



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 06:08 am BST

PDB ID : 4UZM
Title : Shotgun proteolysis: A practical application
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Deposited on : 2014-09-05

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 ⓘ symbol.

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

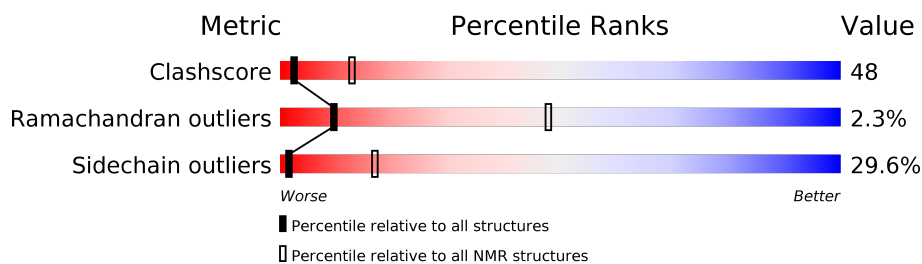
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 91%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	120	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:59, A:78-A:152 (98)	0.20	13

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. No single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1848 atoms, of which 910 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	119	1848	591	910	156	189	2	0

There is a discrepancy between the modelled and reference sequences:

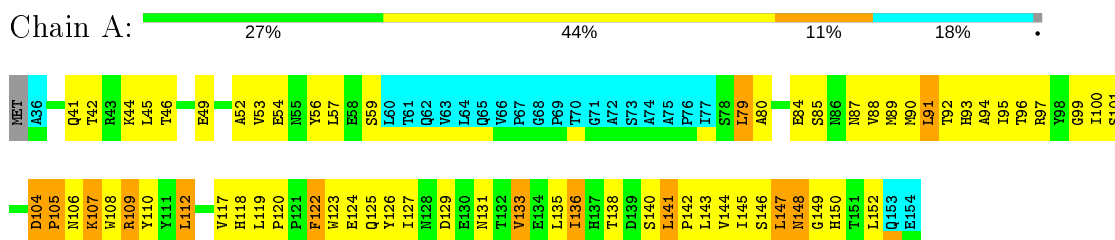
Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MET	-	expression tag	UNP P45800

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: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG

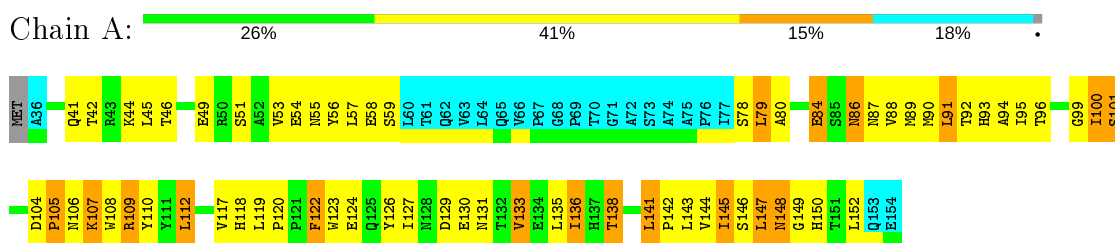


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

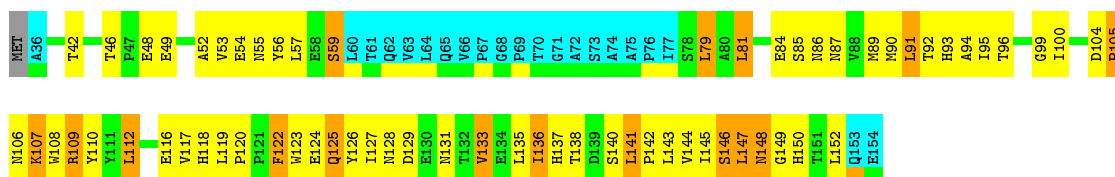
- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



4.2.2 Score per residue for model 2

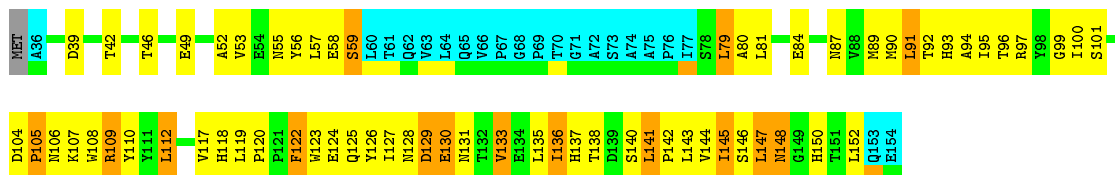
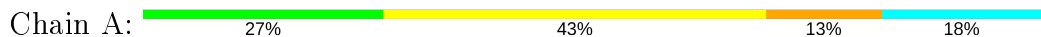
- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG





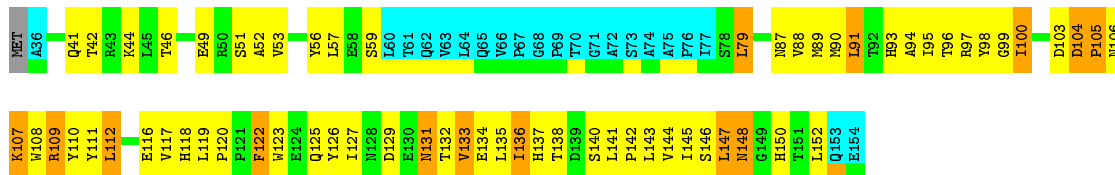
4.2.3 Score per residue for model 3

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



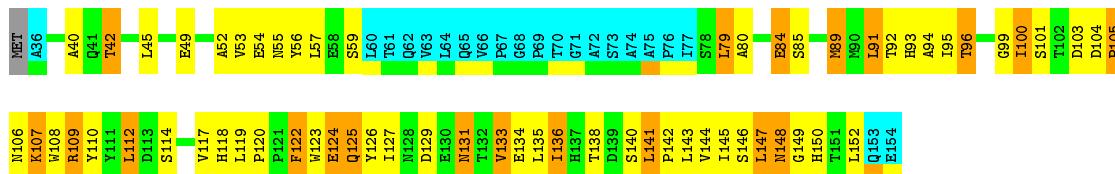
4.2.4 Score per residue for model 4

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



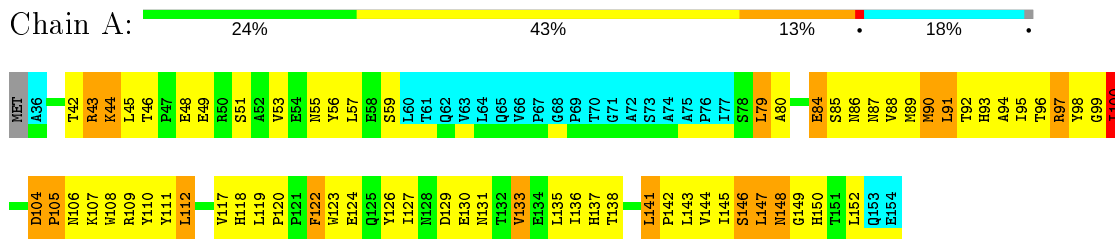
4.2.5 Score per residue for model 5

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



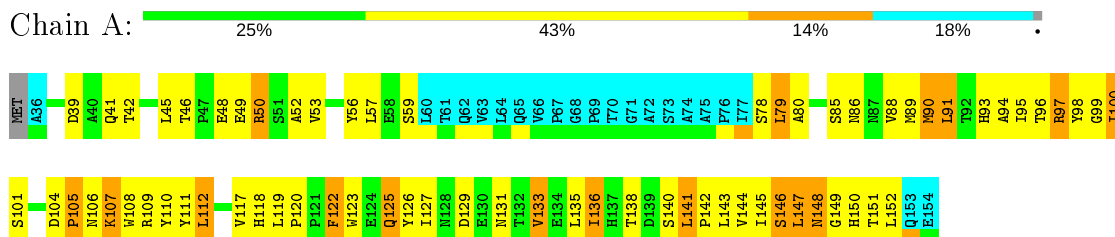
4.2.6 Score per residue for model 6

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



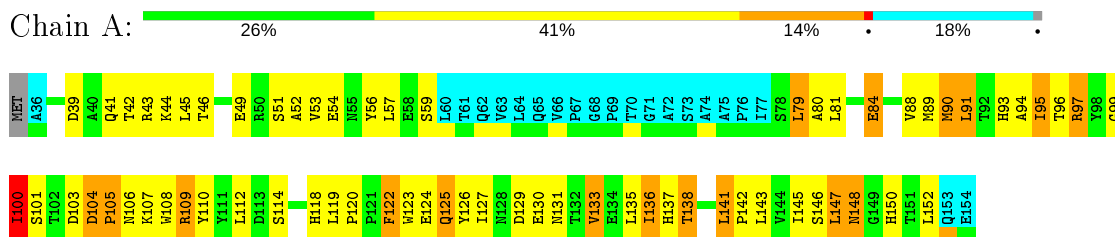
4.2.7 Score per residue for model 7

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



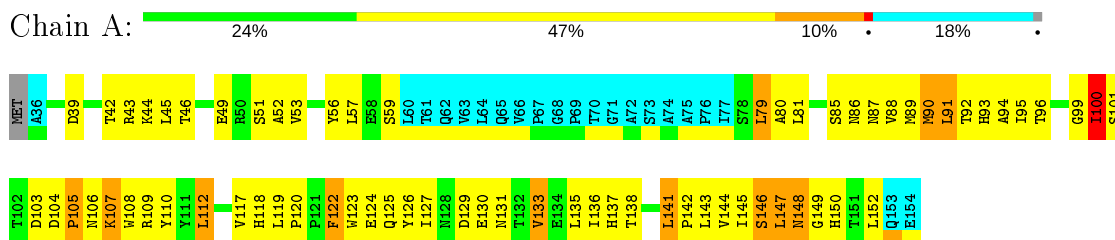
4.2.8 Score per residue for model 8

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



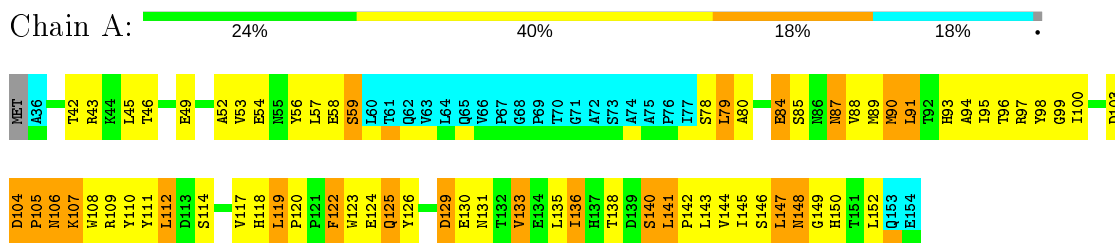
4.2.9 Score per residue for model 9

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



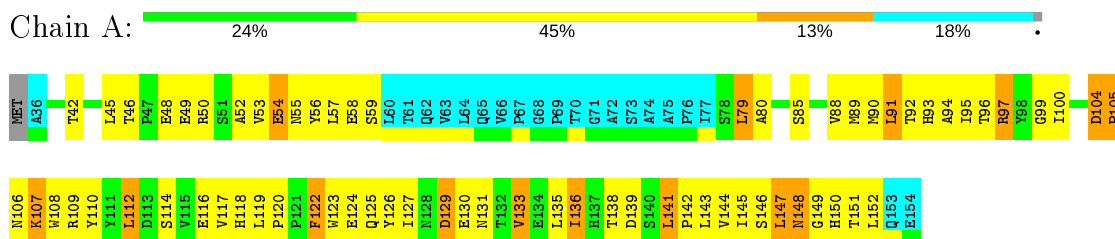
4.2.10 Score per residue for model 10

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



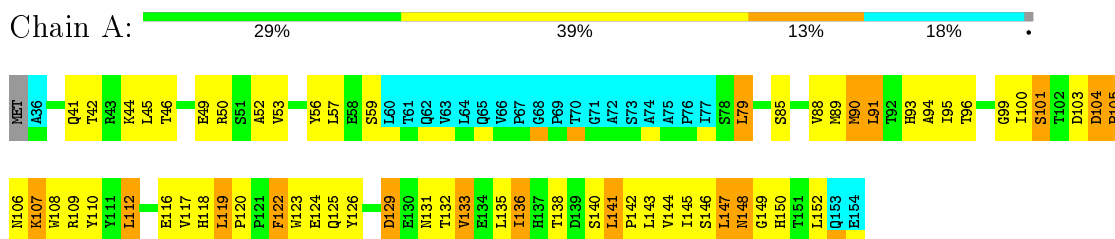
4.2.11 Score per residue for model 11

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



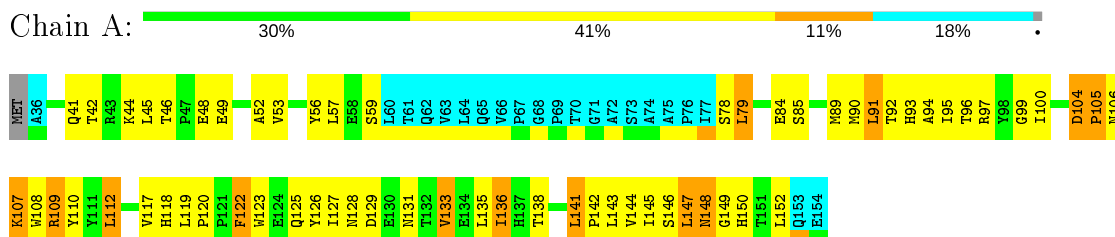
4.2.12 Score per residue for model 12

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



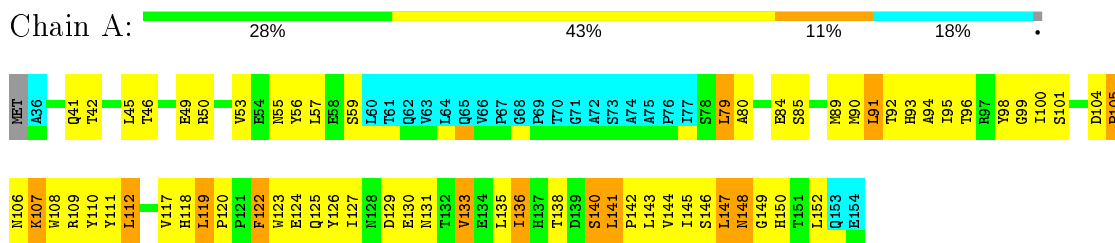
4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



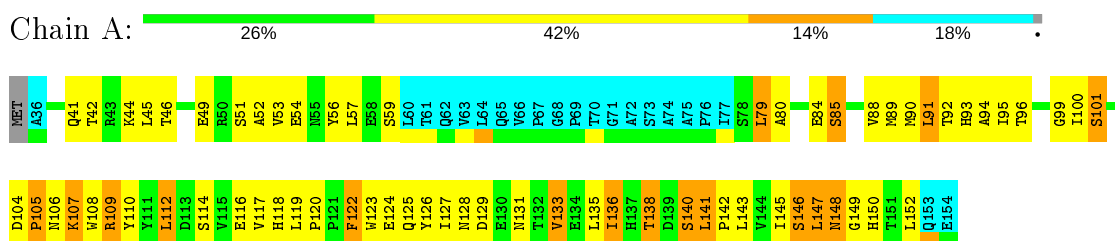
4.2.14 Score per residue for model 14

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



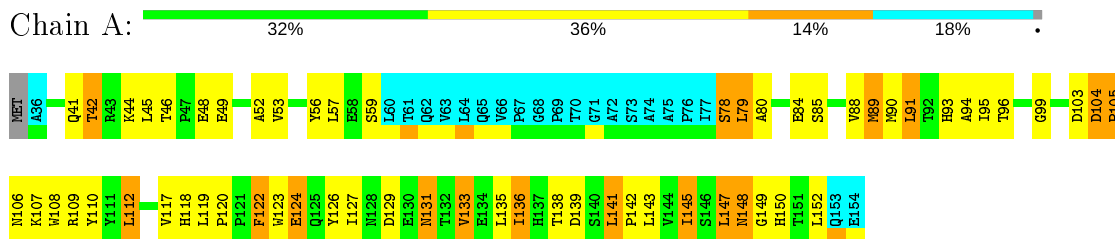
4.2.15 Score per residue for model 15

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



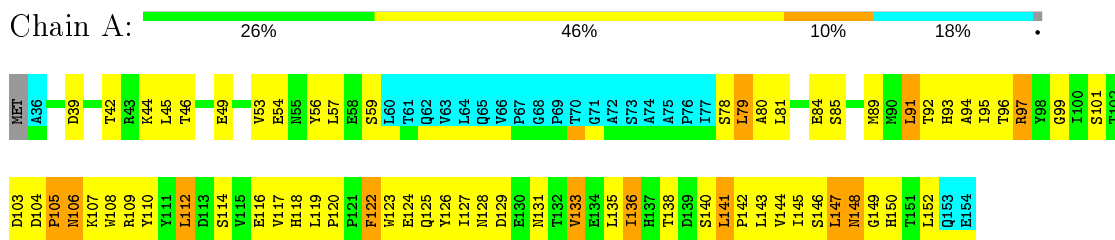
4.2.16 Score per residue for model 16

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



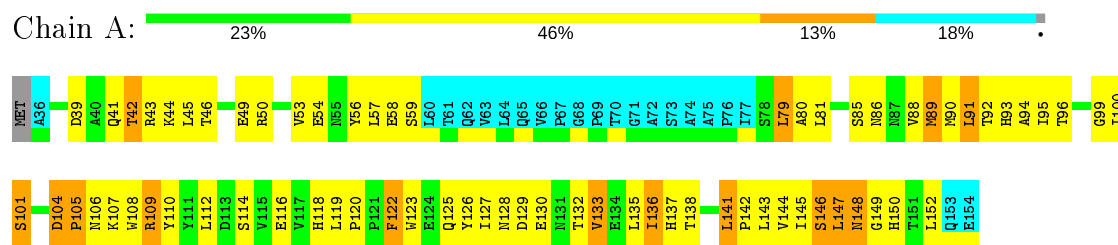
4.2.17 Score per residue for model 17

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



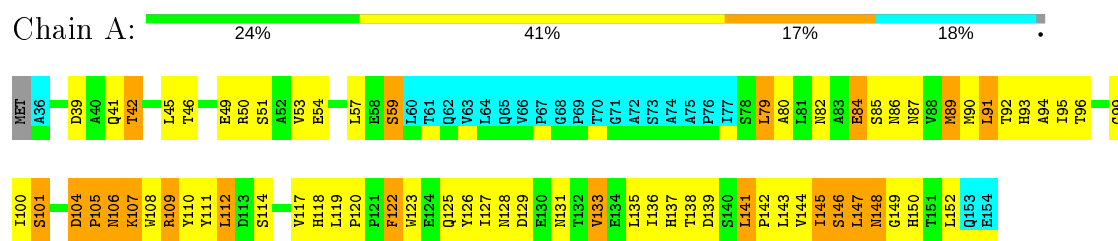
4.2.18 Score per residue for model 18

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



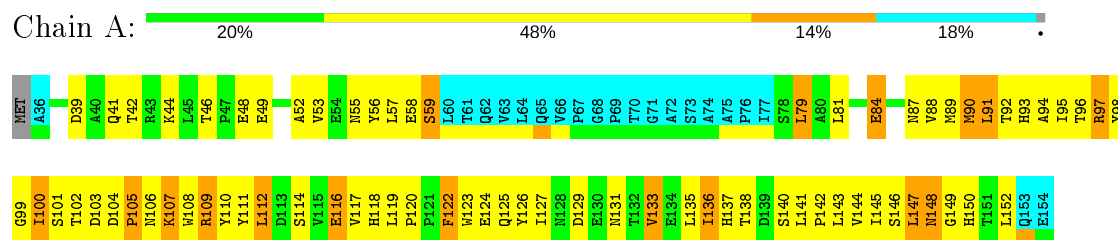
4.2.19 Score per residue for model 19

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



4.2.20 Score per residue for model 20

- Molecule 1: PUTATIVE MEMBRANE PROTEIN IGAA HOMOLOG



5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 20 calculated structures, 20 were deposited, based on the following criterion: *NO VIOLATIONS*.

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

Software name	Classification	Version
CNS	refinement	
ANSIG	structure solution	
CNS	structure solution	

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	1502
Number of shifts mapped to atoms	1494
Number of unparsed shifts	8
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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	794	761	757	75±6
All	All	15880	15220	15140	1495

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ILE:HG21	1:A:119:LEU:HD13	1.03	1.24	14	8
1:A:88:VAL:HG13	1:A:145:ILE:HD11	0.97	1.33	1	1
1:A:79:LEU:HD23	1:A:141:LEU:HD12	0.96	1.37	7	3
1:A:57:LEU:HD22	1:A:79:LEU:HD21	0.95	1.37	19	1
1:A:57:LEU:HD13	1:A:79:LEU:HD23	0.93	1.39	11	4
1:A:100:ILE:HD11	1:A:109:ARG:NH1	0.83	1.88	3	3
1:A:79:LEU:HD13	1:A:138:THR:HG21	0.82	1.49	5	7
1:A:79:LEU:HD23	1:A:141:LEU:CD1	0.82	2.04	7	3
1:A:57:LEU:HD21	1:A:143:LEU:HG	0.78	1.55	17	4
1:A:53:VAL:HG12	1:A:57:LEU:HD11	0.75	1.58	17	6
1:A:135:LEU:HD13	1:A:142:PRO:CB	0.74	2.11	8	20
1:A:100:ILE:HD12	1:A:101:SER:N	0.74	1.96	12	5
1:A:91:LEU:HD12	1:A:93:HIS:HB2	0.74	1.59	3	20
1:A:79:LEU:HD21	1:A:143:LEU:HD23	0.74	1.59	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:85:SER:O	1:A:136:ILE:HG21	0.74	1.82	14	8
1:A:136:ILE:HD11	1:A:145:ILE:CG2	0.74	2.12	10	10
1:A:79:LEU:N	1:A:79:LEU:HD13	0.74	1.98	17	3
1:A:88:VAL:CG1	1:A:145:ILE:HD11	0.74	2.13	1	1
1:A:145:ILE:HA	1:A:152:LEU:HD12	0.73	1.61	9	18
1:A:79:LEU:HD13	1:A:79:LEU:N	0.73	1.99	4	3
1:A:94:ALA:HB2	1:A:129:ASP:O	0.73	1.83	19	19
1:A:95:ILE:HD13	1:A:119:LEU:HD12	0.73	1.61	15	1
1:A:79:LEU:HD11	1:A:143:LEU:HD23	0.72	1.61	8	8
1:A:95:ILE:HD11	1:A:133:VAL:HG11	0.72	1.60	15	9
1:A:87:ASN:O	1:A:136:ILE:HG23	0.70	1.85	9	7
1:A:57:LEU:HD21	1:A:143:LEU:CD2	0.70	2.16	7	6
1:A:95:ILE:HG21	1:A:119:LEU:CD1	0.70	2.17	2	15
1:A:100:ILE:HD11	1:A:109:ARG:CZ	0.70	2.17	2	2
1:A:57:LEU:HD12	1:A:81:LEU:HD11	0.69	1.61	20	3
1:A:80:ALA:HB3	1:A:139:ASP:HB3	0.69	1.63	19	3
1:A:49:GLU:O	1:A:53:VAL:HG23	0.69	1.88	5	20
1:A:119:LEU:HD21	1:A:123:TRP:HB2	0.69	1.63	18	17
1:A:117:VAL:HG12	1:A:142:PRO:HD2	0.69	1.63	13	12
1:A:79:LEU:HG	1:A:138:THR:HG21	0.68	1.62	19	1
1:A:79:LEU:HD21	1:A:118:HIS:HB2	0.68	1.63	14	2
1:A:135:LEU:O	1:A:135:LEU:HD12	0.68	1.89	9	11
1:A:79:LEU:HD21	1:A:118:HIS:CB	0.68	2.18	15	3
1:A:57:LEU:CD2	1:A:79:LEU:HD21	0.68	2.17	19	1
1:A:53:VAL:HG12	1:A:57:LEU:CD1	0.67	2.19	3	6
1:A:57:LEU:HD13	1:A:79:LEU:CD1	0.67	2.19	10	2
1:A:57:LEU:HD13	1:A:79:LEU:CD2	0.67	2.19	13	3
1:A:133:VAL:HG12	1:A:144:VAL:CG1	0.67	2.20	13	2
1:A:135:LEU:HD12	1:A:135:LEU:O	0.67	1.88	10	7
1:A:135:LEU:HD13	1:A:142:PRO:HB3	0.67	1.67	17	19
1:A:88:VAL:HG13	1:A:145:ILE:CD1	0.66	2.19	1	1
1:A:42:THR:HG23	1:A:89:MET:HG2	0.66	1.67	16	3
1:A:138:THR:HG23	1:A:141:LEU:O	0.66	1.91	15	20
1:A:79:LEU:HD12	1:A:138:THR:HG21	0.65	1.69	3	1
1:A:99:GLY:C	1:A:100:ILE:HD13	0.65	2.11	4	3
1:A:118:HIS:HB3	1:A:143:LEU:HD22	0.64	1.68	17	20
1:A:136:ILE:HD11	1:A:145:ILE:HG21	0.64	1.66	8	8
1:A:56:TYR:CD1	1:A:57:LEU:HD23	0.64	2.28	10	9
1:A:79:LEU:HB2	1:A:138:THR:HG21	0.64	1.69	11	17
1:A:88:VAL:HG12	1:A:90:MET:HE2	0.64	1.68	10	3
1:A:79:LEU:HD23	1:A:141:LEU:HG	0.64	1.70	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:SER:HB2	1:A:141:LEU:HD23	0.63	1.70	15	5
1:A:45:LEU:HD11	1:A:49:GLU:HB3	0.63	1.71	11	4
1:A:110:TYR:CG	1:A:119:LEU:HB3	0.63	2.29	15	20
1:A:99:GLY:O	1:A:100:ILE:HD13	0.63	1.93	10	3
1:A:45:LEU:HD23	1:A:50:ARG:HG3	0.62	1.71	18	2
1:A:118:HIS:CD2	1:A:143:LEU:CD2	0.62	2.81	14	20
1:A:123:TRP:HB3	1:A:147:LEU:HD22	0.62	1.72	7	11
1:A:100:ILE:HD12	1:A:100:ILE:O	0.62	1.95	3	1
1:A:85:SER:HA	1:A:136:ILE:HG21	0.62	1.69	6	4
1:A:56:TYR:CD2	1:A:57:LEU:HD23	0.62	2.30	13	3
1:A:79:LEU:HD12	1:A:141:LEU:HD11	0.62	1.72	4	1
1:A:79:LEU:N	1:A:79:LEU:HD23	0.61	2.09	3	1
1:A:79:LEU:N	1:A:79:LEU:HD22	0.61	2.10	6	2
1:A:57:LEU:HD22	1:A:79:LEU:CD2	0.61	2.22	19	2
1:A:135:LEU:HD13	1:A:142:PRO:HB2	0.61	1.70	18	13
1:A:123:TRP:CE3	1:A:147:LEU:HD13	0.61	2.30	10	14
1:A:79:LEU:H	1:A:79:LEU:HD22	0.61	1.56	11	4
1:A:100:ILE:HD11	1:A:109:ARG:HD2	0.61	1.72	20	2
1:A:143:LEU:HD11	1:A:152:LEU:HD11	0.61	1.73	15	18
1:A:119:LEU:HD11	1:A:127:ILE:CG2	0.61	2.26	15	14
1:A:45:LEU:HD13	1:A:88:VAL:HG21	0.61	1.72	18	2
1:A:79:LEU:CD2	1:A:143:LEU:HD23	0.60	2.25	17	4
1:A:84:GLU:O	1:A:136:ILE:HG22	0.60	1.95	1	7
1:A:88:VAL:HG11	1:A:145:ILE:HD11	0.59	1.72	10	2
1:A:79:LEU:CD2	1:A:141:LEU:HD12	0.59	2.23	7	1
1:A:79:LEU:HD22	1:A:79:LEU:H	0.59	1.57	16	3
1:A:46:THR:HG23	1:A:49:GLU:OE1	0.59	1.98	11	19
1:A:53:VAL:HG12	1:A:57:LEU:HD12	0.59	1.73	3	4
1:A:93:HIS:CG	1:A:112:LEU:HD11	0.59	2.32	13	17
1:A:100:ILE:N	1:A:100:ILE:HD13	0.59	2.13	9	5
1:A:119:LEU:HD11	1:A:127:ILE:HG21	0.58	1.75	16	9
1:A:99:GLY:HA2	1:A:108:TRP:CG	0.58	2.33	4	19
1:A:133:VAL:HG12	1:A:144:VAL:HG11	0.58	1.75	13	2
1:A:95:ILE:CG2	1:A:119:LEU:HD13	0.58	2.15	14	2
1:A:133:VAL:CG1	1:A:147:LEU:HD12	0.58	2.28	3	11
1:A:91:LEU:O	1:A:133:VAL:HG23	0.58	1.99	6	18
1:A:95:ILE:HD11	1:A:133:VAL:CG1	0.58	2.28	15	1
1:A:45:LEU:HD22	1:A:136:ILE:CD1	0.57	2.29	6	2
1:A:136:ILE:O	1:A:142:PRO:HA	0.57	1.99	18	19
1:A:105:PRO:HA	1:A:108:TRP:CH2	0.57	2.35	18	20
1:A:80:ALA:O	1:A:138:THR:HB	0.57	2.00	8	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:LEU:HD12	1:A:144:VAL:HG21	0.57	1.77	14	3
1:A:116:GLU:OE2	1:A:141:LEU:HD22	0.57	2.00	18	1
1:A:118:HIS:O	1:A:144:VAL:HG23	0.56	1.99	17	3
1:A:145:ILE:HD12	1:A:146:SER:HB3	0.56	1.75	7	5
1:A:57:LEU:HD21	1:A:143:LEU:HD23	0.56	1.76	7	3
1:A:91:LEU:HD11	1:A:112:LEU:CD2	0.56	2.31	8	2
1:A:126:TYR:CD1	1:A:150:HIS:CG	0.56	2.93	7	8
1:A:118:HIS:CD2	1:A:143:LEU:HD21	0.56	2.35	5	20
1:A:133:VAL:HG12	1:A:147:LEU:HD12	0.56	1.77	19	16
1:A:79:LEU:HD12	1:A:79:LEU:O	0.55	2.01	5	2
1:A:45:LEU:HD23	1:A:85:SER:O	0.55	2.02	9	5
1:A:99:GLY:O	1:A:100:ILE:HG23	0.55	2.02	7	2
1:A:45:LEU:HD22	1:A:136:ILE:HG12	0.55	1.78	11	3
1:A:57:LEU:HD22	1:A:79:LEU:HD11	0.55	1.78	9	2
1:A:79:LEU:O	1:A:79:LEU:HD12	0.54	2.02	18	2
1:A:104:ASP:O	1:A:106:ASN:N	0.54	2.40	3	20
1:A:79:LEU:HD22	1:A:79:LEU:N	0.54	2.16	19	3
1:A:95:ILE:HG21	1:A:119:LEU:HD12	0.54	1.79	2	4
1:A:122:PHE:CE2	1:A:152:LEU:HD23	0.54	2.37	7	3
1:A:146:SER:HB2	1:A:151:THR:HG22	0.54	1.79	7	2
1:A:119:LEU:HD23	1:A:120:PRO:O	0.54	2.03	19	16
1:A:88:VAL:HG12	1:A:90:MET:HE3	0.54	1.80	6	3
1:A:104:ASP:O	1:A:108:TRP:CZ2	0.54	2.61	17	20
1:A:45:LEU:CD2	1:A:136:ILE:HD13	0.54	2.33	8	4
1:A:120:PRO:HG2	1:A:123:TRP:CD2	0.54	2.38	11	19
1:A:53:VAL:CG1	1:A:57:LEU:HD11	0.54	2.32	19	4
1:A:123:TRP:O	1:A:127:ILE:HG23	0.54	2.03	17	5
1:A:79:LEU:CD1	1:A:138:THR:HG21	0.54	2.29	5	3
1:A:110:TYR:CZ	1:A:119:LEU:HD22	0.54	2.37	17	2
1:A:57:LEU:CD2	1:A:79:LEU:HD11	0.53	2.33	9	2
1:A:57:LEU:HD22	1:A:79:LEU:HD23	0.53	1.80	17	1
1:A:91:LEU:HD11	1:A:112:LEU:HD23	0.53	1.80	18	2
1:A:42:THR:HG23	1:A:89:MET:HG3	0.53	1.79	18	1
1:A:126:TYR:CD2	1:A:150:HIS:CG	0.53	2.97	20	12
1:A:145:ILE:HD12	1:A:146:SER:OG	0.53	2.02	19	3
1:A:136:ILE:O	1:A:142:PRO:CA	0.53	2.57	9	8
1:A:107:LYS:O	1:A:108:TRP:CD1	0.52	2.62	4	20
1:A:79:LEU:HD11	1:A:118:HIS:HB2	0.52	1.80	11	2
1:A:100:ILE:O	1:A:100:ILE:HD12	0.52	2.05	2	2
1:A:135:LEU:C	1:A:135:LEU:HD12	0.52	2.25	6	5
1:A:57:LEU:HD12	1:A:81:LEU:CD1	0.52	2.34	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:79:LEU:HD12	1:A:138:THR:CG2	0.52	2.35	3	1
1:A:112:LEU:HB2	1:A:117:VAL:HG11	0.52	1.81	5	6
1:A:140:SER:CB	1:A:141:LEU:HD23	0.52	2.35	3	3
1:A:79:LEU:CG	1:A:138:THR:HG21	0.52	2.33	19	1
1:A:88:VAL:HG12	1:A:90:MET:CE	0.51	2.35	7	3
1:A:79:LEU:HD13	1:A:79:LEU:H	0.51	1.65	19	4
1:A:53:VAL:O	1:A:57:LEU:HG	0.51	2.05	11	8
1:A:57:LEU:HD13	1:A:79:LEU:HD12	0.51	1.82	10	1
1:A:135:LEU:HA	1:A:145:ILE:HD13	0.50	1.83	1	1
1:A:98:TYR:CD1	1:A:111:TYR:CD2	0.50	3.00	4	1
1:A:85:SER:C	1:A:136:ILE:HG21	0.50	2.27	2	4
1:A:104:ASP:O	1:A:106:ASN:OD1	0.50	2.30	19	2
1:A:118:HIS:CG	1:A:143:LEU:CD2	0.50	2.95	15	20
1:A:126:TYR:CD2	1:A:150:HIS:ND1	0.50	2.80	20	12
1:A:100:ILE:HD13	1:A:100:ILE:H	0.50	1.65	6	1
1:A:98:TYR:CD2	1:A:111:TYR:CD2	0.49	3.00	7	3
1:A:100:ILE:H	1:A:100:ILE:HD13	0.49	1.67	8	2
1:A:135:LEU:HD12	1:A:135:LEU:C	0.49	2.26	9	3
1:A:148:ASN:O	1:A:148:ASN:CG	0.49	2.51	8	4
1:A:119:LEU:HD23	1:A:119:LEU:C	0.49	2.28	13	7
1:A:126:TYR:CD1	1:A:150:HIS:ND1	0.49	2.81	13	8
1:A:43:ARG:HB3	1:A:90:MET:HE3	0.49	1.83	8	1
1:A:119:LEU:C	1:A:119:LEU:HD23	0.49	2.28	17	7
1:A:143:LEU:HD11	1:A:152:LEU:CD1	0.49	2.37	12	2
1:A:140:SER:OG	1:A:141:LEU:HD23	0.49	2.07	2	2
1:A:98:TYR:CD1	1:A:111:TYR:CD1	0.48	3.00	6	2
1:A:127:ILE:HG22	1:A:147:LEU:HD21	0.48	1.84	19	4
1:A:57:LEU:HD21	1:A:143:LEU:HD21	0.48	1.81	7	2
1:A:97:ARG:CG	1:A:110:TYR:CE2	0.48	2.96	20	3
1:A:79:LEU:HD12	1:A:141:LEU:CD1	0.48	2.38	19	1
1:A:79:LEU:HD11	1:A:118:HIS:ND1	0.48	2.23	4	2
1:A:100:ILE:N	1:A:100:ILE:CD1	0.48	2.76	6	3
1:A:122:PHE:HE2	1:A:152:LEU:HD23	0.48	1.68	7	2
1:A:120:PRO:HG2	1:A:123:TRP:CE3	0.48	2.43	5	16
1:A:122:PHE:CD1	1:A:122:PHE:N	0.48	2.82	3	4
1:A:85:SER:CA	1:A:136:ILE:HG21	0.48	2.39	6	4
1:A:122:PHE:N	1:A:122:PHE:CD1	0.48	2.82	17	9
1:A:100:ILE:HD13	1:A:109:ARG:NH2	0.48	2.24	7	1
1:A:45:LEU:HD22	1:A:136:ILE:HD11	0.48	1.86	6	1
1:A:79:LEU:HB3	1:A:140:SER:OG	0.47	2.09	3	1
1:A:95:ILE:CD1	1:A:133:VAL:HG11	0.47	2.35	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ILE:HD11	1:A:145:ILE:HG23	0.47	1.86	7	6
1:A:97:ARG:HG3	1:A:110:TYR:CE2	0.47	2.45	17	4
1:A:82:ASN:H	1:A:85:SER:HG	0.47	1.53	19	1
1:A:57:LEU:CD1	1:A:79:LEU:HD23	0.47	2.28	11	1
1:A:136:ILE:CD1	1:A:145:ILE:HG21	0.47	2.40	6	1
1:A:122:PHE:CD2	1:A:122:PHE:N	0.47	2.83	8	6
1:A:137:HIS:CD2	1:A:137:HIS:N	0.47	2.83	9	5
1:A:148:ASN:CG	1:A:148:ASN:O	0.47	2.53	11	5
1:A:79:LEU:H	1:A:79:LEU:HD13	0.47	1.70	4	1
1:A:57:LEU:HD22	1:A:79:LEU:CD1	0.47	2.40	9	2
1:A:97:ARG:CG	1:A:110:TYR:CE1	0.47	2.98	7	1
1:A:79:LEU:CB	1:A:138:THR:HG21	0.47	2.39	11	4
1:A:137:HIS:N	1:A:137:HIS:CD2	0.47	2.83	6	4
1:A:143:LEU:HD13	1:A:144:VAL:N	0.47	2.25	7	9
1:A:79:LEU:HD21	1:A:118:HIS:ND1	0.47	2.25	3	1
1:A:128:ASN:ND2	1:A:131:ASN:OD1	0.47	2.48	3	2
1:A:93:HIS:CG	1:A:112:LEU:CD1	0.47	2.98	3	14
1:A:148:ASN:O	1:A:150:HIS:CD2	0.46	2.69	2	18
1:A:110:TYR:CG	1:A:119:LEU:CB	0.46	2.99	14	3
1:A:95:ILE:HD13	1:A:112:LEU:HD22	0.46	1.86	19	4
1:A:56:TYR:OH	1:A:120:PRO:HA	0.46	2.10	7	4
1:A:95:ILE:HD13	1:A:112:LEU:CD2	0.46	2.41	14	5
1:A:127:ILE:CG2	1:A:147:LEU:HD21	0.46	2.40	6	3
1:A:79:LEU:HD12	1:A:141:LEU:HG	0.46	1.86	11	2
1:A:40:ALA:HB3	1:A:89:MET:SD	0.46	2.51	5	1
1:A:110:TYR:CD2	1:A:119:LEU:HB3	0.46	2.45	10	3
1:A:149:GLY:C	1:A:150:HIS:CG	0.46	2.89	7	17
1:A:100:ILE:HD11	1:A:109:ARG:NH2	0.46	2.25	2	1
1:A:100:ILE:HG21	1:A:109:ARG:NH1	0.46	2.26	1	2
1:A:110:TYR:OH	1:A:124:GLU:HB3	0.46	2.10	5	2
1:A:119:LEU:HD11	1:A:147:LEU:CD1	0.45	2.41	12	2
1:A:95:ILE:CD1	1:A:119:LEU:HD12	0.45	2.42	18	1
1:A:84:GLU:O	1:A:136:ILE:CG2	0.45	2.64	2	3
1:A:53:VAL:HG21	1:A:145:ILE:CG2	0.45	2.42	18	1
1:A:54:GLU:HG3	1:A:55:ASN:N	0.45	2.27	11	1
1:A:126:TYR:CD1	1:A:126:TYR:N	0.45	2.83	1	5
1:A:117:VAL:HG12	1:A:142:PRO:CD	0.45	2.39	4	4
1:A:110:TYR:CD1	1:A:119:LEU:HB3	0.45	2.47	20	7
1:A:109:ARG:HH11	1:A:109:ARG:HB2	0.45	1.71	4	1
1:A:119:LEU:CD1	1:A:127:ILE:HG21	0.45	2.40	16	8
1:A:87:ASN:O	1:A:136:ILE:CG2	0.45	2.65	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:TYR:N	1:A:126:TYR:CD2	0.45	2.84	12	5
1:A:100:ILE:CD1	1:A:100:ILE:N	0.45	2.79	9	1
1:A:79:LEU:CD1	1:A:79:LEU:N	0.45	2.70	17	2
1:A:99:GLY:CA	1:A:108:TRP:CG	0.45	3.00	15	2
1:A:126:TYR:N	1:A:126:TYR:CD1	0.45	2.84	11	7
1:A:126:TYR:CD2	1:A:126:TYR:N	0.45	2.84	16	3
1:A:136:ILE:HG12	1:A:145:ILE:HD12	0.45	1.88	1	1
1:A:141:LEU:N	1:A:141:LEU:HD23	0.44	2.27	3	1
1:A:110:TYR:CE2	1:A:119:LEU:O	0.44	2.70	10	3
1:A:125:GLN:CG	1:A:126:TYR:CD1	0.44	3.00	8	2
1:A:53:VAL:HG21	1:A:145:ILE:HG22	0.44	1.88	16	3
1:A:127:ILE:HG13	1:A:127:ILE:O	0.44	2.12	15	1
1:A:122:PHE:N	1:A:122:PHE:CD2	0.44	2.84	1	1
1:A:125:GLN:HG3	1:A:126:TYR:CE1	0.44	2.48	8	3
1:A:133:VAL:CG1	1:A:147:LEU:CD1	0.44	2.95	4	11
1:A:45:LEU:HD22	1:A:136:ILE:HD13	0.44	1.88	8	1
1:A:136:ILE:HG22	1:A:137:HIS:N	0.44	2.27	19	1
1:A:92:THR:O	1:A:92:THR:HG23	0.44	2.12	14	8
1:A:143:LEU:C	1:A:143:LEU:HD13	0.44	2.33	1	9
1:A:79:LEU:N	1:A:79:LEU:CD1	0.44	2.71	16	1
1:A:45:LEU:HD11	1:A:49:GLU:CB	0.44	2.43	1	2
1:A:85:SER:O	1:A:136:ILE:CG2	0.44	2.64	11	1
1:A:95:ILE:CD1	1:A:112:LEU:CD2	0.43	2.96	14	15
1:A:100:ILE:HG13	1:A:109:ARG:NH1	0.43	2.27	4	1
1:A:110:TYR:O	1:A:111:TYR:CD2	0.43	2.71	7	2
1:A:110:TYR:CE1	1:A:119:LEU:O	0.43	2.72	14	2
1:A:92:THR:HG23	1:A:92:THR:O	0.43	2.13	20	6
1:A:56:TYR:CD1	1:A:57:LEU:CD2	0.43	3.00	10	1
1:A:93:HIS:CB	1:A:112:LEU:HD11	0.43	2.43	3	4
1:A:79:LEU:HB2	1:A:138:THR:OG1	0.43	2.14	9	5
1:A:110:TYR:CE2	1:A:119:LEU:HD22	0.43	2.49	17	1
1:A:132:THR:HG22	1:A:134:GLU:OE1	0.43	2.14	4	1
1:A:125:GLN:CG	1:A:126:TYR:CE1	0.43	3.02	8	2
1:A:79:LEU:HD13	1:A:138:THR:CG2	0.43	2.37	9	1
1:A:104:ASP:O	1:A:106:ASN:CG	0.43	2.57	15	1
1:A:88:VAL:CG1	1:A:90:MET:CE	0.43	2.96	7	2
1:A:127:ILE:O	1:A:127:ILE:HG13	0.43	2.14	17	2
1:A:88:VAL:HA	1:A:136:ILE:HG23	0.43	1.90	7	3
1:A:141:LEU:HD23	1:A:141:LEU:N	0.43	2.28	17	1
1:A:148:ASN:OD1	1:A:148:ASN:N	0.42	2.52	2	4
1:A:131:ASN:HB3	1:A:148:ASN:OD1	0.42	2.14	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLN:HG3	1:A:126:TYR:CE2	0.42	2.48	7	3
1:A:134:GLU:HB2	1:A:146:SER:OG	0.42	2.14	5	1
1:A:135:LEU:HB3	1:A:144:VAL:HA	0.42	1.92	9	8
1:A:143:LEU:HD13	1:A:143:LEU:C	0.42	2.35	16	2
1:A:94:ALA:CB	1:A:129:ASP:O	0.42	2.68	18	3
1:A:99:GLY:HA2	1:A:108:TRP:HB3	0.42	1.91	15	1
1:A:43:ARG:HG2	1:A:44:LYS:N	0.42	2.29	6	2
1:A:100:ILE:CG1	1:A:109:ARG:NH1	0.42	2.83	19	1
1:A:120:PRO:CB	1:A:122:PHE:CZ	0.41	3.03	11	1
1:A:97:ARG:HD2	1:A:110:TYR:CE2	0.41	2.50	6	1
1:A:45:LEU:CD2	1:A:136:ILE:CD1	0.41	2.98	13	4
1:A:122:PHE:CE1	1:A:152:LEU:HD23	0.41	2.50	16	1
1:A:111:TYR:CE1	1:A:116:GLU:CG	0.41	3.03	20	1
1:A:95:ILE:HD12	1:A:119:LEU:CD1	0.41	2.45	18	1
1:A:88:VAL:CG1	1:A:90:MET:HE2	0.41	2.44	10	1
1:A:56:TYR:CD2	1:A:57:LEU:CD2	0.41	3.03	13	1
1:A:56:TYR:CE1	1:A:152:LEU:HD21	0.41	2.51	15	1
1:A:51:SER:O	1:A:54:GLU:HG2	0.41	2.15	15	1
1:A:148:ASN:N	1:A:148:ASN:OD1	0.41	2.54	5	3
1:A:100:ILE:CD1	1:A:109:ARG:NH2	0.41	2.83	7	1
1:A:100:ILE:CG2	1:A:109:ARG:NH1	0.41	2.84	1	2
1:A:128:ASN:OD1	1:A:130:GLU:O	0.41	2.39	3	1
1:A:97:ARG:HG3	1:A:110:TYR:CE1	0.41	2.50	7	1
1:A:105:PRO:CA	1:A:108:TRP:CH2	0.41	3.04	20	2
1:A:79:LEU:HD22	1:A:138:THR:HG21	0.41	1.93	18	1
1:A:102:THR:HG22	1:A:103:ASP:N	0.41	2.31	20	1
1:A:96:THR:O	1:A:110:TYR:HA	0.41	2.16	5	1
1:A:122:PHE:O	1:A:126:TYR:CE2	0.41	2.74	19	1
1:A:57:LEU:HD21	1:A:143:LEU:CG	0.41	2.38	17	1
1:A:79:LEU:HD22	1:A:138:THR:CG2	0.41	2.46	18	1
1:A:50:ARG:NH2	1:A:86:ASN:ND2	0.40	2.69	7	1
1:A:86:ASN:OD1	1:A:86:ASN:N	0.40	2.54	1	1
1:A:127:ILE:HA	1:A:131:ASN:OD1	0.40	2.17	13	1
1:A:119:LEU:CD2	1:A:123:TRP:HB2	0.40	2.45	14	1
1:A:125:GLN:CG	1:A:126:TYR:CD2	0.40	3.05	13	1
1:A:136:ILE:CD1	1:A:145:ILE:CG2	0.40	2.99	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	98/120 (82%)	88±1 (90±1%)	7±1 (8±1%)	2±0 (2±0%)	9	48
All	All	1960/2400 (82%)	1768 (90%)	147 (8%)	45 (2%)	9	48

All 3 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	148	ASN	20
1	A	105	PRO	20
1	A	100	ILE	5

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	90/106 (85%)	63±3 (70±3%)	27±3 (30±3%)	1	17
All	All	1800/2120 (85%)	1267 (70%)	533 (30%)	1	17

All 52 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	133	VAL	20
1	A	79	LEU	20
1	A	96	THR	20
1	A	89	MET	20
1	A	147	LEU	20
1	A	91	LEU	20
1	A	122	PHE	20

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Mol	Chain	Res	Type	Models (Total)
1	A	42	THR	20
1	A	141	LEU	18
1	A	112	LEU	18
1	A	90	MET	17
1	A	109	ARG	17
1	A	136	ILE	17
1	A	131	ASN	16
1	A	146	SER	16
1	A	124	GLU	15
1	A	125	GLN	15
1	A	107	LYS	14
1	A	101	SER	13
1	A	41	GLN	12
1	A	44	LYS	11
1	A	84	GLU	11
1	A	104	ASP	10
1	A	97	ARG	10
1	A	114	SER	9
1	A	130	GLU	9
1	A	54	GLU	9
1	A	103	ASP	8
1	A	140	SER	8
1	A	39	ASP	8
1	A	116	GLU	7
1	A	48	GLU	7
1	A	55	ASN	7
1	A	59	SER	6
1	A	86	ASN	6
1	A	58	GLU	6
1	A	100	ILE	6
1	A	51	SER	6
1	A	128	ASN	5
1	A	145	ILE	4
1	A	81	LEU	4
1	A	50	ARG	4
1	A	129	ASP	4
1	A	43	ARG	3
1	A	106	ASN	3
1	A	78	SER	3
1	A	138	THR	3
1	A	119	LEU	3
1	A	132	THR	2

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Mol	Chain	Res	Type	Models (Total)
1	A	87	ASN	1
1	A	95	ILE	1
1	A	85	SER	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *yrf.dep_3.data.csh*

7.1.1 Bookkeeping [i](#)

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	1502
Number of shifts mapped to atoms	1494
Number of unparsed shifts	8
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 8 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
272	A	57	LEU	HD11	0.783	0.01	2
273	A	57	LEU	HD12	0.783	0.01	2
274	A	57	LEU	HD13	0.783	0.01	2
558	A	81	LEU	HD11	0.731	0.01	2
559	A	81	LEU	HD12	0.731	0.01	2
560	A	81	LEU	HD13	0.731	0.01	2
1185	A	129	ASP	HB2	2.641	0.01	1
1195	A	130	GLU	HB2	1.763	0.01	2

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	118	-0.20 \pm 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\beta$	114	0.11 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	118	-0.13 ± 0.07	None needed (< 0.5 ppm)
^{15}N	111	0.09 ± 0.16	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 91%, i.e. 1106 atoms were assigned a chemical shift out of a possible 1212. 15 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	478/480 (100%)	191/191 (100%)	194/196 (99%)	93/93 (100%)
Sidechain	535/618 (87%)	341/359 (95%)	194/235 (83%)	0/24 (0%)
Aromatic	93/114 (82%)	51/58 (88%)	42/46 (91%)	0/10 (0%)
Overall	1106/1212 (91%)	583/608 (96%)	430/477 (90%)	93/127 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1313 atoms were assigned a chemical shift out of a possible 1433. 19 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	576/579 (99%)	229/230 (100%)	236/238 (99%)	111/111 (100%)
Sidechain	644/740 (87%)	410/430 (95%)	234/283 (83%)	0/27 (0%)
Aromatic	93/114 (82%)	51/58 (88%)	42/46 (91%)	0/10 (0%)
Overall	1313/1433 (92%)	690/718 (96%)	512/567 (90%)	111/148 (75%)

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	120	PRO	HB3	-0.37	3.81 – 0.21	-6.6
1	A	125	GLN	HG3	0.82	3.75 – 0.85	-5.1

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:

