



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 09:08 am BST

PDB ID : 5YFG  
Title : SOLUTION STRUCTURE OF HUMAN MOG1  
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Deposited on : 2017-09-21

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

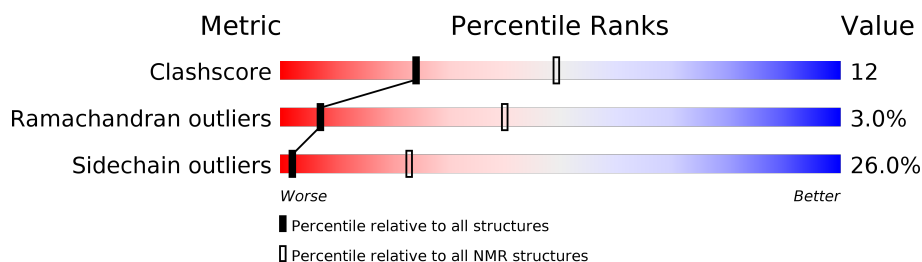
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 65%.

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	194	<div>48% 29% • 16% •</div>

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 17 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:5-A:112, A:119-A:145, A:162-A:180 (154)	0.45	17

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

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

The models can be grouped into 2 clusters and 14 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2858 atoms, of which 1418 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ran guanine nucleotide release factor.

Mol	Chain	Residues	Atoms						Trace
1	A	186	Total	C	H	N	O	S	0
			2858	907	1418	253	275	5	

There are 8 discrepancies between the modelled and reference sequences:

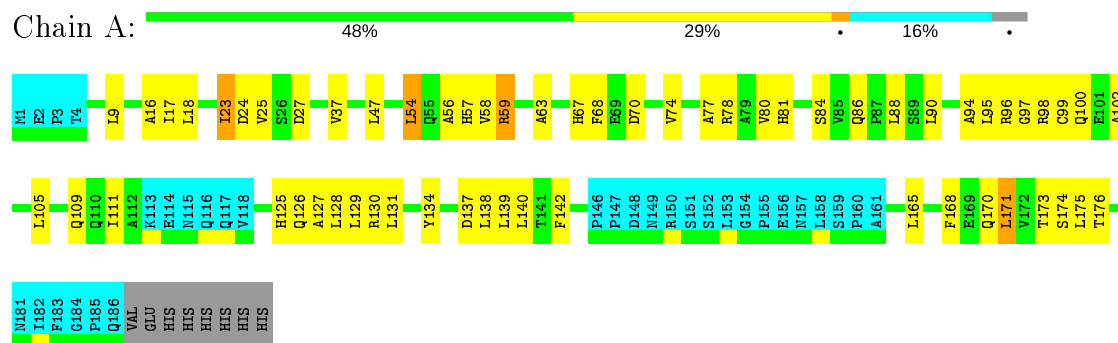
Chain	Residue	Modelled	Actual	Comment	Reference
A	187	VAL	-	expression tag	UNP Q9HD47
A	188	GLU	-	expression tag	UNP Q9HD47
A	189	HIS	-	expression tag	UNP Q9HD47
A	190	HIS	-	expression tag	UNP Q9HD47
A	191	HIS	-	expression tag	UNP Q9HD47
A	192	HIS	-	expression tag	UNP Q9HD47
A	193	HIS	-	expression tag	UNP Q9HD47
A	194	HIS	-	expression tag	UNP Q9HD47

## 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: Ran guanine nucleotide release factor

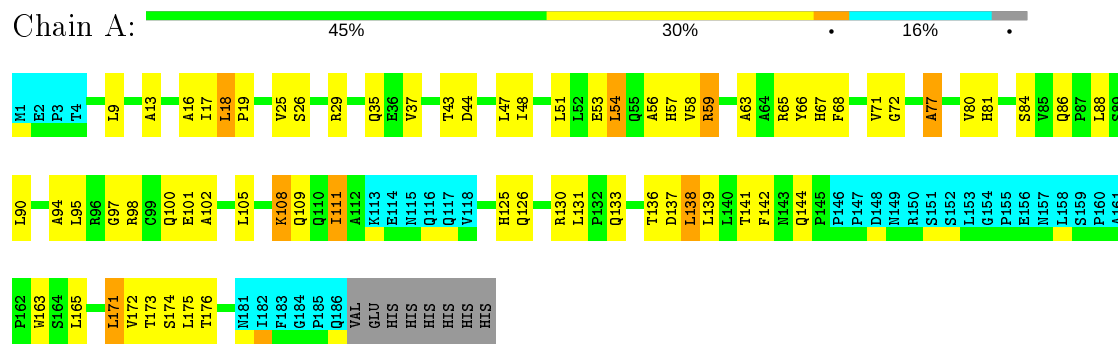


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

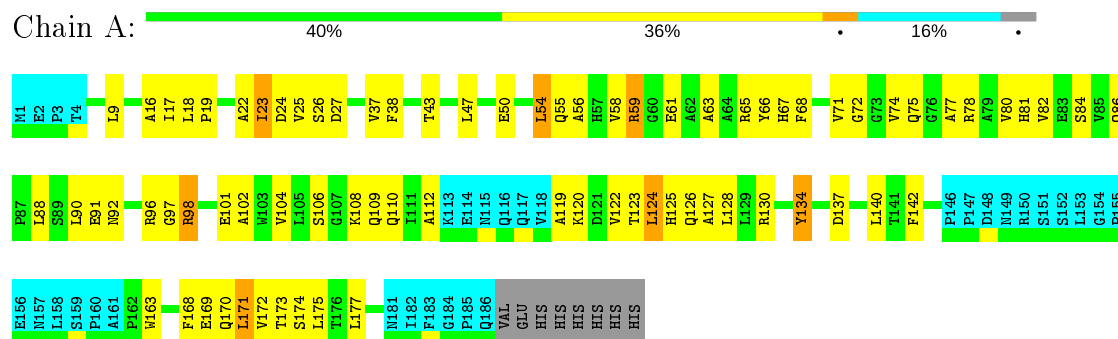
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ran guanine nucleotide release factor



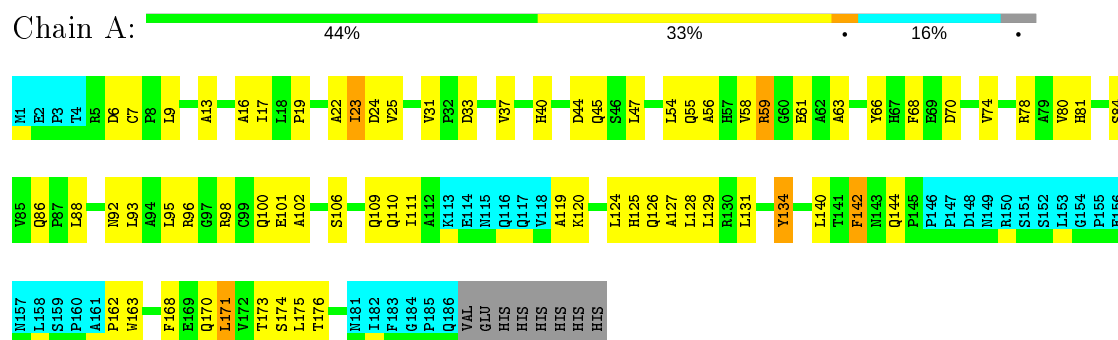
### 4.2.2 Score per residue for model 2

- Molecule 1: Ran guanine nucleotide release factor



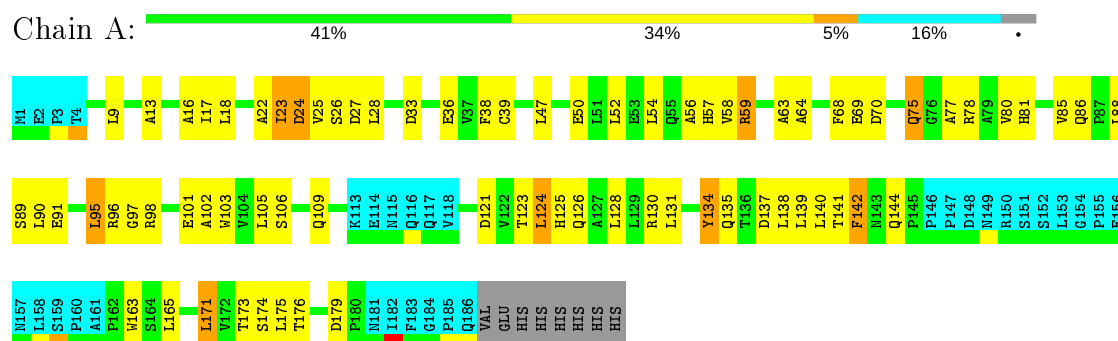
### 4.2.3 Score per residue for model 3

- Molecule 1: Ran guanine nucleotide release factor



### 4.2.4 Score per residue for model 4

- Molecule 1: Ran guanine nucleotide release factor



- Molecule 1: Ran guanine nucleotide release factor

V172	A94	M1
T173	L95	E2
S174	R96	P3
T175	G97	T4
T176	R98	B5
L177	C99	D6
H178	Q100	
D179		L9
P180	L105	
M181	K108	A13
L182	Q109	F14
F183	Q110	S15
G184		A16
P185	K113	I17
Q186	E114	I23
VAL	N115	D24
GLU	Q116	V25
HIS	Q117	
HIS	V118	V37
HIS	A119	F38
HIS	K120	C39
HIS		
	L124	T43
	H125	D44
	Q126	Q45
	A127	S46
	L128	L47
	L129	I48
		V49
	D137	E50
	L138	
	L139	L54
	L140	G55
	T141	A56
	F142	H57
	P146	H67
	P147	
	D148	D70
	M149	
	A150	V74
	S151	Q75
	S152	G76
	L153	A77
	G154	R78
	P155	A79
	E156	V80
	M157	H81
	L158	V82
	S159	E83
	P160	S84
	A161	V85
		Q86
	S164	P87
	L165	L88
	S89	S90
	F168	L90
	T174	L93

- Molecule 1: Ran guanine nucleotide release factor

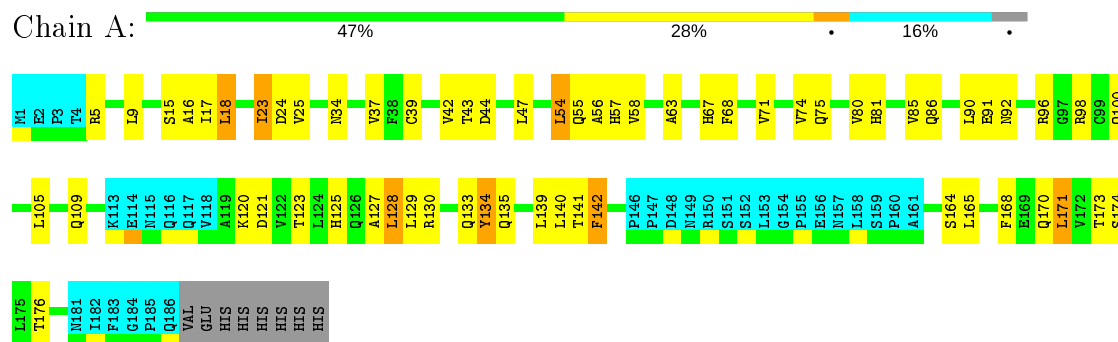
L165	M1
L170	P2
L171	E3
L172	T4
T173	B5
S174	A16
T175	I17
T176	L18
L177	P19
H178	X20
D179	G21
P180	A22
N181	T23
I182	D24
F183	V25
G184	L28
P185	D33
Q186	N34
VAL	Q35
GLU	R36
HIS	V37
HIS	R40
HIS	Q45
HIS	S46
HIS	L47
HIS	L51
HIS	L52
HIS	E53
HIS	L54
HIS	Q55
HIS	A56
HIS	H57
HIS	V58
HIS	B59
HIS	A63
HIS	D70
HIS	V74
HIS	O75
HIS	G76
HIS	A77
HIS	R78
HIS	A79
HIS	V80
HIS	B81
HIS	V82
HIS	E83
HIS	Q86
HIS	P87
HIS	L88
HIS	S89

- Molecule 1: Ran guanine nucleotide release factor

M181	Q100	M1
I182	E101	E2
F183	A102	P3
G184		T4
F185	S106	
Q186		I9
VAL	Q109	A16
GLU	I110	I17
HIS	A112	
HIS	K113	X20
HIS	E114	
HIS	M115	I23
HIS	Q116	D24
HIS	Q117	V25
	V118	
	A119	D83
	K120	K34
		Q35
	H125	E36
	Q126	V37
	A127	
		D44
	R130	Q45
	L131	S46
	Y134	L51
		L52
	L138	P53
	L139	L54
	L140	Q55
		A56
	P146	B59
	P147	
	D148	
	N149	A63
	R150	
	S151	H67
	S152	F68
	L153	
	G154	Q75
	P155	G76
	E156	A77
	M157	
	L158	V80
	S159	B81
	P160	
	A161	Q86
		P87
		L88
	G165	S89
	L166	
	D167	L90
	F168	
		L93
	L171	A94
	V172	L95
	T173	R96
	S174	G97
	L175	R98
	T176	G99

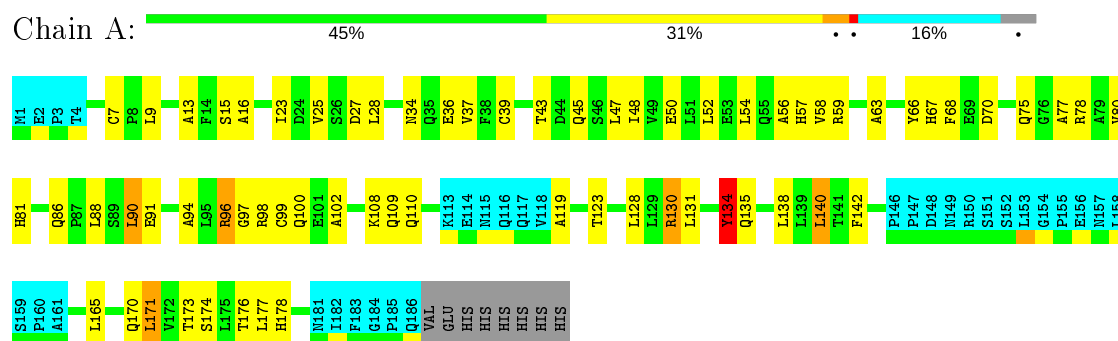
### 4.2.8 Score per residue for model 8

- Molecule 1: Ran guanine nucleotide release factor



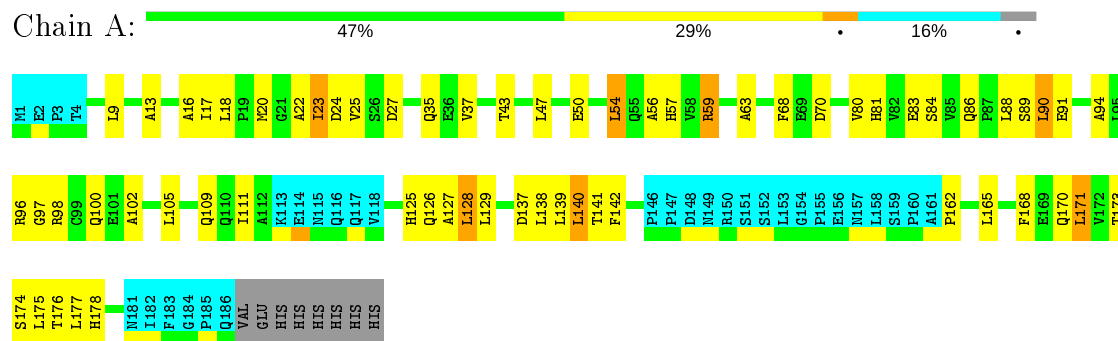
### 4.2.9 Score per residue for model 9

- Molecule 1: Ran guanine nucleotide release factor



### 4.2.10 Score per residue for model 10

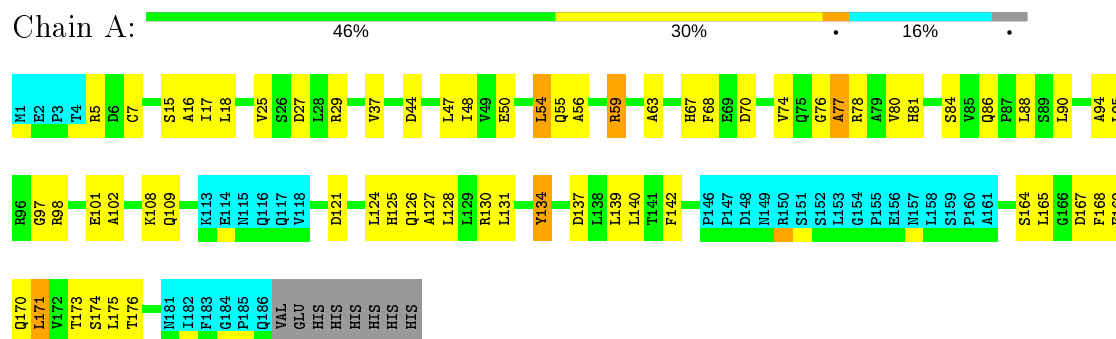
- Molecule 1: Ran guanine nucleotide release factor





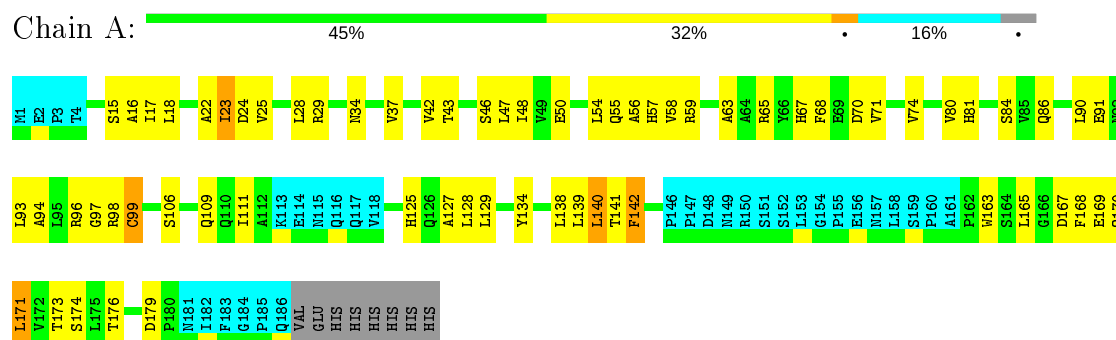
### 4.2.11 Score per residue for model 11

- Molecule 1: Ran guanine nucleotide release factor



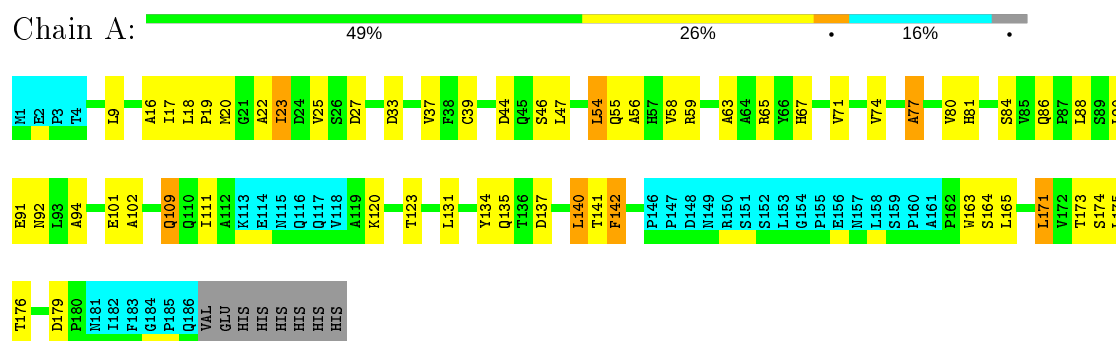
### 4.2.12 Score per residue for model 12

- Molecule 1: Ran guanine nucleotide release factor



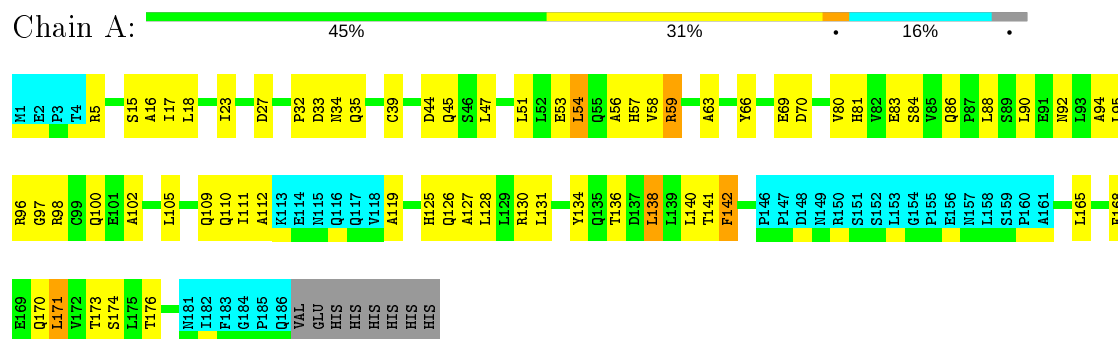
### 4.2.13 Score per residue for model 13

- Molecule 1: Ran guanine nucleotide release factor



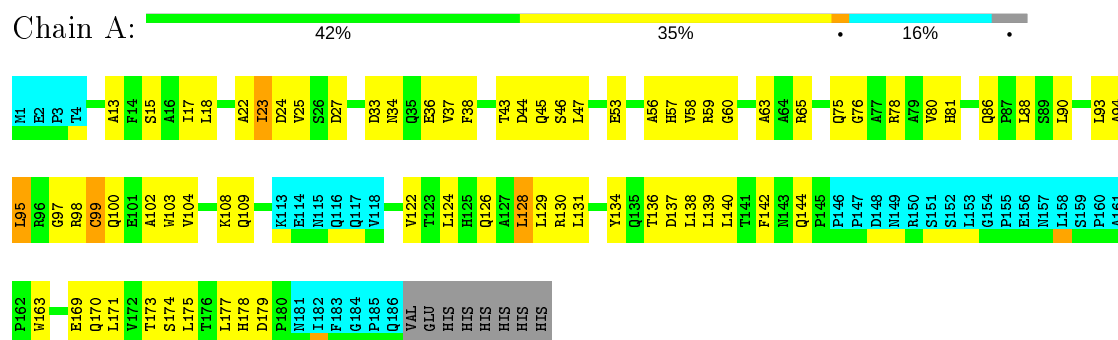
### 4.2.14 Score per residue for model 14

- Molecule 1: Ran guanine nucleotide release factor



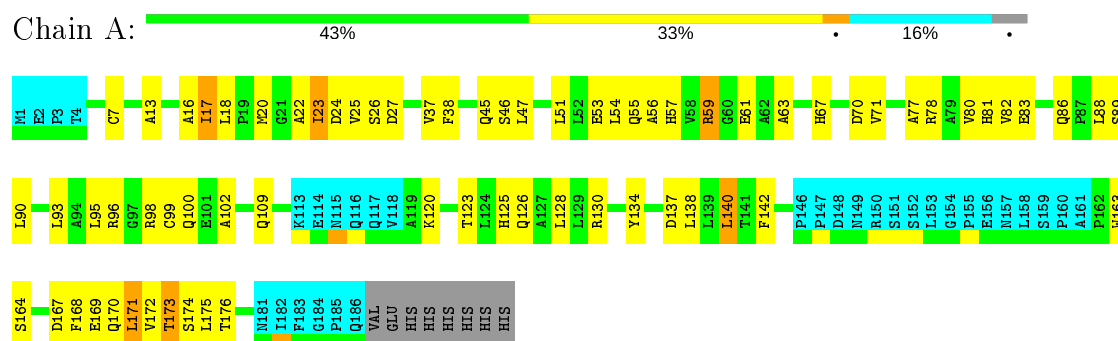
### 4.2.15 Score per residue for model 15

- Molecule 1: Ran guanine nucleotide release factor



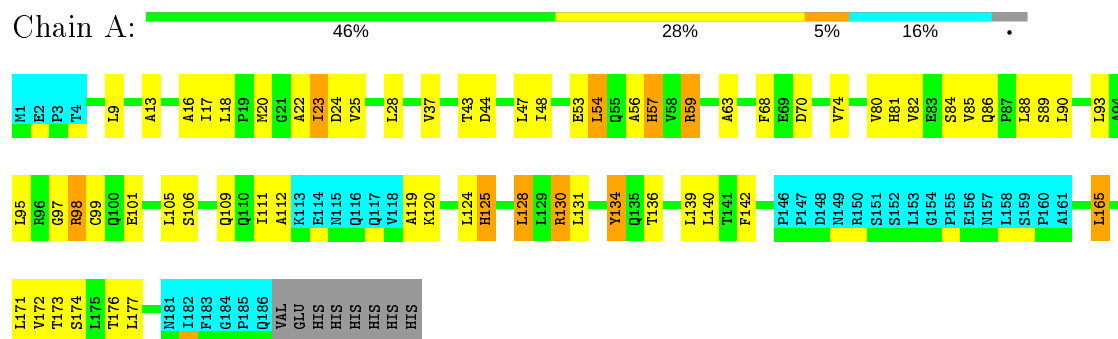
### 4.2.16 Score per residue for model 16

- Molecule 1: Ran guanine nucleotide release factor



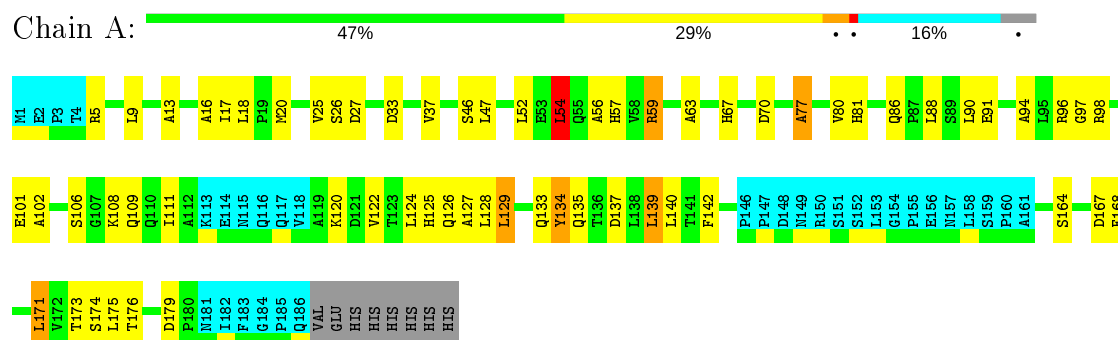
### 4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Ran guanine nucleotide release factor



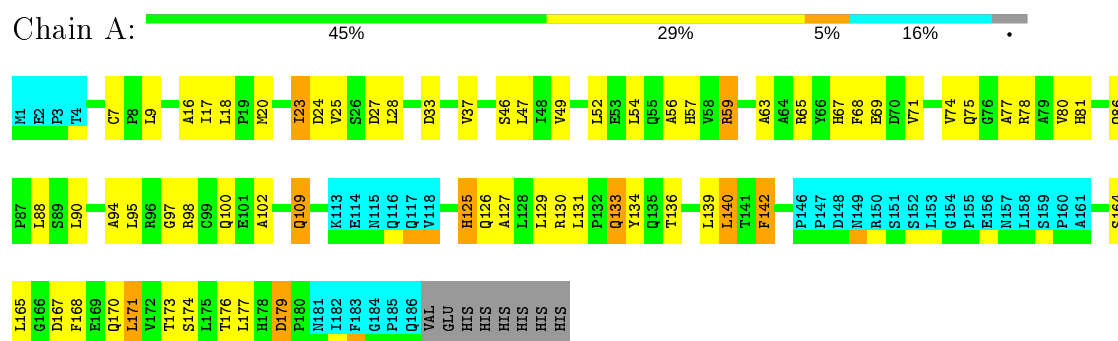
### 4.2.18 Score per residue for model 18

- Molecule 1: Ran guanine nucleotide release factor



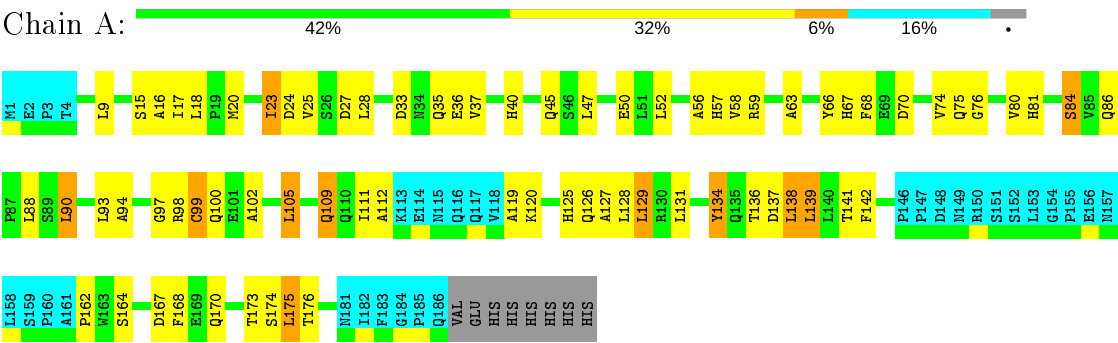
### 4.2.19 Score per residue for model 19

- Molecule 1: Ran guanine nucleotide release factor



4.2.20 Score per residue for model 20

- Molecule 1: Ran guanine nucleotide release factor



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING, DISTANCE GEOMETRY, torsion angle dynamics*.

Of the 200 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
CNS	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1638
Number of shifts mapped to atoms	1638
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	65%

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	1196	1185	1179	28±3
All	All	23920	23700	23580	563

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:138:LEU:HD22	1:A:175:LEU:HD21	0.97	1.34	1	1
1:A:112:ALA:HB2	1:A:119:ALA:HB2	0.94	1.38	17	4
1:A:140:LEU:HD21	1:A:171:LEU:HD12	0.93	1.37	10	5
1:A:129:LEU:HD11	1:A:175:LEU:HD13	0.72	1.58	3	1
1:A:88:LEU:HB2	1:A:102:ALA:HB3	0.72	1.61	2	8
1:A:140:LEU:CD1	1:A:171:LEU:HD12	0.71	2.16	2	1
1:A:19:PRO:HD2	1:A:22:ALA:HB2	0.70	1.61	3	3
1:A:177:LEU:HD13	1:A:177:LEU:C	0.70	2.07	9	3
1:A:127:ALA:HB2	1:A:168:PHE:CZ	0.70	2.21	3	11
1:A:47:LEU:HD21	1:A:171:LEU:HG	0.70	1.63	4	2
1:A:177:LEU:C	1:A:177:LEU:HD13	0.70	2.08	6	1
1:A:95:LEU:HD22	1:A:176:THR:HB	0.69	1.64	16	2
1:A:47:LEU:HD13	1:A:142:PHE:CD2	0.69	2.21	4	2
1:A:58:VAL:HG11	1:A:66:TYR:CD2	0.69	2.23	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:VAL:HG22	1:A:109:GLN:CB	0.67	2.19	9	18
1:A:127:ALA:HB3	1:A:140:LEU:HD22	0.67	1.66	2	1
1:A:47:LEU:HD11	1:A:142:PHE:CZ	0.66	2.26	14	6
1:A:59:ARG:HA	1:A:63:ALA:HB2	0.65	1.69	20	15
1:A:37:VAL:HG12	1:A:48:ILE:HG12	0.65	1.67	12	1
1:A:68:PHE:CE1	1:A:80:VAL:HG11	0.64	2.27	9	12
1:A:140:LEU:HD23	1:A:171:LEU:HD12	0.64	1.68	6	1
1:A:88:LEU:HD21	1:A:172:VAL:HG11	0.64	1.69	17	1
1:A:58:VAL:HG12	1:A:63:ALA:HA	0.64	1.69	1	5
1:A:74:VAL:HG13	1:A:75:GLN:HG3	0.62	1.72	20	1
1:A:140:LEU:CD2	1:A:171:LEU:HD12	0.62	2.24	8	5
1:A:88:LEU:HB3	1:A:102:ALA:HB3	0.62	1.71	19	8
1:A:17:ILE:HD12	1:A:174:SER:HA	0.62	1.69	5	3
1:A:52:LEU:HD13	1:A:139:LEU:HD13	0.61	1.72	7	1
1:A:140:LEU:HD21	1:A:171:LEU:HB3	0.61	1.70	12	1
1:A:128:LEU:HD21	1:A:139:LEU:HD12	0.61	1.71	15	1
1:A:99:CYS:SG	1:A:129:LEU:HD11	0.61	2.35	20	1
1:A:37:VAL:HG13	1:A:48:ILE:CD1	0.61	2.25	11	2
1:A:173:THR:O	1:A:176:THR:HG23	0.60	1.95	12	15
1:A:18:LEU:HD12	1:A:22:ALA:CB	0.60	2.27	17	5
1:A:124:LEU:HD22	1:A:124:LEU:C	0.60	2.17	4	1
1:A:23:ILE:HD13	1:A:24:ASP:N	0.60	2.11	8	13
1:A:140:LEU:HD13	1:A:171:LEU:HB3	0.59	1.73	3	2
1:A:67:HIS:O	1:A:71:VAL:HG23	0.59	1.97	8	7
1:A:88:LEU:CD2	1:A:172:VAL:HG11	0.59	2.28	1	2
1:A:56:ALA:O	1:A:58:VAL:HG23	0.59	1.98	8	1
1:A:47:LEU:HD21	1:A:142:PHE:CE2	0.58	2.33	13	1
1:A:110:GLN:HG3	1:A:119:ALA:HB1	0.58	1.74	9	3
1:A:77:ALA:HB1	1:A:109:GLN:HB2	0.58	1.76	19	6
1:A:95:LEU:HB2	1:A:176:THR:HG23	0.58	1.73	4	1
1:A:70:ASP:O	1:A:74:VAL:HG23	0.58	1.98	5	2
1:A:79:ALA:HB3	1:A:110:GLN:HB2	0.58	1.75	6	1
1:A:54:LEU:HD21	1:A:59:ARG:HD3	0.58	1.74	1	2
1:A:138:LEU:CD2	1:A:175:LEU:HD21	0.57	2.21	1	1
1:A:94:ALA:H	1:A:173:THR:HG22	0.57	1.60	12	12
1:A:88:LEU:HD22	1:A:92:ASN:ND2	0.57	2.15	6	1
1:A:25:VAL:HG22	1:A:37:VAL:O	0.56	2.00	5	18
1:A:68:PHE:CE1	1:A:80:VAL:HG21	0.56	2.34	1	1
1:A:54:LEU:HD11	1:A:59:ARG:HG2	0.56	1.76	6	1
1:A:68:PHE:HE1	1:A:80:VAL:HG11	0.56	1.60	4	9
1:A:63:ALA:HB3	1:A:128:LEU:CD2	0.56	2.31	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:177:LEU:HD13	1:A:178:HIS:N	0.56	2.14	15	4
1:A:168:PHE:O	1:A:172:VAL:HG23	0.56	2.01	5	2
1:A:127:ALA:HB2	1:A:168:PHE:HZ	0.56	1.60	3	8
1:A:95:LEU:HD23	1:A:178:HIS:CE1	0.56	2.35	15	1
1:A:98:ARG:HD3	1:A:177:LEU:HD23	0.55	1.76	17	1
1:A:138:LEU:HD11	1:A:175:LEU:HD22	0.55	1.77	20	1
1:A:54:LEU:HD11	1:A:130:ARG:HG3	0.55	1.75	17	1
1:A:54:LEU:HD11	1:A:59:ARG:HD3	0.55	1.77	13	1
1:A:110:GLN:HG3	1:A:119:ALA:HB3	0.55	1.77	14	1
1:A:80:VAL:HG22	1:A:109:GLN:HB3	0.55	1.79	17	5
1:A:16:ALA:HA	1:A:174:SER:O	0.55	2.02	16	18
1:A:127:ALA:HB3	1:A:140:LEU:HB2	0.55	1.76	12	3
1:A:125:HIS:CE1	1:A:165:LEU:HD21	0.55	2.36	17	1
1:A:59:ARG:CA	1:A:63:ALA:HB2	0.54	2.31	7	13
1:A:47:LEU:HD13	1:A:142:PHE:CZ	0.54	2.37	18	1
1:A:37:VAL:HG22	1:A:48:ILE:HG23	0.54	1.78	17	2
1:A:80:VAL:HG22	1:A:109:GLN:HB2	0.54	1.80	7	6
1:A:90:LEU:HD22	1:A:96:ARG:HD2	0.54	1.79	9	1
1:A:140:LEU:HD11	1:A:171:LEU:HD12	0.53	1.79	2	2
1:A:54:LEU:HD21	1:A:59:ARG:HB3	0.53	1.80	12	3
1:A:138:LEU:HG	1:A:175:LEU:HD22	0.53	1.79	16	1
1:A:37:VAL:HG13	1:A:48:ILE:HG12	0.53	1.79	5	2
1:A:129:LEU:HD12	1:A:138:LEU:CB	0.53	2.33	15	1
1:A:63:ALA:HB3	1:A:128:LEU:HG	0.53	1.80	6	3
1:A:7:CYS:SG	1:A:18:LEU:HD23	0.53	2.44	19	2
1:A:49:VAL:CG2	1:A:171:LEU:HD11	0.53	2.33	19	1
1:A:138:LEU:HD22	1:A:175:LEU:CD1	0.52	2.34	5	1
1:A:67:HIS:CD2	1:A:139:LEU:HD11	0.52	2.39	11	1
1:A:47:LEU:HD21	1:A:171:LEU:CG	0.52	2.33	4	1
1:A:122:VAL:HG13	1:A:122:VAL:O	0.52	2.05	18	1
1:A:17:ILE:C	1:A:18:LEU:HD22	0.52	2.25	14	9
1:A:124:LEU:HD21	1:A:126:GLN:NE2	0.52	2.20	5	1
1:A:52:LEU:HD11	1:A:139:LEU:HD12	0.52	1.82	20	1
1:A:47:LEU:HD11	1:A:142:PHE:CE2	0.51	2.40	5	8
1:A:177:LEU:CD1	1:A:177:LEU:C	0.51	2.79	9	2
1:A:76:GLY:O	1:A:77:ALA:HB2	0.51	2.05	11	1
1:A:68:PHE:CD2	1:A:105:LEU:HD22	0.51	2.40	20	1
1:A:18:LEU:N	1:A:18:LEU:HD22	0.51	2.20	18	2
1:A:23:ILE:HG22	1:A:39:CYS:O	0.51	2.04	5	5
1:A:88:LEU:CB	1:A:102:ALA:HB3	0.51	2.35	4	3
1:A:80:VAL:HG13	1:A:108:LYS:O	0.51	2.06	2	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ALA:HB2	1:A:173:THR:HB	0.50	1.82	15	1
1:A:111:ILE:HD13	1:A:111:ILE:C	0.50	2.25	1	1
1:A:127:ALA:HB3	1:A:140:LEU:HD21	0.50	1.83	19	1
1:A:140:LEU:HD13	1:A:171:LEU:HD12	0.50	1.83	19	2
1:A:72:GLY:O	1:A:77:ALA:HB3	0.50	2.07	1	1
1:A:68:PHE:CZ	1:A:80:VAL:HG21	0.50	2.42	1	1
1:A:177:LEU:HD22	1:A:178:HIS:N	0.50	2.22	10	4
1:A:25:VAL:CG2	1:A:37:VAL:HG23	0.50	2.37	15	2
1:A:17:ILE:HG21	1:A:170:GLN:NE2	0.49	2.22	19	2
1:A:95:LEU:HD22	1:A:176:THR:HG22	0.49	1.84	14	1
1:A:177:LEU:C	1:A:177:LEU:CD1	0.49	2.80	15	2
1:A:19:PRO:CD	1:A:22:ALA:HB2	0.49	2.38	13	1
1:A:140:LEU:HD22	1:A:171:LEU:HD12	0.48	1.83	3	2
1:A:67:HIS:CG	1:A:139:LEU:HD21	0.48	2.43	5	2
1:A:17:ILE:C	1:A:18:LEU:HD23	0.48	2.29	6	3
1:A:177:LEU:HD22	1:A:178:HIS:H	0.48	1.67	15	3
1:A:74:VAL:HG12	1:A:74:VAL:O	0.48	2.08	13	5
1:A:177:LEU:HD11	1:A:179:ASP:O	0.48	2.08	19	1
1:A:85:VAL:HG12	1:A:105:LEU:HA	0.48	1.85	17	3
1:A:122:VAL:HG13	1:A:124:LEU:HD11	0.48	1.86	2	2
1:A:77:ALA:HB1	1:A:109:GLN:CG	0.48	2.39	5	1
1:A:140:LEU:HD21	1:A:171:LEU:CD1	0.48	2.26	10	3
1:A:80:VAL:HG23	1:A:108:LYS:O	0.47	2.09	1	1
1:A:51:LEU:O	1:A:52:LEU:HD22	0.47	2.09	6	1
1:A:58:VAL:HG21	1:A:66:TYR:CD2	0.47	2.44	20	2
1:A:17:ILE:HD13	1:A:170:GLN:NE2	0.47	2.24	3	1
1:A:63:ALA:HB3	1:A:128:LEU:HD21	0.47	1.84	10	1
1:A:18:LEU:HD12	1:A:22:ALA:HB3	0.47	1.85	16	2
1:A:64:ALA:HB2	1:A:103:TRP:CD1	0.47	2.45	4	1
1:A:47:LEU:HD22	1:A:142:PHE:CE2	0.47	2.44	12	1
1:A:32:PRO:HG2	1:A:35:GLN:HB2	0.47	1.86	14	1
1:A:129:LEU:HD12	1:A:138:LEU:HB2	0.47	1.86	15	1
1:A:131:LEU:N	1:A:131:LEU:HD12	0.47	2.25	6	4
1:A:54:LEU:HB2	1:A:135:GLN:HB3	0.47	1.86	8	2
1:A:40:HIS:CE1	1:A:47:LEU:HD13	0.47	2.45	20	1
1:A:37:VAL:HG13	1:A:48:ILE:CG1	0.47	2.39	5	1
1:A:90:LEU:HD23	1:A:93:LEU:HD13	0.47	1.86	5	1
1:A:47:LEU:HD23	1:A:171:LEU:HG	0.47	1.87	11	2
1:A:17:ILE:N	1:A:17:ILE:HD13	0.47	2.25	17	1
1:A:129:LEU:HD22	1:A:129:LEU:N	0.47	2.24	5	1
1:A:47:LEU:HD21	1:A:142:PHE:CZ	0.47	2.45	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:VAL:HG21	1:A:37:VAL:CG1	0.47	2.40	18	1
1:A:74:VAL:O	1:A:74:VAL:HG12	0.46	2.10	2	3
1:A:93:LEU:HD21	1:A:99:CYS:SG	0.46	2.50	12	2
1:A:7:CYS:O	1:A:9:LEU:HD12	0.46	2.10	3	1
1:A:94:ALA:HB2	1:A:173:THR:CG2	0.46	2.41	9	1
1:A:88:LEU:HD13	1:A:172:VAL:HG11	0.46	1.87	2	1
1:A:47:LEU:HD21	1:A:171:LEU:CD2	0.46	2.41	12	1
1:A:47:LEU:HD11	1:A:142:PHE:CE1	0.46	2.46	13	1
1:A:17:ILE:HD13	1:A:17:ILE:N	0.46	2.26	16	2
1:A:111:ILE:HG23	1:A:111:ILE:O	0.46	2.11	1	5
1:A:90:LEU:HD23	1:A:96:ARG:HG2	0.46	1.86	10	2
1:A:131:LEU:HB2	1:A:136:THR:CG2	0.45	2.41	20	6
1:A:95:LEU:HD13	1:A:177:LEU:O	0.45	2.11	6	1
1:A:138:LEU:HD22	1:A:175:LEU:HD13	0.45	1.87	5	1
1:A:128:LEU:CD2	1:A:139:LEU:HD12	0.45	2.41	8	2
1:A:54:LEU:HD11	1:A:130:ARG:CG	0.45	2.40	17	1
1:A:47:LEU:HD11	1:A:142:PHE:CD2	0.45	2.46	3	2
1:A:7:CYS:SG	1:A:16:ALA:HB3	0.45	2.51	16	1
1:A:22:ALA:HB1	1:A:38:PHE:CD2	0.45	2.47	2	2
1:A:47:LEU:HD23	1:A:171:LEU:CD2	0.45	2.41	5	1
1:A:78:ARG:O	1:A:80:VAL:HG23	0.45	2.12	5	1
1:A:127:ALA:HB3	1:A:140:LEU:CD2	0.44	2.41	19	1
1:A:22:ALA:HB1	1:A:38:PHE:CD1	0.44	2.47	4	1
1:A:93:LEU:HD11	1:A:99:CYS:SG	0.44	2.52	16	2
1:A:65:ARG:NH1	1:A:105:LEU:HD12	0.44	2.27	1	1
1:A:31:VAL:HG13	1:A:31:VAL:O	0.44	2.13	3	1
1:A:173:THR:O	1:A:174:SER:C	0.44	2.56	5	1
1:A:52:LEU:HD13	1:A:67:HIS:CE1	0.44	2.47	20	1
1:A:54:LEU:HD13	1:A:135:GLN:HG3	0.44	1.88	13	1
1:A:129:LEU:HD21	1:A:140:LEU:HD13	0.44	1.89	18	1
1:A:67:HIS:CD2	1:A:128:LEU:HD11	0.44	2.47	20	1
1:A:54:LEU:HD21	1:A:59:ARG:CD	0.44	2.41	1	1
1:A:58:VAL:HG12	1:A:63:ALA:CA	0.44	2.42	4	1
1:A:67:HIS:CG	1:A:139:LEU:HD11	0.44	2.47	18	1
1:A:47:LEU:HD12	1:A:141:THR:O	0.44	2.12	4	1
1:A:15:SER:O	1:A:175:LEU:HA	0.44	2.13	5	2
1:A:19:PRO:HG2	1:A:22:ALA:HB2	0.44	1.89	13	1
1:A:60:GLY:HA2	1:A:103:TRP:CD1	0.44	2.48	15	1
1:A:111:ILE:O	1:A:111:ILE:HG23	0.44	2.12	20	4
1:A:40:HIS:CB	1:A:163:TRP:CH2	0.43	3.01	3	1
1:A:51:LEU:HD13	1:A:138:LEU:HG	0.43	1.89	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:171:LEU:O	1:A:171:LEU:HD13	0.43	2.13	1	3
1:A:82:VAL:HG23	1:A:82:VAL:O	0.43	2.14	17	3
1:A:139:LEU:C	1:A:140:LEU:HD12	0.43	2.34	18	1
1:A:95:LEU:HD12	1:A:176:THR:HB	0.43	1.90	5	1
1:A:59:ARG:N	1:A:63:ALA:HB2	0.43	2.28	7	2
1:A:171:LEU:O	1:A:174:SER:HB2	0.43	2.14	5	4
1:A:25:VAL:O	1:A:25:VAL:HG22	0.43	2.14	4	1
1:A:15:SER:O	1:A:174:SER:O	0.43	2.37	15	2
1:A:140:LEU:CB	1:A:171:LEU:HD12	0.43	2.44	3	1
1:A:131:LEU:HD12	1:A:131:LEU:N	0.43	2.29	13	3
1:A:90:LEU:HD11	1:A:99:CYS:O	0.43	2.13	20	1
1:A:52:LEU:CD1	1:A:139:LEU:HD12	0.42	2.44	18	1
1:A:52:LEU:HD23	1:A:67:HIS:CE1	0.42	2.48	9	1
1:A:52:LEU:HD22	1:A:67:HIS:CE1	0.42	2.49	19	1
1:A:127:ALA:CB	1:A:140:LEU:HD22	0.42	2.42	2	1
1:A:85:VAL:HG12	1:A:105:LEU:HG	0.42	1.91	5	1
1:A:88:LEU:HD12	1:A:102:ALA:CB	0.42	2.45	16	1
1:A:88:LEU:HD12	1:A:102:ALA:HB1	0.42	1.90	16	1
1:A:128:LEU:HD23	1:A:139:LEU:HD12	0.42	1.91	17	1
1:A:40:HIS:HB3	1:A:163:TRP:CH2	0.42	2.50	3	1
1:A:63:ALA:HB3	1:A:130:ARG:NH1	0.42	2.30	9	1
1:A:111:ILE:HG23	1:A:120:LYS:HD2	0.42	1.92	13	1
1:A:104:VAL:HG13	1:A:168:PHE:CZ	0.41	2.50	2	1
1:A:25:VAL:HG23	1:A:37:VAL:HG23	0.41	1.92	6	2
1:A:58:VAL:HG11	1:A:66:TYR:CB	0.41	2.45	1	1
1:A:35:GLN:HG3	1:A:50:GLU:HG3	0.41	1.91	10	1
1:A:47:LEU:CD2	1:A:171:LEU:HD23	0.41	2.45	3	1
1:A:47:LEU:HD13	1:A:142:PHE:CE1	0.41	2.50	18	1
1:A:58:VAL:HG21	1:A:66:TYR:CE2	0.41	2.49	20	1
1:A:54:LEU:HD11	1:A:59:ARG:CD	0.41	2.46	13	1
1:A:14:PHE:CE1	1:A:177:LEU:HD13	0.41	2.50	5	1
1:A:51:LEU:C	1:A:52:LEU:HD12	0.41	2.36	7	1
1:A:51:LEU:HD12	1:A:138:LEU:CD2	0.41	2.44	14	1
1:A:129:LEU:HD11	1:A:175:LEU:CD1	0.41	2.40	3	1
1:A:55:GLN:O	1:A:58:VAL:HG23	0.41	2.16	13	1
1:A:18:LEU:HD11	1:A:38:PHE:CD2	0.41	2.50	16	1
1:A:125:HIS:HB3	1:A:168:PHE:CE1	0.41	2.50	19	1
1:A:129:LEU:N	1:A:129:LEU:HD22	0.41	2.30	19	1
1:A:98:ARG:HG2	1:A:98:ARG:O	0.41	2.16	2	1
1:A:140:LEU:HD13	1:A:171:LEU:CB	0.41	2.43	3	1
1:A:46:SER:O	1:A:47:LEU:HD12	0.41	2.15	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:HIS:HE1	1:A:47:LEU:HD13	0.41	1.75	6	1
1:A:125:HIS:HB3	1:A:168:PHE:CE2	0.41	2.51	7	1
1:A:72:GLY:HA2	1:A:77:ALA:HB3	0.40	1.93	2	1
1:A:79:ALA:N	1:A:110:GLN:HB3	0.40	2.31	5	1
1:A:88:LEU:HD13	1:A:104:VAL:HG23	0.40	1.93	15	1
1:A:56:ALA:O	1:A:57:HIS:CG	0.40	2.74	8	1
1:A:23:ILE:HD13	1:A:23:ILE:C	0.40	2.37	17	1
1:A:82:VAL:O	1:A:82:VAL:HG23	0.40	2.17	2	1
1:A:54:LEU:HD21	1:A:59:ARG:NH1	0.40	2.31	7	1
1:A:134:TYR:CD1	1:A:134:TYR:N	0.40	2.89	9	1
1:A:54:LEU:HD11	1:A:59:ARG:HD2	0.40	1.94	10	1
1:A:55:GLN:O	1:A:58:VAL:HG22	0.40	2.16	12	1
1:A:94:ALA:N	1:A:173:THR:HG22	0.40	2.31	15	1
1:A:124:LEU:C	1:A:124:LEU:HD12	0.40	2.36	18	1
1:A:49:VAL:HG22	1:A:171:LEU:HD11	0.40	1.93	19	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	154/194 (79%)	134±2 (87±1%)	15±2 (10±1%)	5±1 (3±1%)	7	40
All	All	3080/3880 (79%)	2684 (87%)	305 (10%)	91 (3%)	7	40

All 12 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	56	ALA	19
1	A	134	TYR	17
1	A	97	GLY	16
1	A	57	HIS	14
1	A	77	ALA	9
1	A	75	GLN	5
1	A	76	GLY	4

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Mol	Chain	Res	Type	Models (Total)
1	A	54	LEU	3
1	A	84	SER	1
1	A	23	ILE	1
1	A	162	PRO	1
1	A	19	PRO	1

### 6.3.2 Protein sidechains ⓘ

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	130/167 (78%)	96±4 (74±3%)	34±4 (26±3%)	2	23
All	All	2600/3340 (78%)	1925 (74%)	675 (26%)	2	23

All 89 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	86	GLN	20
1	A	81	HIS	20
1	A	171	LEU	19
1	A	98	ARG	19
1	A	90	LEU	17
1	A	125	HIS	16
1	A	54	LEU	16
1	A	59	ARG	15
1	A	128	LEU	14
1	A	165	LEU	14
1	A	126	GLN	14
1	A	23	ILE	13
1	A	130	ARG	13
1	A	100	GLN	13
1	A	9	LEU	13
1	A	27	ASP	12
1	A	142	PHE	12
1	A	137	ASP	11
1	A	134	TYR	11
1	A	70	ASP	11

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Mol	Chain	Res	Type	Models (Total)
1	A	84	SER	10
1	A	101	GLU	10
1	A	78	ARG	10
1	A	44	ASP	10
1	A	33	ASP	10
1	A	96	ARG	10
1	A	170	GLN	10
1	A	46	SER	9
1	A	120	LYS	9
1	A	175	LEU	9
1	A	45	GLN	9
1	A	140	LEU	9
1	A	43	THR	9
1	A	20	MET	9
1	A	95	LEU	8
1	A	164	SER	8
1	A	91	GLU	8
1	A	179	ASP	8
1	A	138	LEU	8
1	A	139	LEU	8
1	A	141	THR	7
1	A	28	LEU	7
1	A	15	SER	7
1	A	50	GLU	7
1	A	123	THR	7
1	A	163	TRP	7
1	A	167	ASP	7
1	A	106	SER	7
1	A	34	ASN	6
1	A	109	GLN	6
1	A	5	ARG	6
1	A	99	CYS	6
1	A	129	LEU	6
1	A	169	GLU	5
1	A	26	SER	5
1	A	53	GLU	5
1	A	55	GLN	5
1	A	144	GLN	5
1	A	108	LYS	5
1	A	124	LEU	5
1	A	83	GLU	5
1	A	65	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	92	ASN	5
1	A	105	LEU	4
1	A	89	SER	4
1	A	36	GLU	4
1	A	35	GLN	4
1	A	133	GLN	4
1	A	61	GLU	3
1	A	29	ARG	3
1	A	75	GLN	3
1	A	69	GLU	3
1	A	18	LEU	3
1	A	93	LEU	3
1	A	173	THR	3
1	A	121	ASP	3
1	A	47	LEU	2
1	A	42	VAL	2
1	A	6	ASP	2
1	A	57	HIS	2
1	A	7	CYS	2
1	A	51	LEU	2
1	A	135	GLN	2
1	A	17	ILE	2
1	A	111	ILE	1
1	A	24	ASP	1
1	A	39	CYS	1
1	A	88	LEU	1
1	A	52	LEU	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 65% for the well-defined parts and 64% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *mog1-shifts\_gaiHB1\_HB3.txt*

#### 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	1638
Number of shifts mapped to atoms	1638
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	172	$-0.19 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	151	$-0.12 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	152	$0.28 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	160	$-0.27 \pm 0.27$	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 65%, i.e. 1210 atoms were assigned a chemical shift out of a possible 1874. 18 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	687/750 (92%)	276/298 (93%)	273/308 (89%)	138/144 (96%)
Sidechain	523/982 (53%)	329/572 (58%)	194/368 (53%)	0/42 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/142 (0%)	0/74 (0%)	0/54 (0%)	0/14 (0%)
Overall	1210/1874 (65%)	605/944 (64%)	467/730 (64%)	138/200 (69%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 64%, i.e. 1444 atoms were assigned a chemical shift out of a possible 2258. 19 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	806/898 (90%)	322/356 (90%)	324/372 (87%)	160/170 (94%)
Sidechain	638/1209 (53%)	400/709 (56%)	238/447 (53%)	0/53 (0%)
Aromatic	0/151 (0%)	0/79 (0%)	0/58 (0%)	0/14 (0%)
Overall	1444/2258 (64%)	722/1144 (63%)	562/877 (64%)	160/237 (68%)

#### 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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	123	THR	CB	29.62	78.10 – 61.30	-23.9
1	A	96	ARG	CD	23.59	47.57 – 38.77	-22.2
1	A	74	VAL	CG1	41.21	28.40 – 14.60	14.3
1	A	17	ILE	CG2	37.26	24.63 – 10.43	13.9
1	A	74	VAL	CG2	41.21	29.20 – 13.40	12.6
1	A	17	ILE	CD1	32.92	21.91 – 5.01	11.5

#### 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:

