Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:51 AM BST

PDB ID	:	2RR8
Title	:	Solution structure of calponin homology domain of IQGAP1
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Deposited on	:	2010-06-09

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

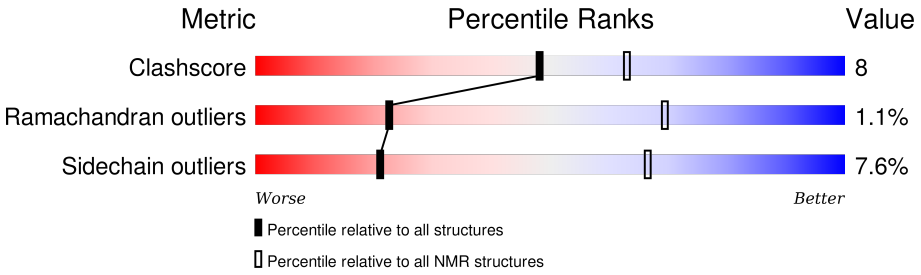
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 80%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	190	76% 11% • 13%

2 Ensemble composition and analysis

This entry contains 20 models. Model 4 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:37-A:202 (166)	0.69	4

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 4 clusters and 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3078 atoms, of which 1532 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called IQGAP1 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	190	3078	989	1532	258	289	10	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	EXPRESSION TAG	UNP Q6P1N4
A	22	PRO	-	EXPRESSION TAG	UNP Q6P1N4
A	23	LEU	-	EXPRESSION TAG	UNP Q6P1N4
A	24	GLY	-	EXPRESSION TAG	UNP Q6P1N4
A	25	SER	-	EXPRESSION TAG	UNP Q6P1N4

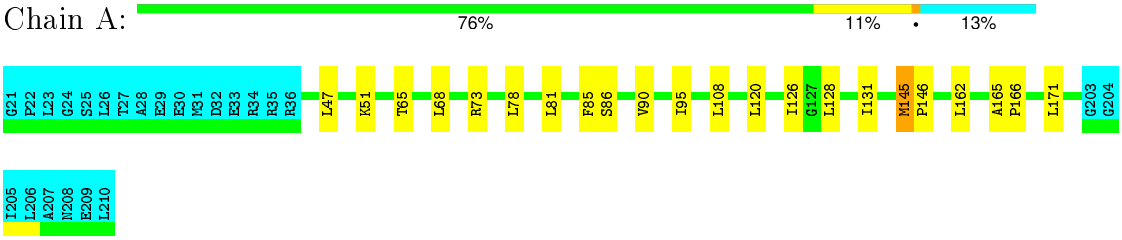
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: IQGAP1 protein

Chain A:



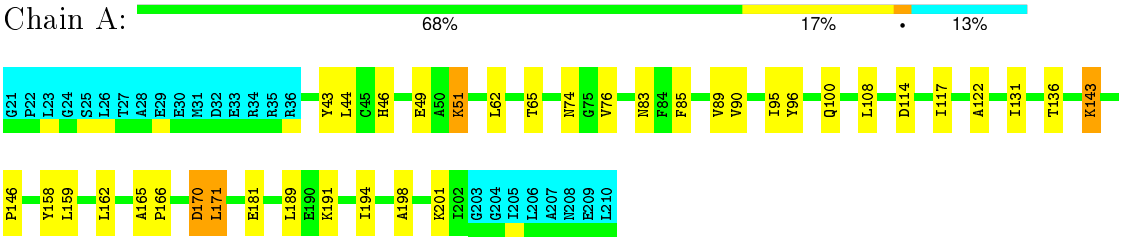
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: IQGAP1 protein

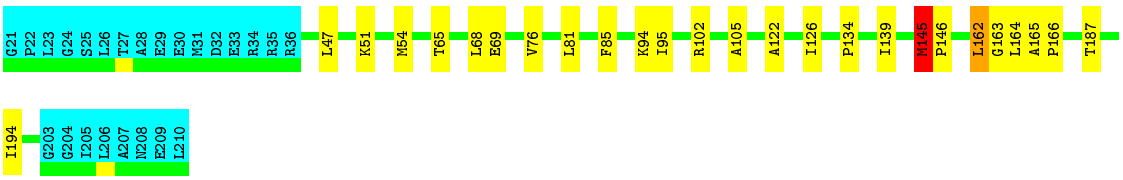
Chain A:



4.2.2 Score per residue for model 2

- Molecule 1: IQGAP1 protein

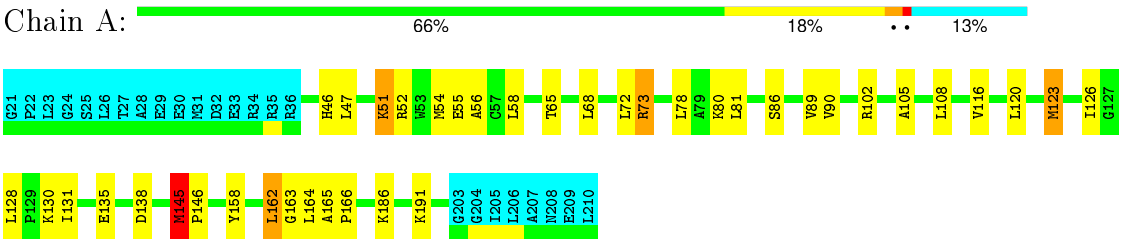
Chain A:



4.2.3 Score per residue for model 3

- Molecule 1: IQGAP1 protein

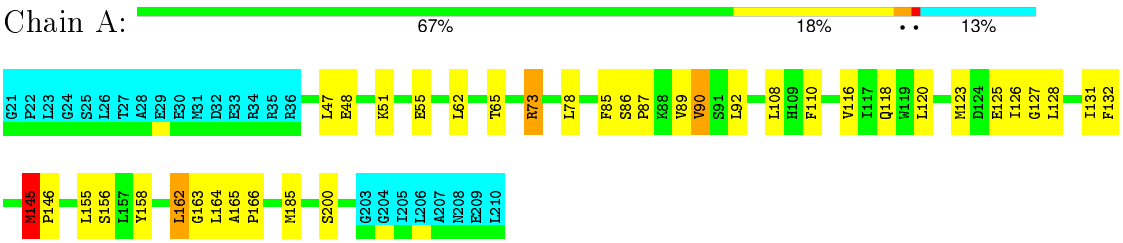
Chain A:



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: IQGAP1 protein

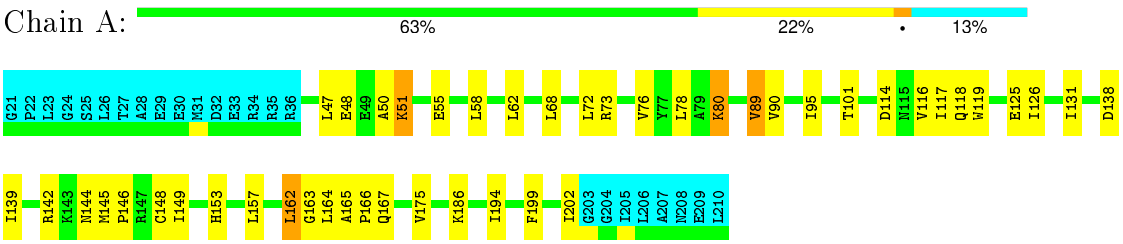
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: IQGAP1 protein

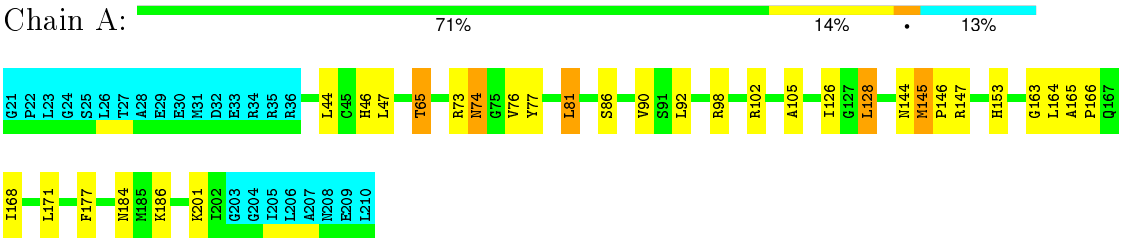
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: IQGAP1 protein

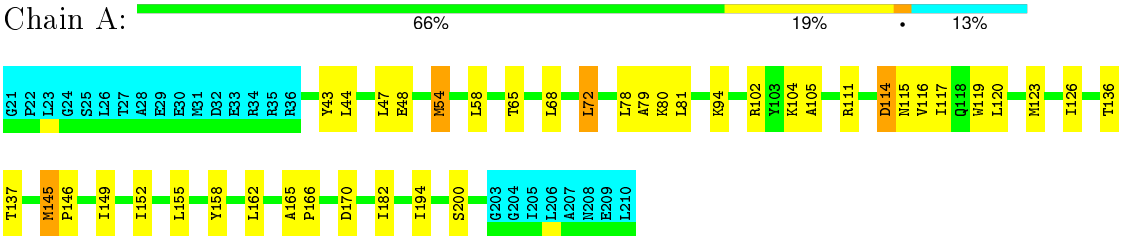
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: IQGAP1 protein

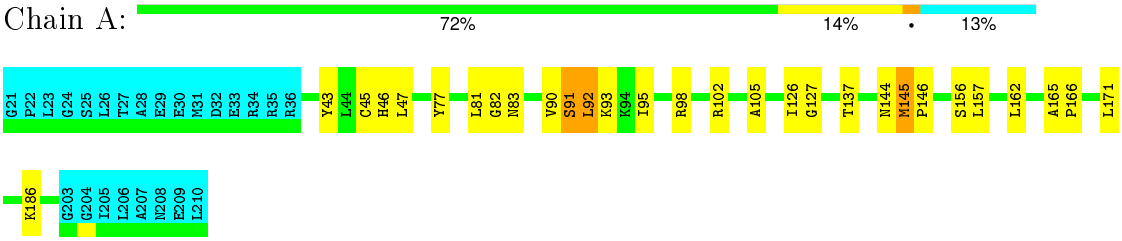
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: IQGAP1 protein

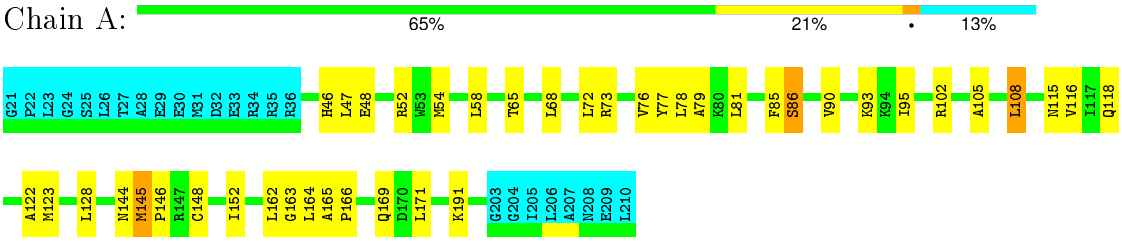
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: IQGAP1 protein

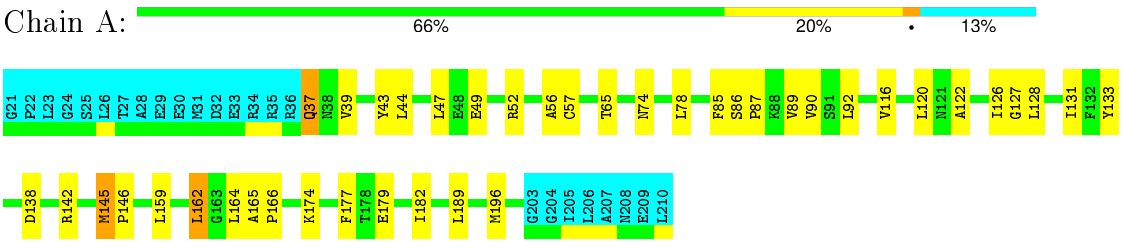
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: IQGAP1 protein

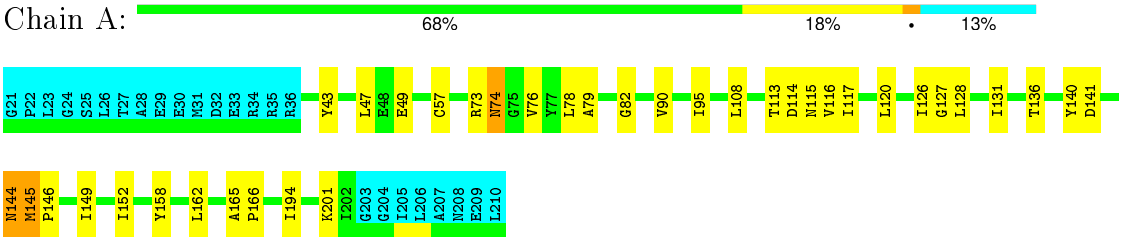
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: IQGAP1 protein

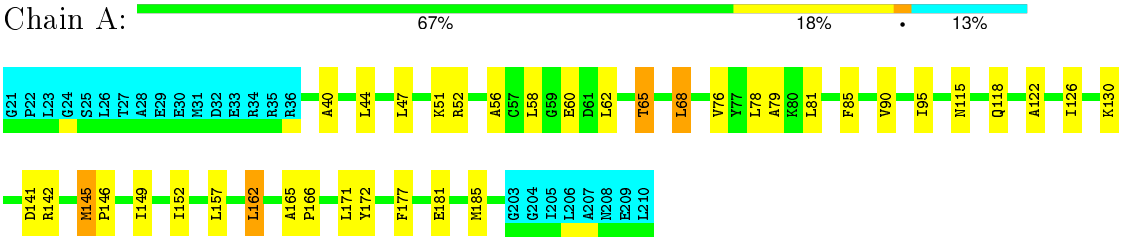
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: IQGAP1 protein

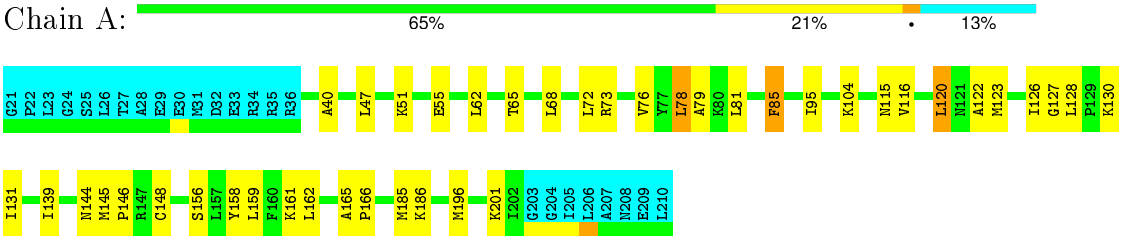
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: IQGAP1 protein

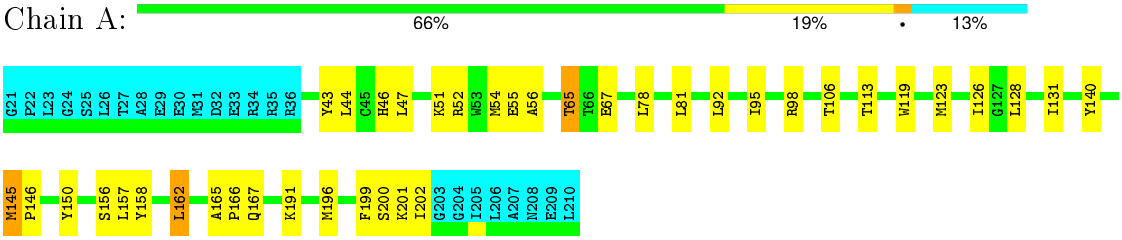
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: IQGAP1 protein

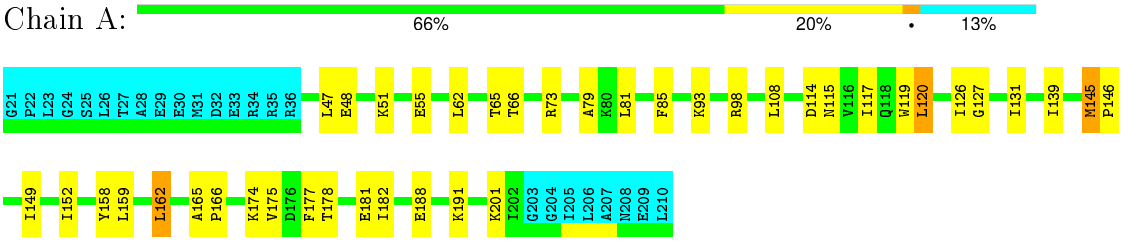
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: IQGAP1 protein

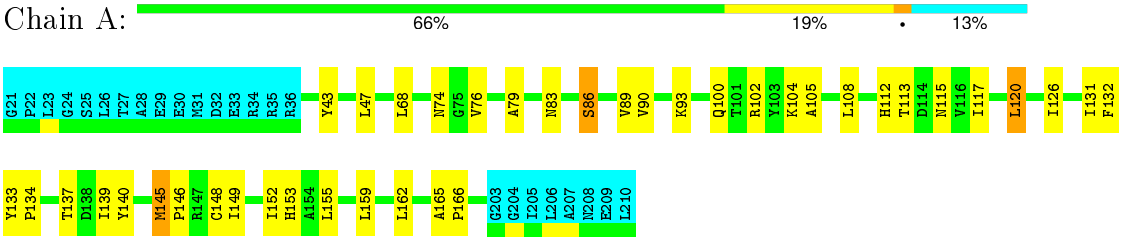
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: IQGAP1 protein

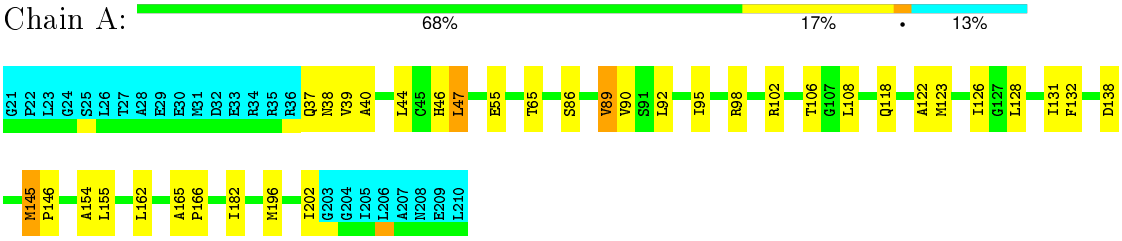
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: IQGAP1 protein

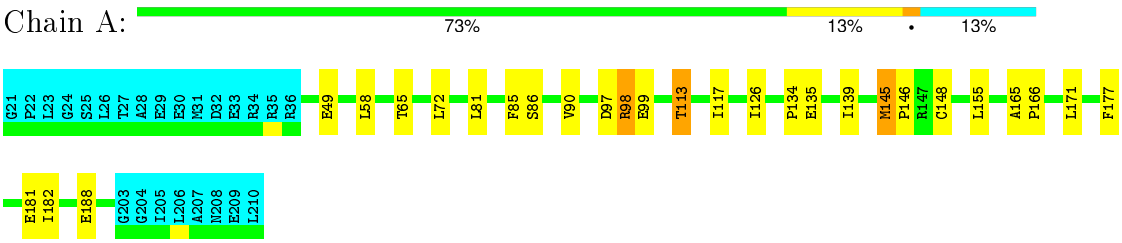
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: IQGAP1 protein

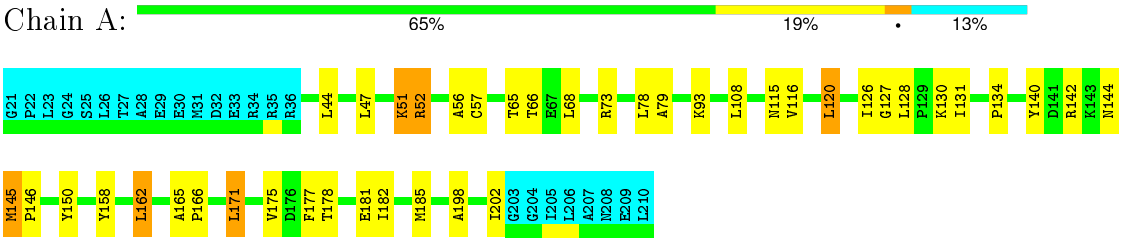
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: IQGAP1 protein

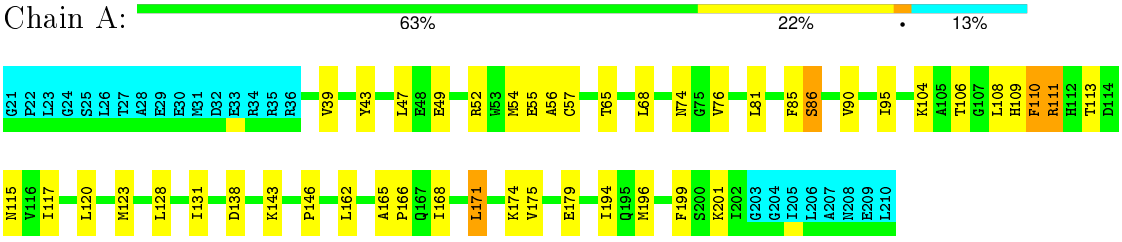
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: IQGAP1 protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 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
CYANA	refinement	2.1

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

Chemical shift file(s)	BMRB entry 11175
Number of chemical shift lists	1
Total number of shifts	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	1367	1354	1354	21±5
All	All	27340	27080	27080	412

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:VAL:HG13	1:A:95:ILE:HG21	0.96	1.37	5	2
1:A:126:ILE:HG21	1:A:162:LEU:HD22	0.90	1.42	13	2
1:A:159:LEU:HD13	1:A:162:LEU:HD11	0.87	1.45	15	1
1:A:159:LEU:HD12	1:A:162:LEU:HD11	0.86	1.48	10	1
1:A:47:LEU:HD23	1:A:65:THR:HG22	0.81	1.50	12	1
1:A:47:LEU:HD22	1:A:68:LEU:HD23	0.76	1.56	3	7
1:A:126:ILE:HD11	1:A:162:LEU:HD13	0.76	1.58	7	5
1:A:76:VAL:HG13	1:A:95:ILE:HG23	0.73	1.61	12	4
1:A:126:ILE:HD13	1:A:162:LEU:HD13	0.71	1.63	19	1
1:A:123:MET:HE1	1:A:155:LEU:HD21	0.70	1.61	7	1
1:A:108:LEU:HD13	1:A:140:TYR:CD2	0.68	2.24	19	1
1:A:73:ARG:HD2	1:A:108:LEU:HD13	0.66	1.66	3	1
1:A:47:LEU:HB3	1:A:65:THR:HG23	0.65	1.67	17	3
1:A:90:VAL:HG12	1:A:118:GLN:HB3	0.65	1.68	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD13	1:A:158:TYR:CE1	0.65	2.27	19	1
1:A:123:MET:CE	1:A:155:LEU:HD21	0.64	2.23	7	1
1:A:108:LEU:HD13	1:A:140:TYR:CE2	0.64	2.28	11	2
1:A:44:LEU:HD22	1:A:177:PHE:CE2	0.64	2.28	10	2
1:A:76:VAL:HG13	1:A:95:ILE:CG2	0.63	2.22	20	4
1:A:85:PHE:CE1	1:A:155:LEU:HD21	0.63	2.29	18	1
1:A:131:ILE:HD11	1:A:132:PHE:CE2	0.63	2.29	4	2
1:A:43:TYR:CE2	1:A:47:LEU:HD11	0.62	2.30	8	6
1:A:73:ARG:O	1:A:108:LEU:HD11	0.62	1.95	9	1
1:A:43:TYR:CZ	1:A:47:LEU:HD11	0.62	2.30	11	3
1:A:116:VAL:CG1	1:A:136:THR:HG23	0.61	2.25	11	1
1:A:120:LEU:HD11	1:A:133:TYR:CE1	0.61	2.30	16	1
1:A:146:PRO:HG3	1:A:194:ILE:HG21	0.61	1.70	5	2
1:A:86:SER:O	1:A:90:VAL:HG22	0.61	1.96	6	8
1:A:126:ILE:CG2	1:A:162:LEU:HD22	0.60	2.26	4	1
1:A:44:LEU:HD13	1:A:177:PHE:CD2	0.60	2.32	10	1
1:A:76:VAL:HG23	1:A:95:ILE:CG2	0.60	2.26	1	1
1:A:158:TYR:CE1	1:A:162:LEU:HD21	0.59	2.33	14	2
1:A:131:ILE:HD11	1:A:132:PHE:CZ	0.59	2.33	4	1
1:A:78:LEU:HG	1:A:116:VAL:HG22	0.59	1.74	13	8
1:A:51:LYS:NZ	1:A:68:LEU:HD22	0.58	2.13	13	1
1:A:126:ILE:HG21	1:A:162:LEU:CD2	0.58	2.28	11	1
1:A:126:ILE:HG13	1:A:162:LEU:HD21	0.58	1.75	5	1
1:A:149:ILE:HA	1:A:152:ILE:HD12	0.58	1.76	15	3
1:A:114:ASP:HA	1:A:117:ILE:HD12	0.58	1.73	7	4
1:A:148:CYS:O	1:A:152:ILE:HD12	0.57	1.99	9	2
1:A:123:MET:HB3	1:A:128:LEU:HD12	0.57	1.75	9	2
1:A:58:LEU:HD11	1:A:81:LEU:HA	0.56	1.76	12	1
1:A:154:ALA:HB2	1:A:202:ILE:HG21	0.56	1.77	17	1
1:A:126:ILE:CG1	1:A:162:LEU:HD21	0.56	2.30	5	1
1:A:128:LEU:HD23	1:A:133:TYR:CE1	0.56	2.36	10	1
1:A:159:LEU:HD13	1:A:162:LEU:CD1	0.56	2.27	15	1
1:A:134:PRO:HG2	1:A:139:ILE:HD11	0.56	1.76	16	2
1:A:85:PHE:CE2	1:A:159:LEU:HD13	0.56	2.36	13	1
1:A:113:THR:HG23	1:A:140:TYR:CE2	0.56	2.36	14	2
1:A:123:MET:HB2	1:A:128:LEU:HD12	0.56	1.76	20	1
1:A:163:GLY:C	1:A:164:LEU:HD22	0.56	2.21	4	4
1:A:146:PRO:HG3	1:A:194:ILE:HG23	0.56	1.75	1	1
1:A:77:TYR:O	1:A:81:LEU:HD23	0.56	2.01	9	3
1:A:116:VAL:CG1	1:A:139:ILE:HD12	0.56	2.31	5	1
1:A:120:LEU:O	1:A:120:LEU:HD13	0.55	2.01	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:189:LEU:HD22	1:A:196:MET:HG3	0.55	1.77	10	1
1:A:81:LEU:HD21	1:A:85:PHE:CE2	0.55	2.36	15	1
1:A:74:ASN:HB2	1:A:76:VAL:HG22	0.55	1.77	6	1
1:A:74:ASN:HB3	1:A:76:VAL:HG22	0.55	1.77	16	1
1:A:163:GLY:C	1:A:164:LEU:HD12	0.55	2.21	5	2
1:A:54:MET:HE2	1:A:72:LEU:HD21	0.55	1.79	7	1
1:A:85:PHE:CE1	1:A:122:ALA:HB1	0.55	2.37	10	2
1:A:78:LEU:HD21	1:A:139:ILE:HD13	0.55	1.79	13	1
1:A:89:VAL:HG23	1:A:125:GLU:OE1	0.55	2.01	5	1
1:A:44:LEU:HD11	1:A:181:GLU:HG3	0.55	1.79	12	2
1:A:178:THR:O	1:A:182:ILE:HD12	0.54	2.02	19	2
1:A:95:ILE:HD13	1:A:98:ARG:NH1	0.54	2.18	17	1
1:A:90:VAL:HG12	1:A:118:GLN:CB	0.54	2.32	17	2
1:A:126:ILE:CD1	1:A:162:LEU:HD13	0.54	2.32	17	5
1:A:58:LEU:HD11	1:A:80:LYS:CG	0.54	2.32	5	1
1:A:158:TYR:O	1:A:162:LEU:HD12	0.54	2.03	4	2
1:A:126:ILE:HG22	1:A:162:LEU:HD22	0.54	1.78	4	1
1:A:120:LEU:HD21	1:A:133:TYR:CD1	0.53	2.38	16	1
1:A:49:GLU:OE1	1:A:171:LEU:HD12	0.53	2.04	18	1
1:A:47:LEU:CB	1:A:65:THR:HG22	0.53	2.34	6	1
1:A:153:HIS:CE1	1:A:168:ILE:HD13	0.53	2.38	6	1
1:A:73:ARG:O	1:A:139:ILE:HG22	0.53	2.03	15	1
1:A:37:GLN:NE2	1:A:182:ILE:HG21	0.53	2.18	10	1
1:A:73:ARG:HD3	1:A:108:LEU:HD12	0.53	1.79	9	1
1:A:126:ILE:HD11	1:A:162:LEU:HD22	0.53	1.81	7	1
1:A:44:LEU:O	1:A:65:THR:HG21	0.53	2.04	14	1
1:A:146:PRO:HG2	1:A:194:ILE:HG21	0.53	1.81	7	2
1:A:126:ILE:CD1	1:A:162:LEU:HD22	0.53	2.34	7	1
1:A:170:ASP:C	1:A:171:LEU:HD13	0.52	2.24	1	1
1:A:73:ARG:CD	1:A:108:LEU:HD12	0.52	2.34	9	1
1:A:86:SER:OG	1:A:122:ALA:HB1	0.52	2.04	17	1
1:A:120:LEU:HD21	1:A:134:PRO:HD2	0.52	1.82	19	1
1:A:113:THR:O	1:A:117:ILE:HD12	0.52	2.04	11	4
1:A:74:ASN:CG	1:A:76:VAL:HG12	0.52	2.24	1	1
1:A:126:ILE:HD12	1:A:158:TYR:CE1	0.52	2.40	7	1
1:A:128:LEU:HD11	1:A:158:TYR:CE2	0.52	2.40	13	1
1:A:134:PRO:CG	1:A:139:ILE:HD11	0.52	2.35	2	3
1:A:44:LEU:HD12	1:A:182:ILE:HG12	0.51	1.82	17	3
1:A:55:GLU:CB	1:A:62:LEU:HD13	0.51	2.35	5	2
1:A:171:LEU:HD13	1:A:171:LEU:N	0.51	2.19	1	1
1:A:126:ILE:HD11	1:A:162:LEU:CD1	0.51	2.33	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:GLN:HB3	1:A:40:ALA:HB3	0.51	1.82	17	1
1:A:54:MET:HB2	1:A:81:LEU:HD21	0.51	1.80	14	1
1:A:65:THR:HA	1:A:68:LEU:HD23	0.51	1.82	12	1
1:A:157:LEU:HD21	1:A:202:ILE:HG22	0.51	1.82	5	1
1:A:40:ALA:HB1	1:A:185:MET:HB2	0.51	1.83	13	2
1:A:47:LEU:CD2	1:A:68:LEU:HD23	0.51	2.36	16	2
1:A:73:ARG:HD2	1:A:108:LEU:HD11	0.50	1.81	4	1
1:A:85:PHE:HB2	1:A:159:LEU:HD11	0.50	1.83	1	1
1:A:47:LEU:CB	1:A:65:THR:HG23	0.50	2.37	9	8
1:A:60:GLU:OE2	1:A:62:LEU:HD11	0.50	2.06	12	1
1:A:198:ALA:HB3	1:A:201:LYS:CG	0.50	2.36	1	1
1:A:145:MET:N	1:A:146:PRO:HD2	0.50	2.22	13	17
1:A:44:LEU:HD13	1:A:177:PHE:CG	0.50	2.41	12	2
1:A:78:LEU:HD12	1:A:119:TRP:CE3	0.50	2.41	14	2
1:A:116:VAL:HG11	1:A:139:ILE:HD12	0.50	1.83	5	1
1:A:156:SER:OG	1:A:157:LEU:HD12	0.50	2.06	14	2
1:A:79:ALA:HB2	1:A:115:ASN:HB3	0.50	1.84	7	8
1:A:79:ALA:HB2	1:A:115:ASN:CB	0.50	2.37	11	3
1:A:54:MET:SD	1:A:81:LEU:HD13	0.49	2.47	20	2
1:A:126:ILE:HG21	1:A:162:LEU:HD13	0.49	1.84	4	1
1:A:58:LEU:HD22	1:A:80:LYS:HE2	0.49	1.85	3	2
1:A:82:GLY:C	1:A:90:VAL:HG21	0.49	2.26	8	2
1:A:87:PRO:HB2	1:A:92:LEU:HD12	0.49	1.84	4	1
1:A:91:SER:C	1:A:92:LEU:HD23	0.49	2.28	8	1
1:A:123:MET:HB3	1:A:128:LEU:HD22	0.49	1.83	4	1
1:A:126:ILE:HD12	1:A:162:LEU:CD2	0.49	2.37	3	4
1:A:123:MET:HG2	1:A:155:LEU:HD11	0.49	1.85	4	1
1:A:83:ASN:HB2	1:A:90:VAL:HG21	0.49	1.85	1	1
1:A:48:GLU:OE1	1:A:175:VAL:HG11	0.49	2.06	15	1
1:A:81:LEU:HD12	1:A:119:TRP:HE1	0.48	1.68	15	1
1:A:51:LYS:HG2	1:A:62:LEU:HD22	0.48	1.85	1	1
1:A:149:ILE:HG22	1:A:153:HIS:CD2	0.48	2.43	16	1
1:A:131:ILE:HD11	1:A:132:PHE:CE1	0.48	2.44	16	1
1:A:66:THR:HG22	1:A:181:GLU:OE1	0.48	2.08	19	1
1:A:123:MET:HB3	1:A:128:LEU:HD23	0.47	1.85	14	1
1:A:120:LEU:HA	1:A:123:MET:HE3	0.47	1.85	4	1
1:A:76:VAL:HG21	1:A:100:GLN:NE2	0.47	2.25	16	1
1:A:54:MET:CE	1:A:72:LEU:HD21	0.47	2.39	7	2
1:A:139:ILE:HG23	1:A:145:MET:SD	0.47	2.49	5	1
1:A:149:ILE:HD13	1:A:152:ILE:HD12	0.47	1.84	12	1
1:A:171:LEU:HD23	1:A:174:LYS:CB	0.47	2.39	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:ALA:HB3	1:A:95:ILE:CD1	0.47	2.40	9	1
1:A:55:GLU:OE1	1:A:62:LEU:HD11	0.47	2.09	13	1
1:A:126:ILE:HD12	1:A:162:LEU:HD11	0.47	1.87	5	1
1:A:76:VAL:HG23	1:A:95:ILE:HG21	0.47	1.86	1	1
1:A:163:GLY:O	1:A:164:LEU:HD22	0.47	2.08	3	2
1:A:108:LEU:HD13	1:A:140:TYR:CZ	0.47	2.45	11	1
1:A:145:MET:CB	1:A:146:PRO:CD	0.46	2.93	2	9
1:A:83:ASN:OD1	1:A:90:VAL:HG21	0.46	2.11	16	1
1:A:126:ILE:CG2	1:A:128:LEU:HD12	0.46	2.41	6	2
1:A:54:MET:HG3	1:A:81:LEU:HD13	0.46	1.88	3	1
1:A:128:LEU:HD13	1:A:158:TYR:CZ	0.46	2.45	19	1
1:A:87:PRO:O	1:A:92:LEU:HD21	0.46	2.11	10	1
1:A:126:ILE:HG22	1:A:128:LEU:HD12	0.46	1.88	6	1
1:A:81:LEU:HD22	1:A:119:TRP:HE1	0.45	1.70	7	1
1:A:144:ASN:ND2	1:A:194:ILE:HD13	0.45	2.26	11	1
1:A:189:LEU:HD12	1:A:189:LEU:O	0.45	2.12	1	1
1:A:169:GLN:NE2	1:A:171:LEU:HD11	0.45	2.26	9	1
1:A:90:VAL:HG13	1:A:118:GLN:HB3	0.45	1.87	12	1
1:A:189:LEU:O	1:A:189:LEU:HD12	0.45	2.12	10	1
1:A:146:PRO:CG	1:A:194:ILE:HG21	0.45	2.41	2	1
1:A:51:LYS:O	1:A:62:LEU:HD12	0.45	2.11	15	1
1:A:51:LYS:HB3	1:A:68:LEU:HD13	0.45	1.89	5	1
1:A:123:MET:CB	1:A:128:LEU:HD12	0.45	2.41	9	3
1:A:95:ILE:HD13	1:A:98:ARG:HH11	0.44	1.71	17	1
1:A:171:LEU:HD12	1:A:175:VAL:HG11	0.44	1.88	19	1
1:A:158:TYR:CZ	1:A:162:LEU:HD11	0.44	2.47	4	1
1:A:39:VAL:HG21	1:A:196:MET:HB2	0.44	1.89	10	1
1:A:66:THR:HG22	1:A:181:GLU:CD	0.44	2.32	15	1
1:A:39:VAL:HG13	1:A:196:MET:SD	0.44	2.53	20	1
1:A:85:PHE:CZ	1:A:122:ALA:HB1	0.44	2.47	12	2
1:A:44:LEU:HA	1:A:47:LEU:HD12	0.44	1.88	6	1
1:A:116:VAL:HB	1:A:136:THR:HG23	0.44	1.90	7	1
1:A:165:ALA:HB1	1:A:166:PRO:HD2	0.44	1.90	16	20
1:A:102:ARG:O	1:A:105:ALA:HB3	0.44	2.13	3	7
1:A:40:ALA:HB1	1:A:185:MET:CB	0.44	2.43	13	1
1:A:145:MET:N	1:A:146:PRO:CD	0.44	2.81	5	5
1:A:72:LEU:HD21	1:A:148:CYS:SG	0.44	2.53	18	1
1:A:74:ASN:HA	1:A:108:LEU:HD21	0.43	1.89	20	1
1:A:55:GLU:HB3	1:A:62:LEU:HD13	0.43	1.88	5	1
1:A:171:LEU:HD23	1:A:174:LYS:HB2	0.43	1.90	20	1
1:A:52:ARG:O	1:A:56:ALA:HB2	0.43	2.14	19	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:ILE:HG22	1:A:153:HIS:HD2	0.43	1.73	16	1
1:A:154:ALA:HB2	1:A:202:ILE:CG2	0.43	2.43	17	1
1:A:123:MET:CG	1:A:128:LEU:HD12	0.43	2.44	17	1
1:A:126:ILE:CD1	1:A:162:LEU:HD11	0.43	2.42	8	2
1:A:157:LEU:HD21	1:A:202:ILE:CG2	0.43	2.43	5	1
1:A:126:ILE:CG2	1:A:128:LEU:HD22	0.43	2.44	14	1
1:A:128:LEU:HD13	1:A:158:TYR:CE2	0.43	2.49	11	1
1:A:120:LEU:HD13	1:A:120:LEU:O	0.43	2.14	13	2
1:A:177:PHE:HB2	1:A:182:ILE:HD11	0.43	1.90	15	2
1:A:97:ASP:O	1:A:98:ARG:C	0.43	2.57	18	1
1:A:110:PHE:O	1:A:111:ARG:CB	0.43	2.67	20	1
1:A:48:GLU:OE2	1:A:175:VAL:HG21	0.43	2.14	5	1
1:A:43:TYR:CD2	1:A:47:LEU:HD11	0.43	2.48	7	1
1:A:51:LYS:HB3	1:A:68:LEU:HD11	0.42	1.90	3	1
1:A:113:THR:HG23	1:A:140:TYR:CD2	0.42	2.49	14	1
1:A:150:TYR:CE1	1:A:202:ILE:HD11	0.42	2.48	19	2
1:A:49:GLU:HG3	1:A:168:ILE:HD11	0.42	1.91	20	1
1:A:108:LEU:HD21	1:A:140:TYR:CE2	0.42	2.49	16	1
1:A:83:ASN:ND2	1:A:92:LEU:HD22	0.42	2.29	8	1
1:A:44:LEU:HD22	1:A:177:PHE:CE1	0.42	2.50	6	1
1:A:123:MET:CB	1:A:128:LEU:HD13	0.42	2.44	3	1
1:A:120:LEU:O	1:A:120:LEU:HD23	0.42	2.15	20	2
1:A:74:ASN:O	1:A:78:LEU:HD23	0.42	2.15	11	1
1:A:73:ARG:HH11	1:A:108:LEU:HD22	0.42	1.75	3	1
1:A:81:LEU:C	1:A:81:LEU:HD13	0.42	2.35	15	1
1:A:72:LEU:HD22	1:A:149:ILE:CD1	0.42	2.45	5	1
1:A:58:LEU:CD1	1:A:81:LEU:HD22	0.42	2.45	9	1
1:A:47:LEU:HD21	1:A:68:LEU:CB	0.42	2.45	12	1
1:A:58:LEU:HD11	1:A:81:LEU:HD22	0.42	1.91	9	1
1:A:145:MET:HB3	1:A:146:PRO:HD3	0.42	1.92	15	5
1:A:131:ILE:O	1:A:131:ILE:HD12	0.42	2.15	16	1
1:A:128:LEU:HD21	1:A:158:TYR:CD1	0.41	2.50	13	1
1:A:38:ASN:OD1	1:A:39:VAL:HG23	0.41	2.15	17	1
1:A:158:TYR:CD1	1:A:162:LEU:HD21	0.41	2.49	14	1
1:A:51:LYS:HB2	1:A:68:LEU:HD21	0.41	1.90	19	1
1:A:85:PHE:HE1	1:A:122:ALA:HB1	0.41	1.76	13	1
1:A:171:LEU:HD22	1:A:175:VAL:CG1	0.41	2.45	20	1
1:A:51:LYS:HZ2	1:A:68:LEU:HD22	0.41	1.71	13	1
1:A:158:TYR:O	1:A:162:LEU:HD23	0.41	2.16	1	1
1:A:51:LYS:CB	1:A:68:LEU:HD13	0.41	2.46	5	1
1:A:150:TYR:CD1	1:A:202:ILE:HD11	0.41	2.50	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:ILE:HG12	1:A:162:LEU:HD13	0.41	1.93	11	1
1:A:158:TYR:CD2	1:A:162:LEU:HD21	0.41	2.51	15	1
1:A:89:VAL:HG11	1:A:122:ALA:HA	0.41	1.92	17	2
1:A:50:ALA:HB2	1:A:153:HIS:NE2	0.41	2.31	5	1
1:A:92:LEU:HD12	1:A:95:ILE:HD12	0.40	1.93	14	1
1:A:47:LEU:HG	1:A:68:LEU:HD23	0.40	1.93	5	1
1:A:81:LEU:HD13	1:A:81:LEU:O	0.40	2.16	15	1
1:A:76:VAL:HG23	1:A:95:ILE:HG23	0.40	1.91	1	1
1:A:47:LEU:HD23	1:A:65:THR:O	0.40	2.16	17	1
1:A:85:PHE:HE2	1:A:159:LEU:HD13	0.40	1.73	13	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	166/190 (87%)	149±3 (90±2%)	16±3 (9±2%)	2±1 (1±1%)	23	69
All	All	3320/3800 (87%)	2973 (90%)	312 (9%)	35 (1%)	23	69

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	145	MET	14
1	A	127	GLY	7
1	A	89	VAL	6
1	A	199	PHE	2
1	A	143	LYS	1
1	A	58	LEU	1
1	A	198	ALA	1
1	A	156	SER	1
1	A	95	ILE	1
1	A	90	VAL	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	148/166 (89%)	137±3 (92±2%)	11±3 (8±2%)	21 66
All	All	2960/3320 (89%)	2734 (92%)	226 (8%)	21 66

All 85 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	162	LEU	11
1	A	51	LYS	8
1	A	65	THR	8
1	A	73	ARG	7
1	A	46	HIS	7
1	A	144	ASN	7
1	A	120	LEU	6
1	A	171	LEU	6
1	A	55	GLU	5
1	A	201	LYS	5
1	A	138	ASP	5
1	A	145	MET	5
1	A	98	ARG	5
1	A	191	LYS	5
1	A	186	LYS	5
1	A	93	LYS	5
1	A	142	ARG	4
1	A	108	LEU	4
1	A	130	LYS	4
1	A	57	CYS	4
1	A	137	THR	3
1	A	74	ASN	3
1	A	106	THR	3
1	A	104	LYS	3
1	A	196	MET	3
1	A	86	SER	3
1	A	48	GLU	3
1	A	92	LEU	3
1	A	200	SER	3

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Mol	Chain	Res	Type	Models (Total)
1	A	81	LEU	3
1	A	49	GLU	3
1	A	85	PHE	3
1	A	72	LEU	3
1	A	52	ARG	2
1	A	94	LYS	2
1	A	148	CYS	2
1	A	179	GLU	2
1	A	78	LEU	2
1	A	135	GLU	2
1	A	47	LEU	2
1	A	110	PHE	2
1	A	188	GLU	2
1	A	155	LEU	2
1	A	143	LYS	2
1	A	111	ARG	2
1	A	167	GLN	2
1	A	170	ASP	2
1	A	174	LYS	2
1	A	141	ASP	2
1	A	185	MET	2
1	A	43	TYR	2
1	A	114	ASP	2
1	A	199	PHE	1
1	A	100	GLN	1
1	A	112	HIS	1
1	A	68	LEU	1
1	A	187	THR	1
1	A	123	MET	1
1	A	184	ASN	1
1	A	37	GLN	1
1	A	115	ASN	1
1	A	147	ARG	1
1	A	181	GLU	1
1	A	99	GLU	1
1	A	157	LEU	1
1	A	156	SER	1
1	A	109	HIS	1
1	A	101	THR	1
1	A	164	LEU	1
1	A	80	LYS	1
1	A	113	THR	1

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Mol	Chain	Res	Type	Models (Total)
1	A	45	CYS	1
1	A	67	GLU	1
1	A	128	LEU	1
1	A	54	MET	1
1	A	172	TYR	1
1	A	125	GLU	1
1	A	159	LEU	1
1	A	136	THR	1
1	A	96	TYR	1
1	A	126	ILE	1
1	A	69	GLU	1
1	A	91	SER	1
1	A	161	LYS	1
1	A	102	ARG	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 80% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 11175

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	2093
Number of shifts mapped to atoms	2093
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	190	1.90 ± 0.13	Should be applied
$^{13}C_{\beta}$	177	2.91 ± 0.11	Should be applied
$^{13}C'$	0	—	—
^{15}N	167	0.57 ± 0.30	None needed (imprecise)

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 80%, i.e. 1722 atoms were assigned a chemical shift out of a possible 2140. 25 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	628/814 (77%)	314/324 (97%)	166/332 (50%)	148/158 (94%)
Sidechain	963/1123 (86%)	598/661 (90%)	355/414 (86%)	10/48 (21%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	131/203 (65%)	83/107 (78%)	46/90 (51%)	2/6 (33%)
Overall	1722/2140 (80%)	995/1092 (91%)	567/836 (68%)	160/212 (75%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1939 atoms were assigned a chemical shift out of a possible 2424. 29 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	714/932 (77%)	357/371 (96%)	190/380 (50%)	167/181 (92%)
Sidechain	1094/1289 (85%)	679/758 (90%)	404/473 (85%)	11/58 (19%)
Aromatic	131/203 (65%)	83/107 (78%)	46/90 (51%)	2/6 (33%)
Overall	1939/2424 (80%)	1119/1236 (91%)	640/943 (68%)	180/245 (73%)

7.1.4 Statistically unusual chemical shifts (i)

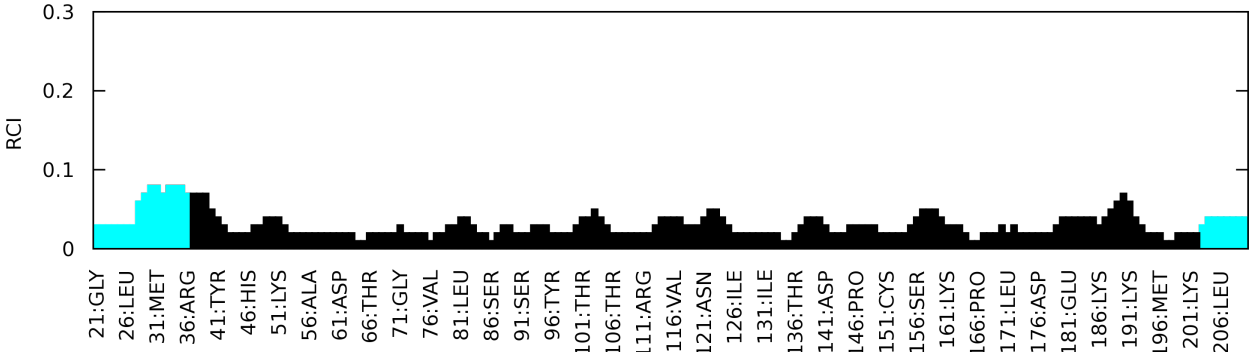
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	146	PRO	CD	19.91	55.31 – 45.41	-30.8
1	A	156	SER	HB3	1.77	5.25 – 2.45	-7.4
1	A	156	SER	HB2	2.26	5.18 – 2.58	-6.2

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:


RCI
0.3
0.2
0.1
0
21:GLY
26:LEU
31:MET
36:ARG
41:TYR
46:HIS
51:LYS
56:ALA
61:ASP
66:THR
71:GLY
76:VAL
81:LEU
86:SER
91:SER
96:TYR
101:THR
106:THR
111:ARG
116:VAL
121:ASN
126:ILE
131:ILE
136:THR
141:ASP
146:PRO
151:CYS
156:SER
161:LYS
166:PRO
171:LEU
176:ASP
181:GLU
186:LYS
191:LYS
196:MET
201:LYS
206:LEU