecule 1: Protein prgI



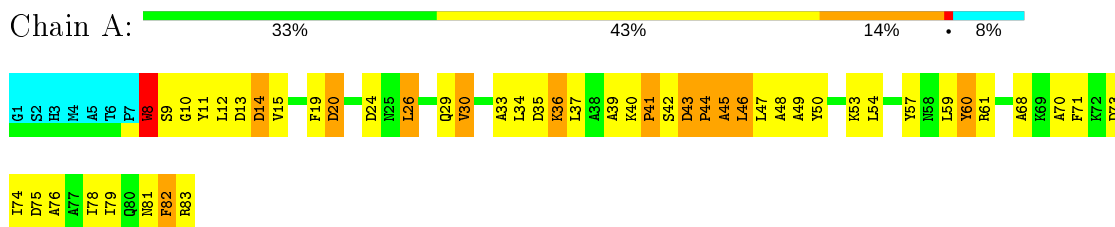
#### 4.2.19 Score per residue for model 19

- Molecule 1: Protein prgI



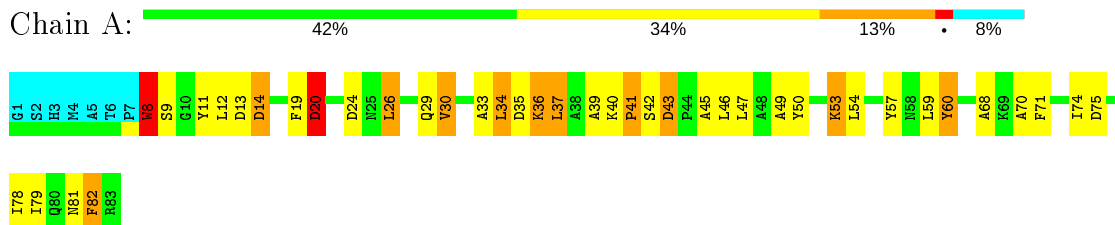
#### 4.2.20 Score per residue for model 20

- Molecule 1: Protein prgI



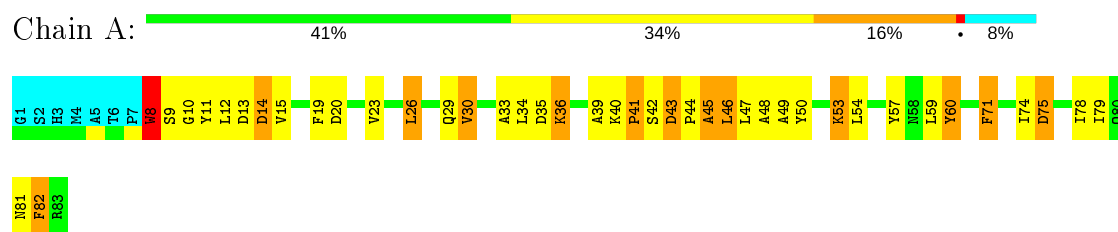
#### 4.2.21 Score per residue for model 21

- Molecule 1: Protein prgI



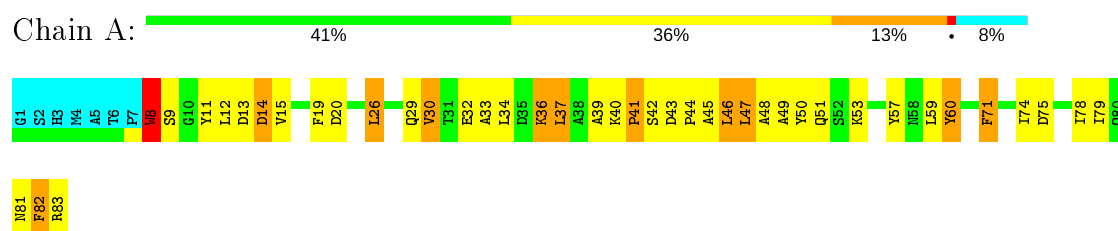
#### 4.2.22 Score per residue for model 22

- Molecule 1: Protein prgI



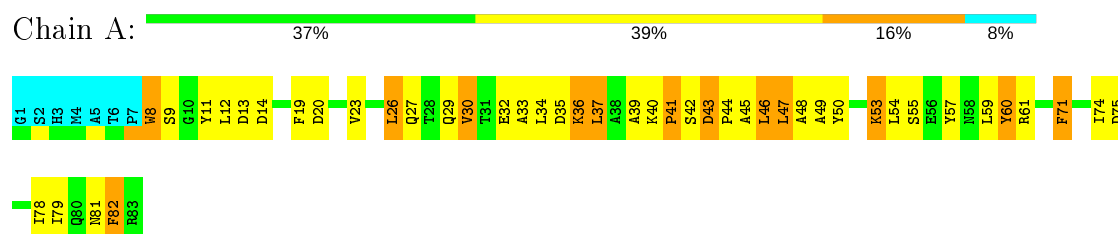
#### 4.2.23 Score per residue for model 23

- Molecule 1: Protein prgI



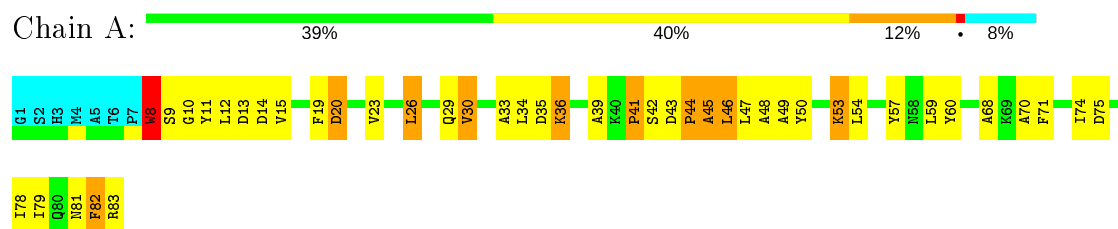
#### 4.2.24 Score per residue for model 24

- Molecule 1: Protein prgI



#### 4.2.25 Score per residue for model 25

- Molecule 1: Protein prgI



## 5 Refinement protocol and experimental data overview i

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

Of the 100 calculated structures, 25 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	
X-PLOR NIH	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	594	577	577	36±3
All	All	14850	14425	14425	906

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 31.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD13	1:A:47:LEU:HD12	0.82	1.50	20	20
1:A:26:LEU:HD22	1:A:57:TYR:HB2	0.78	1.56	10	25
1:A:8:TRP:CE3	1:A:79:ILE:HD13	0.74	2.17	17	15
1:A:30:VAL:HG13	1:A:53:LYS:HB3	0.71	1.62	2	25
1:A:36:LYS:O	1:A:39:ALA:HB3	0.69	1.87	3	21
1:A:37:LEU:CD1	1:A:47:LEU:HD12	0.68	2.19	2	16
1:A:36:LYS:HG2	1:A:46:LEU:HD13	0.67	1.66	22	3
1:A:46:LEU:O	1:A:49:ALA:HB3	0.67	1.89	21	25
1:A:59:LEU:HD13	1:A:59:LEU:O	0.66	1.91	18	14
1:A:9:SER:OG	1:A:12:LEU:HD22	0.66	1.91	21	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:O	1:A:59:LEU:HD13	0.65	1.92	13	11
1:A:36:LYS:C	1:A:46:LEU:HD13	0.65	2.11	21	1
1:A:40:LYS:HB2	1:A:46:LEU:HD12	0.65	1.67	21	1
1:A:34:LEU:HD13	1:A:50:TYR:CE2	0.64	2.28	13	16
1:A:37:LEU:HD13	1:A:47:LEU:CD1	0.64	2.21	20	6
1:A:35:ASP:O	1:A:39:ALA:HB2	0.64	1.92	25	4
1:A:19:PHE:CE1	1:A:68:ALA:HB2	0.63	2.28	5	7
1:A:36:LYS:CG	1:A:46:LEU:HD13	0.63	2.23	25	3
1:A:26:LEU:HD13	1:A:57:TYR:HA	0.62	1.71	19	24
1:A:8:TRP:CZ3	1:A:79:ILE:HG21	0.61	2.31	12	22
1:A:36:LYS:O	1:A:46:LEU:HD12	0.61	1.96	22	3
1:A:30:VAL:HA	1:A:33:ALA:HB3	0.60	1.74	25	25
1:A:9:SER:HA	1:A:12:LEU:HD13	0.59	1.74	21	23
1:A:11:TYR:CE1	1:A:15:VAL:HG11	0.57	2.34	2	5
1:A:36:LYS:HG2	1:A:46:LEU:HD22	0.57	1.77	21	1
1:A:75:ASP:HA	1:A:78:ILE:HD12	0.56	1.77	4	25
1:A:81:ASN:O	1:A:82:PHE:CD2	0.56	2.59	4	25
1:A:23:VAL:HG22	1:A:60:TYR:CD2	0.55	2.36	4	12
1:A:37:LEU:C	1:A:37:LEU:HD23	0.53	2.25	1	1
1:A:37:LEU:HD23	1:A:37:LEU:C	0.53	2.25	3	1
1:A:37:LEU:N	1:A:46:LEU:HD12	0.52	2.19	23	4
1:A:34:LEU:HD12	1:A:50:TYR:CE2	0.51	2.39	21	2
1:A:8:TRP:H	1:A:79:ILE:HD11	0.51	1.66	17	1
1:A:26:LEU:CD1	1:A:60:TYR:CG	0.50	2.94	22	25
1:A:36:LYS:C	1:A:46:LEU:HD12	0.50	2.26	20	20
1:A:33:ALA:HB1	1:A:50:TYR:CA	0.50	2.37	22	4
1:A:44:PRO:O	1:A:48:ALA:HB2	0.49	2.07	25	18
1:A:37:LEU:HD11	1:A:47:LEU:HD12	0.49	1.84	16	15
1:A:70:ALA:O	1:A:74:ILE:HD12	0.49	2.08	17	12
1:A:8:TRP:CZ3	1:A:79:ILE:HD13	0.49	2.43	1	6
1:A:82:PHE:CD1	1:A:82:PHE:C	0.48	2.87	10	14
1:A:82:PHE:C	1:A:82:PHE:CD1	0.48	2.87	7	11
1:A:74:ILE:HG23	1:A:83:ARG:HH12	0.48	1.67	23	1
1:A:26:LEU:HD12	1:A:60:TYR:CG	0.48	2.44	19	22
1:A:37:LEU:HD22	1:A:47:LEU:HD12	0.48	1.85	21	1
1:A:10:GLY:O	1:A:15:VAL:HG23	0.47	2.09	25	6
1:A:26:LEU:HD22	1:A:57:TYR:CB	0.47	2.36	22	3
1:A:50:TYR:CE1	1:A:54:LEU:HD13	0.47	2.45	24	17
1:A:50:TYR:HE1	1:A:54:LEU:HD13	0.47	1.69	18	18
1:A:26:LEU:HD12	1:A:60:TYR:CD2	0.47	2.44	19	20
1:A:30:VAL:O	1:A:34:LEU:N	0.47	2.48	25	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:THR:HG22	1:A:25:ASN:ND2	0.47	2.25	16	2
1:A:37:LEU:HD12	1:A:37:LEU:O	0.47	2.09	21	1
1:A:34:LEU:HD12	1:A:50:TYR:HE2	0.46	1.70	21	2
1:A:26:LEU:CD1	1:A:60:TYR:CD1	0.46	2.99	25	10
1:A:41:PRO:O	1:A:43:ASP:N	0.46	2.49	4	25
1:A:71:PHE:HA	1:A:74:ILE:HD12	0.46	1.87	23	5
1:A:23:VAL:HG22	1:A:60:TYR:HD2	0.46	1.69	4	1
1:A:57:TYR:O	1:A:60:TYR:CB	0.46	2.64	5	25
1:A:8:TRP:HZ3	1:A:79:ILE:HG21	0.45	1.69	24	2
1:A:11:TYR:CZ	1:A:15:VAL:HG11	0.45	2.46	18	3
1:A:34:LEU:CD1	1:A:50:TYR:CE2	0.45	3.00	13	12
1:A:8:TRP:CE3	1:A:79:ILE:CD1	0.45	3.00	11	2
1:A:15:VAL:HG12	1:A:19:PHE:HB2	0.45	1.87	10	1
1:A:37:LEU:HA	1:A:46:LEU:HB3	0.45	1.88	19	4
1:A:11:TYR:CE1	1:A:15:VAL:CG1	0.45	3.00	2	1
1:A:9:SER:O	1:A:11:TYR:N	0.44	2.51	10	25
1:A:59:LEU:C	1:A:59:LEU:HD13	0.44	2.33	20	10
1:A:15:VAL:O	1:A:19:PHE:CB	0.44	2.66	18	1
1:A:20:ASP:O	1:A:24:ASP:CB	0.43	2.66	21	6
1:A:81:ASN:O	1:A:82:PHE:CG	0.43	2.71	8	25
1:A:30:VAL:O	1:A:50:TYR:CE2	0.43	2.71	3	22
1:A:59:LEU:HD13	1:A:59:LEU:C	0.43	2.33	5	15
1:A:57:TYR:HA	1:A:60:TYR:HB2	0.43	1.91	8	10
1:A:36:LYS:CB	1:A:46:LEU:HD13	0.43	2.43	20	3
1:A:44:PRO:O	1:A:48:ALA:CB	0.42	2.67	25	13
1:A:45:ALA:O	1:A:49:ALA:N	0.42	2.52	22	3
1:A:35:ASP:O	1:A:39:ALA:CB	0.42	2.67	25	3
1:A:32:GLU:O	1:A:36:LYS:HB2	0.42	2.14	19	13
1:A:30:VAL:O	1:A:50:TYR:CD2	0.42	2.72	21	6
1:A:47:LEU:HD23	1:A:51:GLN:NE2	0.42	2.29	23	1
1:A:26:LEU:O	1:A:30:VAL:HG22	0.42	2.15	18	1
1:A:60:TYR:CG	1:A:64:GLN:NE2	0.41	2.89	11	1
1:A:36:LYS:O	1:A:46:LEU:HD13	0.41	2.16	21	1
1:A:74:ILE:HG23	1:A:83:ARG:NH2	0.41	2.31	4	1
1:A:50:TYR:CD1	1:A:50:TYR:C	0.41	2.94	18	1
1:A:73:ASP:O	1:A:76:ALA:HB3	0.41	2.16	20	1
1:A:29:GLN:NE2	1:A:53:LYS:CG	0.41	2.84	18	1
1:A:37:LEU:HD12	1:A:37:LEU:C	0.41	2.37	21	1
1:A:36:LYS:HB3	1:A:46:LEU:CD1	0.41	2.46	3	6
1:A:19:PHE:CE2	1:A:64:GLN:O	0.41	2.74	12	3
1:A:19:PHE:CD1	1:A:64:GLN:OE1	0.40	2.75	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LYS:C	1:A:46:LEU:CD1	0.40	2.89	14	5
1:A:19:PHE:CD2	1:A:64:GLN:OE1	0.40	2.74	2	1
1:A:15:VAL:O	1:A:19:PHE:N	0.40	2.54	18	1
1:A:81:ASN:C	1:A:83:ARG:H	0.40	2.20	25	4
1:A:37:LEU:C	1:A:37:LEU:HD12	0.40	2.37	19	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	75/83 (90%)	61±1 (81±1%)	9±1 (12±1%)	5±1 (7±1%)	2	17
All	All	1875/2075 (90%)	1514 (81%)	231 (12%)	130 (7%)	2	17

All 10 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	42	SER	25
1	A	14	ASP	25
1	A	13	ASP	25
1	A	41	PRO	25
1	A	8	TRP	16
1	A	20	ASP	7
1	A	44	PRO	3
1	A	10	GLY	2
1	A	73	ASP	1
1	A	9	SER	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	62/67 (93%)	47±2 (75±4%)	15±2 (25±4%)	2	25
All	All	1550/1675 (93%)	1167 (75%)	383 (25%)	2	25

All 30 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	36	LYS	25
1	A	26	LEU	25
1	A	82	PHE	25
1	A	8	TRP	25
1	A	29	GLN	24
1	A	71	PHE	24
1	A	47	LEU	23
1	A	30	VAL	23
1	A	60	TYR	21
1	A	43	ASP	20
1	A	20	ASP	19
1	A	14	ASP	19
1	A	19	PHE	17
1	A	53	LYS	16
1	A	46	LEU	9
1	A	27	GLN	8
1	A	61	ARG	7
1	A	40	LYS	7
1	A	42	SER	7
1	A	35	ASP	6
1	A	75	ASP	6
1	A	34	LEU	5
1	A	37	LEU	5
1	A	55	SER	4
1	A	72	LYS	4
1	A	9	SER	2
1	A	73	ASP	2
1	A	69	LYS	2
1	A	66	ASN	2
1	A	25	ASN	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.



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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.6 Other polymers [i](#)

There are no such molecules in this entry.

### 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Chemical shift validation

No chemical shift data were provided