WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 27, 2016 – 05:12 AM BST

PDB ID	:	2RPB
Title	:	The solution structure of membrane protein
Authors	:	Kuwahara, Y.; Unzai, S.; Nagata, T.; Hiroaki, H.
Deposited on	:	2008-05-13

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 83%.

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	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		3.4%
Sidechain outliers		9.0%

Worse — *Better*

▌ Percentile relative to all structures

▯ Percentile relative to all NMR structures
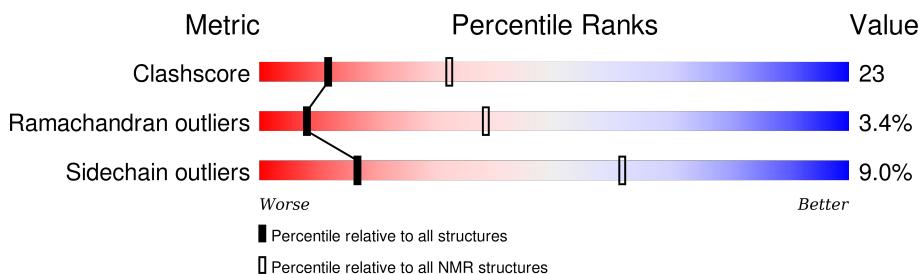
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	113	51% 39% · 8%
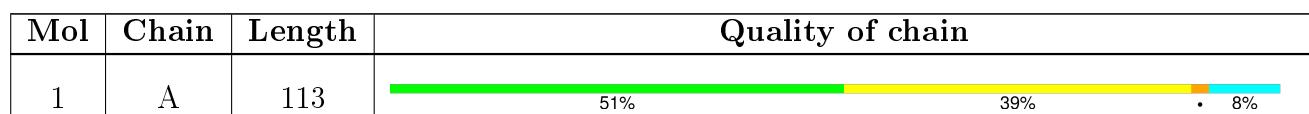
2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average.*

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:69-A:172 (104)	0.25	3

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1825 atoms, of which 923 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical membrane protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	113	1825	569	923	156	174	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	GLY	-	EXPRESSION TAG	UNP O58205
A	63	SER	-	EXPRESSION TAG	UNP O58205
A	64	ASP	-	EXPRESSION TAG	UNP O58205
A	65	HIS	-	EXPRESSION TAG	UNP O58205

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: hypothetical membrane protein
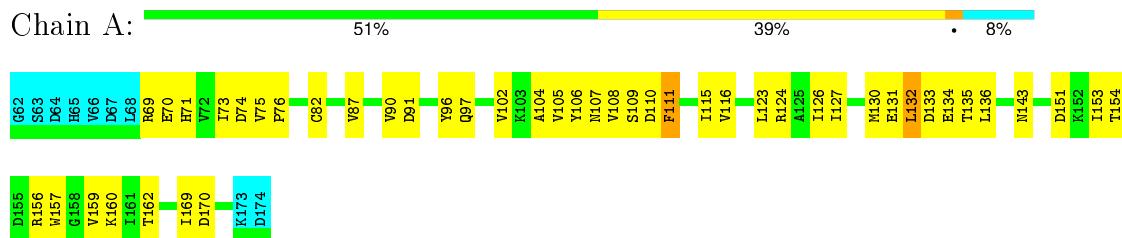
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: hypothetical membrane protein
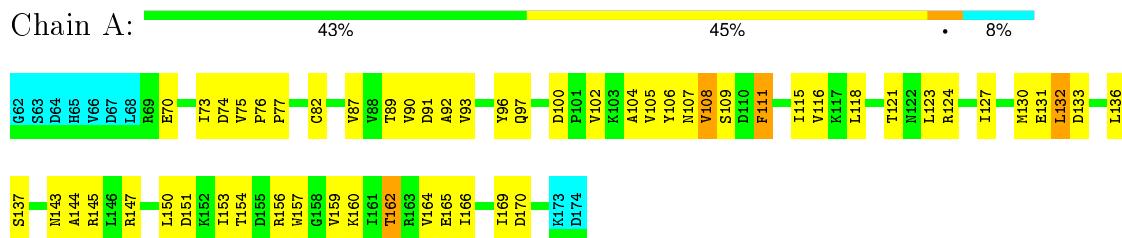

4.2.2 Score per residue for model 2

• Molecule 1: hypothetical membrane protein

G62 S63 D64 H65 V66 D67 L68 H71 V72 I73 D74 V75 P76 C82 V87 A92 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 L118 N122 L123 I126 I127 M130 E131 L132 D133 E134 S137 G138 I142 R145 E148 E149 L150

I153 T154 D155 R156 V159 K160 I161 T162 K173 D174
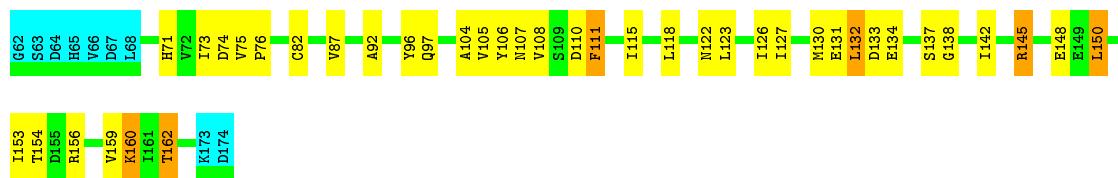
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: hypothetical membrane protein

Chain A: 51% 36% · 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 C82 K83 D84 N85 V86 V87 D91 Y96 Q97 V98 V102 K103 A104 V105 Y106 N107 V108 F111 L112 M113 A114 I115 V116 K117 L118 I126 M130 E131 L132 D133 E134 T135 I141 I142 N143 A144 R147 D151

K152 I153 T154 D155 R156 W157 G158 V159 K160 I161 T162 R168 I169 D170 K173 D174
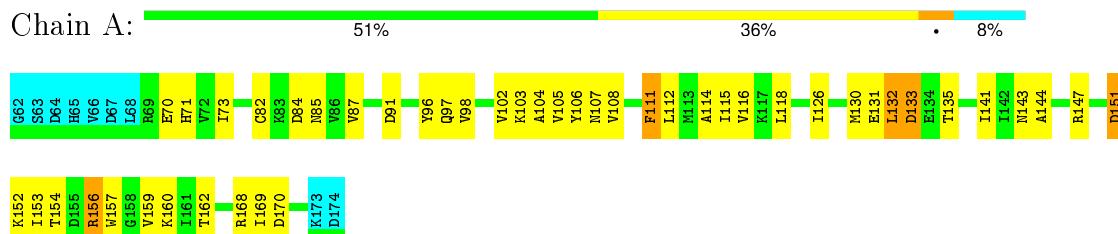
4.2.4 Score per residue for model 4

- Molecule 1: hypothetical membrane protein

Chain A: 51% 33% 8% 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 C82 V87 V90 D91 Y95 Y96 A104 V105 Y106 N107 V108 S109 D110 F111 L112 M113 A114 I115 V116 K117 L123 R124 I127 M130 E131 L132 D133 E134 T135 L136 S137 N143 R147 D151

R156 W157 K160 V164 I169 D170 K173 D174
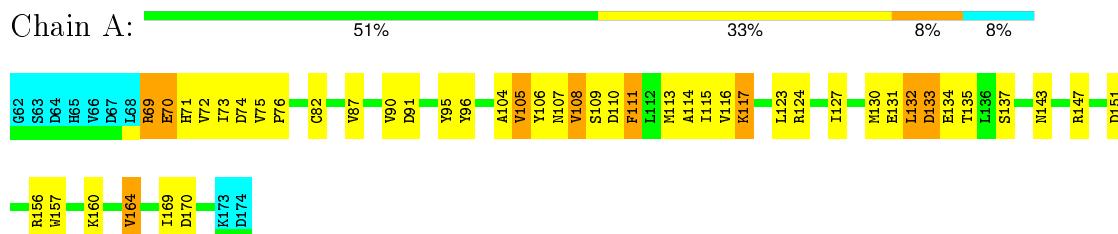
4.2.5 Score per residue for model 5

- Molecule 1: hypothetical membrane protein

Chain A: 53% 34% 5% 8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 P76 C82 V87 V90 Y96 Q97 P101 V102 V105 Y106 N107 V108 S109 D110 F111 I115 V116 K117 L118 A119 L123 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 S137 I141 I142 N143

L150 R156 W157 T162 R163 V164 R168 I169 D170 K173 D174
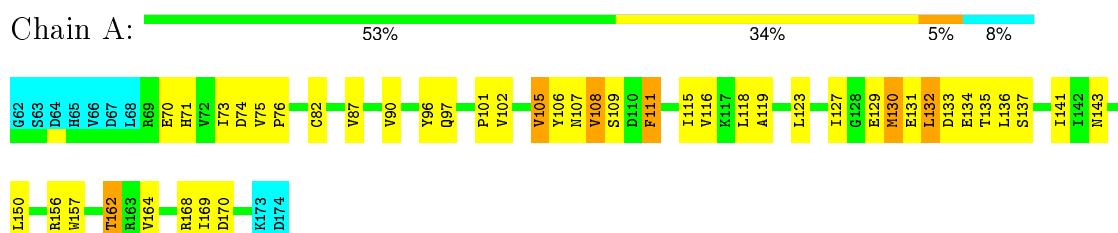
4.2.6 Score per residue for model 6

- Molecule 1: hypothetical membrane protein

Chain A: 47% 42% 8%
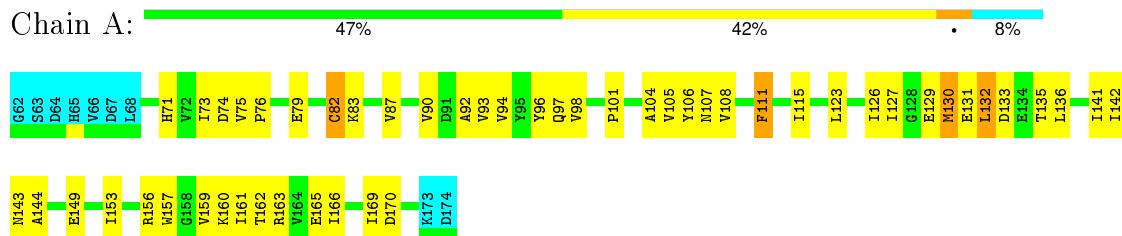
4.2.7 Score per residue for model 7

• Molecule 1: hypothetical membrane protein

Chain A: 42% 45% 8%
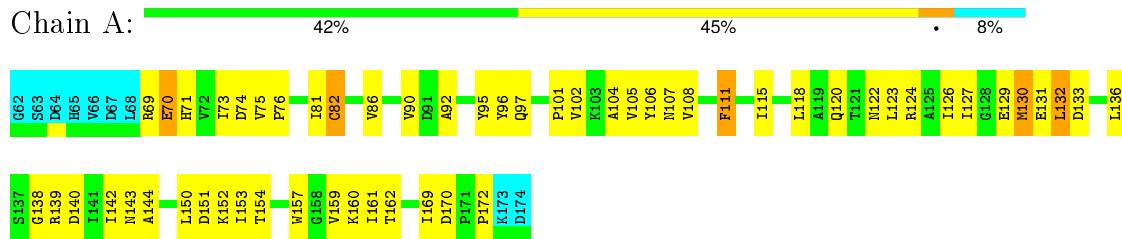
4.2.8 Score per residue for model 8

• Molecule 1: hypothetical membrane protein

Chain A: 52% 36% 8%
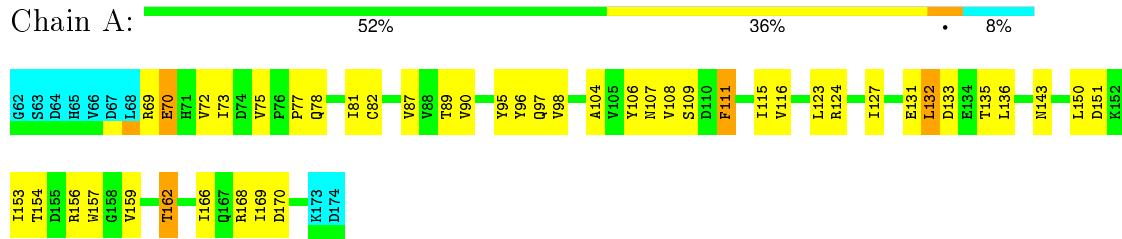
4.2.9 Score per residue for model 9

• Molecule 1: hypothetical membrane protein

Chain A: 47% 38% 7% 8%
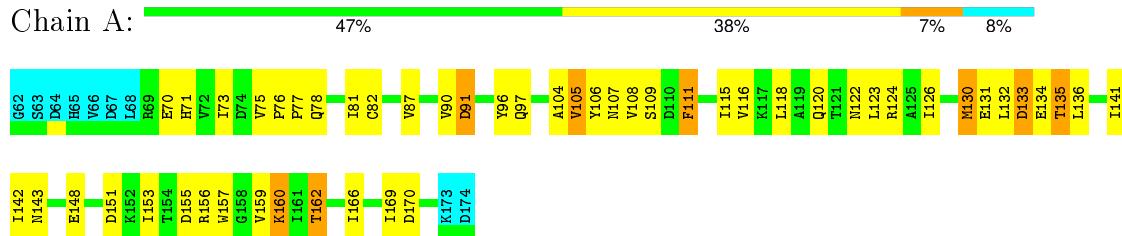
4.2.10 Score per residue for model 10

• Molecule 1: hypothetical membrane protein

Chain A:

47%   40%   8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 I81 C82 V87 V90 D91 A92 Y95 Y96 Q97 V98 I99 D100 A104 V105 Y106 N107 V108 S109 D110 F111 A114 I115 V116 K117 L123 R124 A125 I126 I127 M130 E131 L132 D133 E134 T135 L136 N143

A144 R145 L146 R147 E148 D151 K152 I153 R156 W157 K160 I161 T162 I169 D170 K173 D174
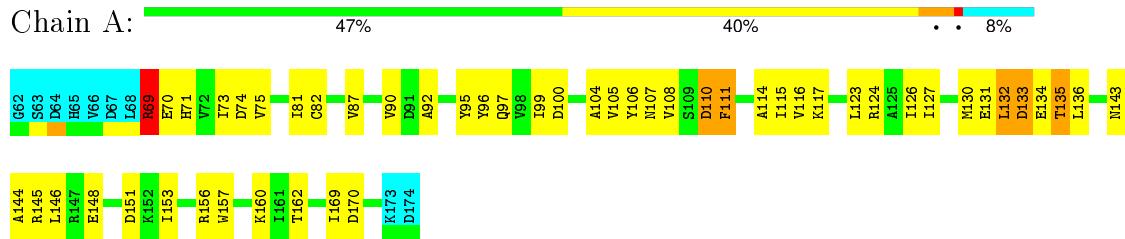
4.2.11 Score per residue for model 11

• Molecule 1: hypothetical membrane protein

Chain A:

46%   41%   5%   8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 H71 V72 I73 D74 V75 Q78 E79 V80 I81 C82 K83 D84 N85 V86 T89 V90 D91 A92 V93 V94 Y95 Y96 Q97 D100 P101 V102 K103 A104 V105 Y106 N107 V108 F111 I115 N122 L123 R124 A125 I126 M130 E131 L132 D133

I141 I142 N143 E148 K152 I153 T154 D155 R156 W157 G158 V159 K160 I161 T162 R163 V164 E165 I169 D170 K173 D174
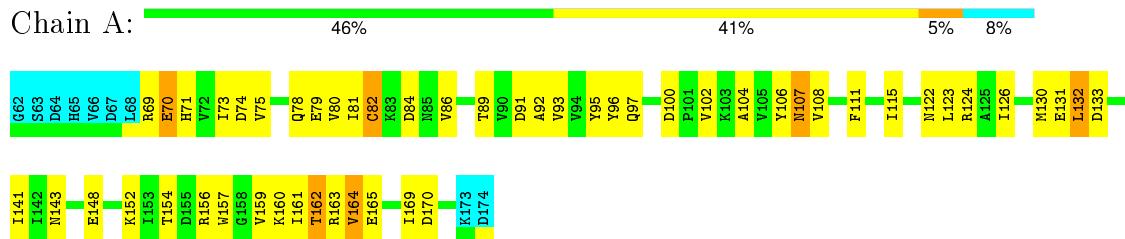
4.2.12 Score per residue for model 12

• Molecule 1: hypothetical membrane protein

Chain A:

50%   37%   5%   8%

G62 S63 D64 H65 V66 D67 L68 R69 E70 I73 D74 V75 P76 P77 Q78 I81 C82 K83 D84 V87 V88 T89 V90 D91 A92 Y96 Q97 A104 V105 Y106 N107 V108 S109 D110 F111 I115 Q120 L123 I126 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 S137 G138

R139 D140 I141 I142 N143 A144 D151 T154 W157 G158 V159 T162 I169 D170 K173 D174
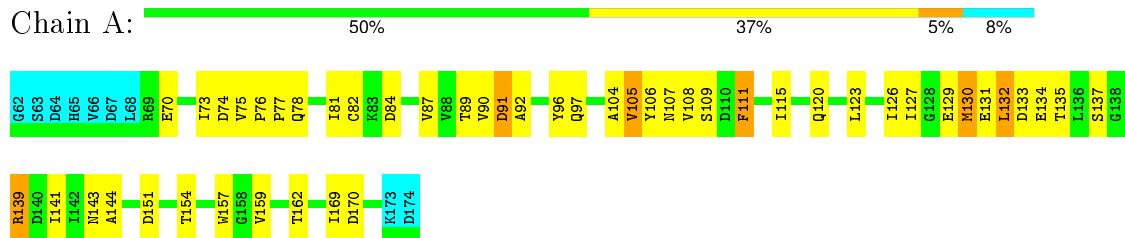
4.2.13 Score per residue for model 13

• Molecule 1: hypothetical membrane protein

Chain A:

46%   41%   5%   8%

G62 S63 D64 H65 V66 D67 L68 V72 I73 D74 V75 P76 P77 Q78 C82 V87 V90 D91 Y95 Y96 Q97 V98 I99 D100 A104 V105 Y106 N107 V108 S109 D110 F111 I115 V116 Q120 L123 I127 G128 E129 M130 E131 L132 D133 E134 T135 L136 S137 G138 R139 D140

I141 I142 N143 A144 R145 L146 R147 E148 E149 L150 D151 K152 K160 I161 T162 I169 D170 K173 D174
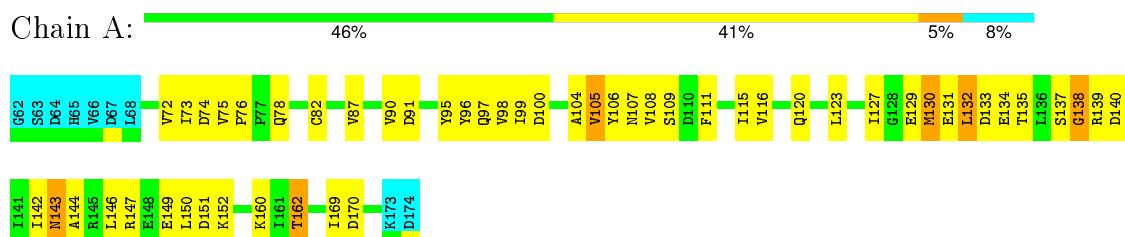
4.2.14 Score per residue for model 14

• Molecule 1: hypothetical membrane protein
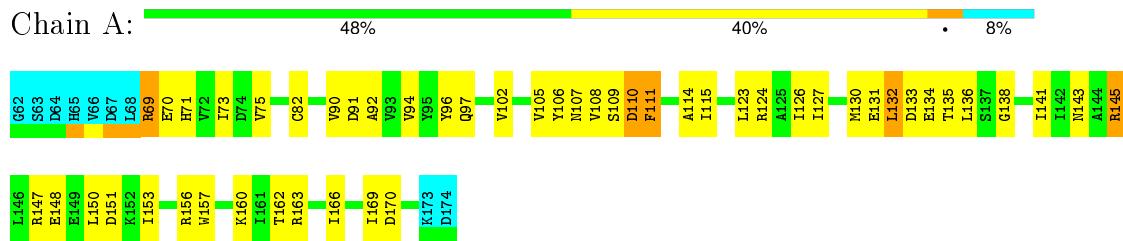
4.2.15 Score per residue for model 15

• Molecule 1: hypothetical membrane protein
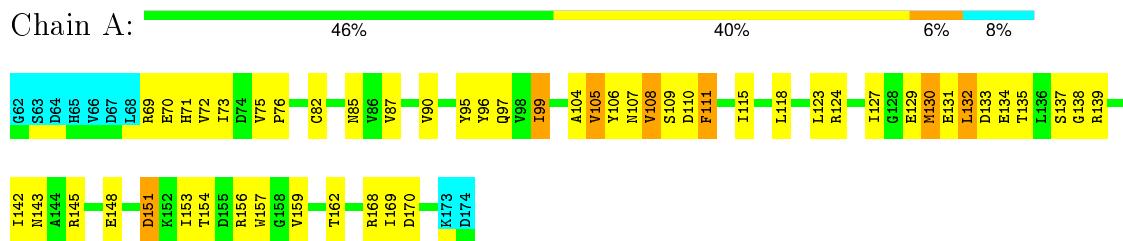
4.2.16 Score per residue for model 16

• Molecule 1: hypothetical membrane protein
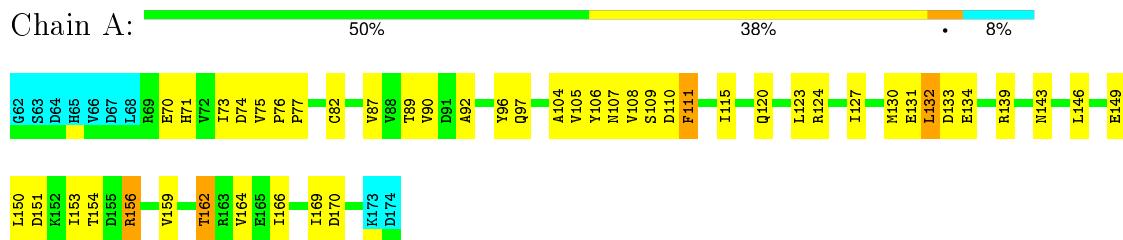
4.2.17 Score per residue for model 17

• Molecule 1: hypothetical membrane protein
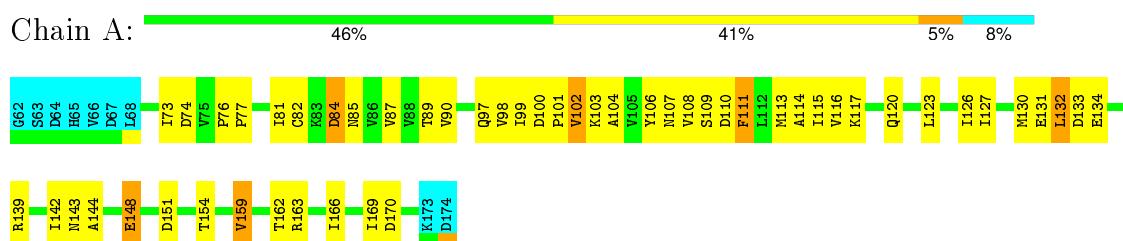
4.2.18 Score per residue for model 18

• Molecule 1: hypothetical membrane protein
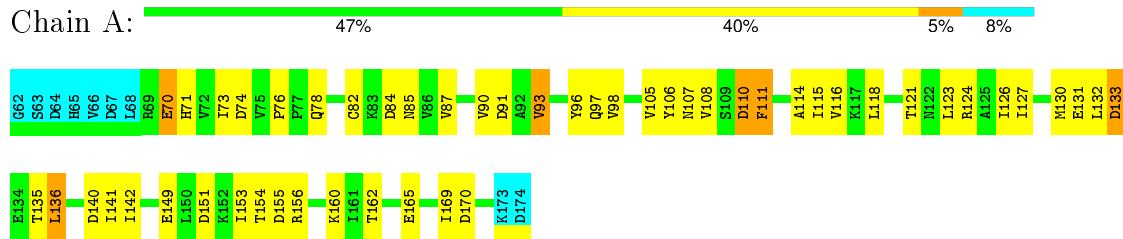
4.2.19 Score per residue for model 19

• Molecule 1: hypothetical membrane protein
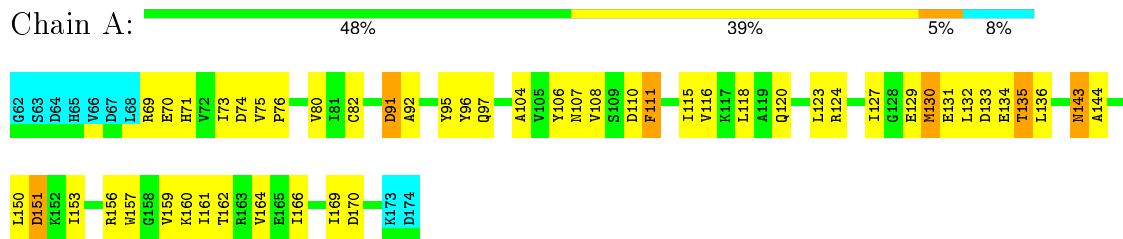
4.2.20 Score per residue for model 20

• Molecule 1: hypothetical membrane protein
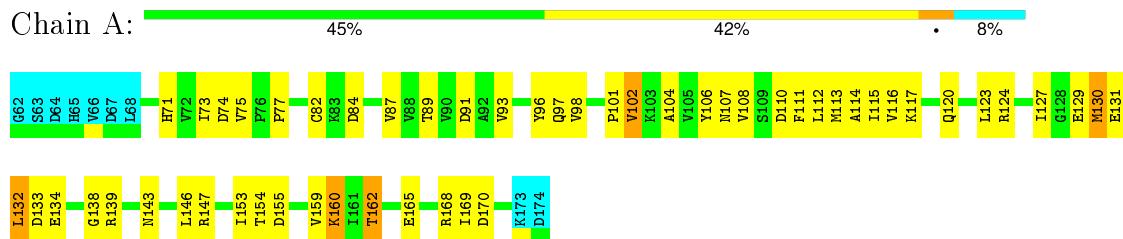
5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *distance geometry, torsion angle dynamics, rigid body restrained molecular dynamics.*

Of the 200 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	structure solution	2.0.17
CYANA	refinement	2.0.17
Molmol	refinement	2K.2
SPARKY	refinement	3.106

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 11060
Number of chemical shift lists	1
Total number of shifts	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality (i)

6.1 Standard geometry (i)

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	834	862	861	39±5
All	All	16680	17240	17220	781

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:73:ILE:HD13	1:A:115:ILE:HG21	1.00	1.31	7	17
1:A:81:ILE:CD1	1:A:87:VAL:HG22	0.87	1.98	9	4
1:A:72:VAL:HG12	1:A:95:TYR:CE1	0.86	2.05	8	3
1:A:154:THR:HB	1:A:159:VAL:HG13	0.81	1.52	3	9
1:A:123:LEU:HB2	1:A:127:ILE:HD13	0.79	1.53	17	5
1:A:90:VAL:HG21	1:A:127:ILE:HG21	0.77	1.55	8	4
1:A:90:VAL:HG11	1:A:127:ILE:HG21	0.77	1.55	18	8
1:A:115:ILE:HD13	1:A:150:LEU:HD12	0.75	1.57	19	5
1:A:111:PHE:CE2	1:A:115:ILE:HD11	0.73	2.19	17	2
1:A:123:LEU:HD12	1:A:124:ARG:N	0.72	2.00	4	12
1:A:76:PRO:HD2	1:A:116:VAL:HG13	0.69	1.65	9	3
1:A:108:VAL:O	1:A:108:VAL:HG13	0.69	1.86	5	1
1:A:113:MET:O	1:A:116:VAL:HG22	0.68	1.88	20	2
1:A:153:ILE:O	1:A:153:ILE:HG22	0.68	1.89	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:GLN:HG2	1:A:162:THR:HG23	0.66	1.68	6	16
1:A:105:VAL:HG13	1:A:105:VAL:O	0.66	1.89	13	2
1:A:123:LEU:C	1:A:123:LEU:HD12	0.65	2.11	10	6
1:A:73:ILE:CD1	1:A:115:ILE:HG21	0.65	2.19	3	4
1:A:102:VAL:O	1:A:105:VAL:HG13	0.65	1.92	14	2
1:A:71:HIS:CB	1:A:96:TYR:CZ	0.65	2.80	20	3
1:A:108:VAL:HG12	1:A:108:VAL:O	0.64	1.93	3	6
1:A:149:GLU:O	1:A:153:ILE:HD12	0.63	1.94	18	2
1:A:73:ILE:HD11	1:A:111:PHE:CE1	0.63	2.27	8	5
1:A:143:ASN:OD1	1:A:164:VAL:HG12	0.62	1.94	5	2
1:A:73:ILE:HD11	1:A:111:PHE:CZ	0.62	2.29	15	16
1:A:111:PHE:CD1	1:A:111:PHE:C	0.62	2.73	19	3
1:A:150:LEU:O	1:A:154:THR:HG23	0.62	1.94	7	3
1:A:71:HIS:CB	1:A:96:TYR:CE2	0.62	2.83	2	5
1:A:97:GLN:NE2	1:A:162:THR:HG21	0.61	2.10	12	6
1:A:141:ILE:HG22	1:A:145:ARG:NE	0.61	2.10	14	1
1:A:114:ALA:O	1:A:118:LEU:HD12	0.61	1.94	3	1
1:A:108:VAL:O	1:A:108:VAL:HG22	0.61	1.96	4	2
1:A:123:LEU:HD12	1:A:123:LEU:C	0.61	2.16	1	8
1:A:111:PHE:C	1:A:111:PHE:CD1	0.60	2.74	7	5
1:A:143:ASN:HB3	1:A:166:ILE:HD11	0.59	1.74	9	2
1:A:93:VAL:HG23	1:A:165:GLU:HB2	0.59	1.74	6	5
1:A:123:LEU:HB3	1:A:146:LEU:HD21	0.59	1.73	20	1
1:A:123:LEU:CB	1:A:146:LEU:HD21	0.59	2.27	20	1
1:A:140:ASP:O	1:A:144:ALA:HB2	0.59	1.98	13	1
1:A:73:ILE:HD13	1:A:115:ILE:CG2	0.58	2.24	3	2
1:A:143:ASN:CB	1:A:164:VAL:HG21	0.58	2.29	11	1
1:A:99:ILE:HD12	1:A:100:ASP:HB2	0.57	1.74	17	3
1:A:105:VAL:O	1:A:105:VAL:HG13	0.57	2.00	9	2
1:A:126:ILE:HD12	1:A:126:ILE:H	0.57	1.59	3	4
1:A:133:ASP:HA	1:A:136:LEU:HD21	0.56	1.76	18	1
1:A:78:GLN:HE21	1:A:123:LEU:HD11	0.56	1.60	18	1
1:A:153:ILE:HG22	1:A:153:ILE:O	0.56	2.00	10	6
1:A:87:VAL:HG13	1:A:87:VAL:O	0.56	2.01	2	4
1:A:157:TRP:O	1:A:159:VAL:HG23	0.56	2.00	19	1
1:A:78:GLN:NE2	1:A:123:LEU:HD11	0.56	2.16	18	2
1:A:123:LEU:HD13	1:A:127:ILE:HD12	0.56	1.78	7	1
1:A:111:PHE:CE2	1:A:115:ILE:CD1	0.56	2.89	17	1
1:A:127:ILE:HD11	1:A:142:ILE:HG23	0.55	1.78	15	4
1:A:105:VAL:HG22	1:A:105:VAL:O	0.55	2.01	10	4
1:A:71:HIS:HB2	1:A:96:TYR:CE2	0.55	2.37	14	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:PRO:O	1:A:105:VAL:HG12	0.55	2.02	7	2
1:A:143:ASN:CB	1:A:164:VAL:CG2	0.55	2.85	11	1
1:A:105:VAL:O	1:A:105:VAL:HG22	0.55	2.01	3	2
1:A:108:VAL:HG22	1:A:108:VAL:O	0.55	2.02	9	1
1:A:100:ASP:OD1	1:A:102:VAL:HG22	0.55	2.02	17	3
1:A:69:ARG:O	1:A:71:HIS:CE1	0.54	2.61	4	1
1:A:145:ARG:N	1:A:145:ARG:CD	0.54	2.70	2	1
1:A:87:VAL:O	1:A:87:VAL:HG13	0.54	2.03	6	7
1:A:107:ASN:O	1:A:108:VAL:C	0.53	2.47	1	20
1:A:71:HIS:HB3	1:A:96:TYR:CE2	0.53	2.39	2	2
1:A:102:VAL:O	1:A:105:VAL:HG23	0.53	2.04	5	1
1:A:80:VAL:HG12	1:A:124:ARG:NH1	0.52	2.19	19	1
1:A:86:VAL:HG13	1:A:172:PRO:HG3	0.52	1.81	7	1
1:A:127:ILE:HD11	1:A:142:ILE:CG2	0.52	2.34	2	2
1:A:153:ILE:H	1:A:153:ILE:HD12	0.52	1.65	19	2
1:A:143:ASN:OD1	1:A:144:ALA:N	0.52	2.43	3	6
1:A:123:LEU:CA	1:A:146:LEU:HD21	0.52	2.35	20	1
1:A:107:ASN:O	1:A:109:SER:N	0.52	2.43	5	11
1:A:73:ILE:CG2	1:A:116:VAL:HG12	0.52	2.34	3	1
1:A:71:HIS:HB2	1:A:96:TYR:CZ	0.51	2.41	20	7
1:A:105:VAL:HG12	1:A:105:VAL:O	0.51	2.05	1	2
1:A:111:PHE:CE1	1:A:115:ILE:HG13	0.51	2.41	13	2
1:A:75:VAL:HG22	1:A:116:VAL:HA	0.51	1.81	20	4
1:A:108:VAL:O	1:A:108:VAL:CG1	0.51	2.58	5	2
1:A:73:ILE:HD11	1:A:111:PHE:HZ	0.51	1.65	19	3
1:A:169:ILE:CG2	1:A:170:ASP:N	0.51	2.74	12	19
1:A:116:VAL:O	1:A:120:GLN:NE2	0.51	2.44	20	2
1:A:131:GLU:O	1:A:133:ASP:N	0.51	2.44	18	20
1:A:134:GLU:O	1:A:136:LEU:N	0.50	2.44	19	3
1:A:75:VAL:HG23	1:A:76:PRO:HD2	0.50	1.82	5	8
1:A:75:VAL:CG1	1:A:92:ALA:O	0.50	2.59	7	9
1:A:97:GLN:O	1:A:99:ILE:HG23	0.50	2.06	13	2
1:A:154:THR:O	1:A:157:TRP:N	0.50	2.44	1	6
1:A:114:ALA:O	1:A:118:LEU:CD1	0.50	2.60	3	1
1:A:102:VAL:CG1	1:A:103:LYS:N	0.50	2.74	3	1
1:A:101:PRO:O	1:A:104:ALA:N	0.50	2.45	17	2
1:A:90:VAL:HG11	1:A:127:ILE:CG2	0.50	2.36	17	1
1:A:105:VAL:O	1:A:105:VAL:CG1	0.50	2.60	13	1
1:A:143:ASN:OD1	1:A:166:ILE:CD1	0.50	2.59	14	4
1:A:71:HIS:CD2	1:A:96:TYR:CE1	0.50	3.00	2	1
1:A:98:VAL:O	1:A:98:VAL:HG12	0.50	2.06	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:106:TYR:CE1	1:A:108:VAL:HA	0.49	2.42	1	14
1:A:139:ARG:O	1:A:143:ASN:ND2	0.49	2.45	13	3
1:A:143:ASN:OD1	1:A:166:ILE:HD11	0.49	2.06	17	3
1:A:130:MET:SD	1:A:142:ILE:HD11	0.49	2.47	9	1
1:A:81:ILE:HD13	1:A:87:VAL:HG22	0.49	1.83	9	3
1:A:149:GLU:O	1:A:153:ILE:CD1	0.49	2.60	6	2
1:A:106:TYR:CE2	1:A:108:VAL:HA	0.49	2.43	16	3
1:A:70:GLU:OE2	1:A:97:GLN:NE2	0.49	2.45	3	4
1:A:118:LEU:HD22	1:A:153:ILE:HD13	0.49	1.84	7	2
1:A:131:GLU:O	1:A:135:THR:HG23	0.49	2.07	12	1
1:A:141:ILE:H	1:A:141:ILE:HD12	0.49	1.67	9	4
1:A:112:LEU:O	1:A:116:VAL:HG13	0.49	2.07	3	1
1:A:111:PHE:CE2	1:A:115:ILE:HG13	0.49	2.43	5	9
1:A:126:ILE:H	1:A:126:ILE:HD12	0.49	1.67	18	6
1:A:76:PRO:O	1:A:120:GLN:NE2	0.49	2.46	7	5
1:A:94:VAL:CG1	1:A:161:ILE:HD12	0.49	2.37	6	1
1:A:122:ASN:O	1:A:126:ILE:HD12	0.49	2.08	11	1
1:A:97:GLN:NE2	1:A:162:THR:CG2	0.48	2.75	12	4
1:A:102:VAL:HG13	1:A:103:LYS:N	0.48	2.22	3	1
1:A:153:ILE:O	1:A:153:ILE:CG2	0.48	2.60	9	2
1:A:139:ARG:HA	1:A:142:ILE:HD12	0.48	1.85	17	1
1:A:110:ASP:O	1:A:114:ALA:CB	0.48	2.61	17	6
1:A:147:ARG:O	1:A:151:ASP:CB	0.48	2.61	1	2
1:A:96:TYR:CG	1:A:111:PHE:CZ	0.48	3.01	5	6
1:A:71:HIS:HB3	1:A:96:TYR:CZ	0.48	2.44	20	2
1:A:95:TYR:O	1:A:161:ILE:HG23	0.48	2.07	7	3
1:A:83:LYS:CB	1:A:130:MET:O	0.48	2.61	6	1
1:A:111:PHE:CZ	1:A:115:ILE:HG13	0.48	2.44	3	5
1:A:134:GLU:O	1:A:135:THR:C	0.48	2.52	4	8
1:A:123:LEU:CD1	1:A:124:ARG:N	0.48	2.76	16	4
1:A:78:GLN:CG	1:A:120:GLN:OE1	0.48	2.61	9	1
1:A:159:VAL:CG2	1:A:160:LYS:N	0.47	2.77	2	1
1:A:156:ARG:HG3	1:A:157:TRP:CD1	0.47	2.44	1	11
1:A:71:HIS:HB2	1:A:96:TYR:CE1	0.47	2.44	7	3
1:A:113:MET:O	1:A:117:LYS:CD	0.47	2.62	4	1
1:A:96:TYR:CE1	1:A:108:VAL:HG21	0.47	2.45	8	1
1:A:106:TYR:C	1:A:107:ASN:CG	0.47	2.73	11	1
1:A:143:ASN:HB2	1:A:164:VAL:CG2	0.47	2.39	11	1
1:A:134:GLU:O	1:A:137:SER:N	0.47	2.47	5	6
1:A:91:ASP:N	1:A:91:ASP:OD1	0.47	2.47	12	2
1:A:102:VAL:HG23	1:A:103:LYS:HG2	0.47	1.86	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:TYR:CD2	1:A:111:PHE:CE1	0.47	3.03	1	3
1:A:131:GLU:O	1:A:134:GLU:N	0.47	2.47	14	5
1:A:72:VAL:HG23	1:A:95:TYR:CE1	0.47	2.45	4	1
1:A:114:ALA:O	1:A:118:LEU:CG	0.47	2.62	3	1
1:A:138:GLY:O	1:A:142:ILE:CD1	0.47	2.63	15	2
1:A:79:GLU:OE2	1:A:89:THR:HG23	0.47	2.10	11	1
1:A:104:ALA:HA	1:A:106:TYR:CE2	0.47	2.45	6	14
1:A:90:VAL:HG22	1:A:91:ASP:N	0.46	2.25	13	2
1:A:78:GLN:CD	1:A:120:GLN:CD	0.46	2.74	12	1
1:A:116:VAL:CG2	1:A:117:LYS:N	0.46	2.77	10	2
1:A:131:GLU:O	1:A:132:LEU:C	0.46	2.54	12	17
1:A:145:ARG:O	1:A:148:GLU:N	0.46	2.48	10	1
1:A:123:LEU:O	1:A:127:ILE:N	0.46	2.48	8	8
1:A:143:ASN:OD1	1:A:143:ASN:C	0.46	2.54	12	7
1:A:118:LEU:HB2	1:A:150:LEU:HD11	0.46	1.87	19	1
1:A:150:LEU:CD1	1:A:150:LEU:N	0.46	2.78	2	1
1:A:153:ILE:CG2	1:A:153:ILE:O	0.46	2.62	1	2
1:A:129:GLU:O	1:A:130:MET:CG	0.46	2.64	15	8
1:A:150:LEU:O	1:A:154:THR:CG2	0.46	2.63	16	1
1:A:101:PRO:O	1:A:103:LYS:N	0.46	2.49	17	1
1:A:113:MET:CG	1:A:114:ALA:N	0.46	2.79	17	1
1:A:82:CYS:HG	1:A:130:MET:C	0.46	2.12	6	1
1:A:102:VAL:O	1:A:105:VAL:CG1	0.45	2.63	7	2
1:A:70:GLU:CD	1:A:70:GLU:O	0.45	2.55	8	2
1:A:154:THR:C	1:A:159:VAL:O	0.45	2.55	11	3
1:A:138:GLY:O	1:A:142:ILE:HD12	0.45	2.12	13	2
1:A:148:GLU:CD	1:A:148:GLU:O	0.45	2.55	14	1
1:A:96:TYR:CD1	1:A:96:TYR:C	0.45	2.90	11	3
1:A:91:ASP:OD1	1:A:91:ASP:N	0.45	2.49	14	1
1:A:99:ILE:HD13	1:A:159:VAL:HA	0.45	1.88	15	1
1:A:139:ARG:O	1:A:143:ASN:CG	0.45	2.55	20	3
1:A:146:LEU:O	1:A:149:GLU:N	0.45	2.50	13	2
1:A:104:ALA:HA	1:A:106:TYR:CE1	0.45	2.46	16	2
1:A:126:ILE:HG23	1:A:145:ARG:NH2	0.45	2.27	14	1
1:A:118:LEU:O	1:A:122:ASN:ND2	0.45	2.50	9	3
1:A:135:THR:O	1:A:136:LEU:C	0.44	2.56	14	2
1:A:126:ILE:CG2	1:A:145:ARG:NH2	0.44	2.80	14	1
1:A:153:ILE:O	1:A:156:ARG:CG	0.44	2.65	3	1
1:A:97:GLN:CG	1:A:162:THR:HG23	0.44	2.42	11	4
1:A:144:ALA:O	1:A:148:GLU:CD	0.44	2.55	17	1
1:A:106:TYR:O	1:A:107:ASN:CG	0.44	2.56	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:PHE:CE1	1:A:115:ILE:CG1	0.44	3.01	13	1
1:A:94:VAL:HG21	1:A:150:LEU:CD1	0.44	2.43	14	1
1:A:101:PRO:O	1:A:102:VAL:C	0.44	2.56	20	2
1:A:92:ALA:HB1	1:A:166:ILE:HD13	0.44	1.89	6	1
1:A:84:ASP:CG	1:A:84:ASP:O	0.44	2.56	20	2
1:A:131:GLU:C	1:A:133:ASP:N	0.44	2.72	19	10
1:A:97:GLN:O	1:A:99:ILE:N	0.44	2.50	17	1
1:A:143:ASN:OD1	1:A:164:VAL:HG23	0.43	2.13	19	1
1:A:111:PHE:CE2	1:A:159:VAL:HG11	0.43	2.48	6	1
1:A:79:GLU:N	1:A:79:GLU:OE1	0.43	2.51	6	1
1:A:144:ALA:O	1:A:145:ARG:C	0.43	2.56	1	1
1:A:93:VAL:HG23	1:A:165:GLU:CB	0.43	2.43	18	1
1:A:70:GLU:HG3	1:A:162:THR:HG21	0.43	1.91	5	1
1:A:101:PRO:O	1:A:105:VAL:HG22	0.43	2.13	5	1
1:A:90:VAL:C	1:A:91:ASP:OD1	0.43	2.57	9	1
1:A:84:ASP:O	1:A:86:VAL:HG23	0.43	2.13	11	1
1:A:115:ILE:CD1	1:A:150:LEU:HD12	0.43	2.35	19	1
1:A:96:TYR:C	1:A:96:TYR:CD1	0.43	2.91	20	3
1:A:76:PRO:CD	1:A:116:VAL:HG13	0.43	2.42	9	1
1:A:78:GLN:OE1	1:A:124:ARG:CZ	0.43	2.67	11	1
1:A:146:LEU:O	1:A:147:ARG:C	0.43	2.57	13	2
1:A:151:ASP:CG	1:A:151:ASP:O	0.43	2.57	19	1
1:A:123:LEU:C	1:A:123:LEU:CD1	0.43	2.84	16	1
1:A:156:ARG:HB2	1:A:156:ARG:CZ	0.43	2.44	16	1
1:A:141:ILE:O	1:A:144:ALA:N	0.42	2.52	6	2
1:A:115:ILE:O	1:A:116:VAL:C	0.42	2.58	8	3
1:A:154:THR:CB	1:A:159:VAL:O	0.42	2.67	7	1
1:A:78:GLN:CD	1:A:123:LEU:HD11	0.42	2.34	13	1
1:A:133:ASP:O	1:A:135:THR:N	0.42	2.53	18	1
1:A:154:THR:CB	1:A:159:VAL:HG13	0.42	2.33	20	3
1:A:159:VAL:HG22	1:A:160:LYS:N	0.42	2.29	20	1
1:A:84:ASP:OD1	1:A:84:ASP:N	0.42	2.50	17	1
1:A:127:ILE:N	1:A:127:ILE:HD12	0.42	2.29	18	1
1:A:115:ILE:HD11	1:A:154:THR:CG2	0.42	2.44	18	1
1:A:118:LEU:O	1:A:121:THR:N	0.42	2.51	18	2
1:A:108:VAL:O	1:A:112:LEU:HD12	0.42	2.14	20	1
1:A:70:GLU:HG3	1:A:95:TYR:CD2	0.42	2.49	10	1
1:A:91:ASP:OD1	1:A:92:ALA:N	0.42	2.53	19	1
1:A:147:ARG:HB2	1:A:164:VAL:HG21	0.42	1.91	4	1
1:A:147:ARG:O	1:A:151:ASP:N	0.42	2.53	3	1
1:A:136:LEU:C	1:A:136:LEU:HD12	0.42	2.35	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:PRO:HG2	1:A:120:GLN:NE2	0.42	2.30	19	1
1:A:78:GLN:NE2	1:A:120:GLN:O	0.42	2.52	9	1
1:A:153:ILE:N	1:A:153:ILE:HD12	0.42	2.30	19	1
1:A:104:ALA:HB1	1:A:108:VAL:HG22	0.42	1.92	11	1
1:A:169:ILE:HG22	1:A:170:ASP:N	0.42	2.30	12	7
1:A:157:TRP:HB2	1:A:159:VAL:HG12	0.42	1.92	7	1
1:A:70:GLU:O	1:A:70:GLU:OE2	0.42	2.38	7	2
1:A:110:ASP:O	1:A:114:ALA:HB2	0.42	2.14	14	1
1:A:96:TYR:CE1	1:A:108:VAL:HG11	0.42	2.50	15	1
1:A:127:ILE:HD12	1:A:127:ILE:H	0.42	1.75	15	1
1:A:107:ASN:C	1:A:109:SER:N	0.41	2.74	4	2
1:A:97:GLN:CD	1:A:162:THR:CG2	0.41	2.88	20	1
1:A:118:LEU:O	1:A:119:ALA:C	0.41	2.58	5	1
1:A:159:VAL:CG1	1:A:160:LYS:N	0.41	2.84	9	1
1:A:108:VAL:O	1:A:108:VAL:HG12	0.41	2.15	13	1
1:A:77:PRO:HB2	1:A:89:THR:CG2	0.41	2.45	17	6
1:A:136:LEU:HD12	1:A:136:LEU:C	0.41	2.35	1	1
1:A:143:ASN:C	1:A:143:ASN:OD1	0.41	2.58	3	1
1:A:77:PRO:CB	1:A:90:VAL:O	0.41	2.68	9	1
1:A:71:HIS:HB2	1:A:96:TYR:CD2	0.41	2.50	2	1
1:A:99:ILE:CD1	1:A:159:VAL:HA	0.41	2.45	15	1
1:A:82:CYS:SG	1:A:130:MET:O	0.41	2.78	6	1
1:A:73:ILE:HD11	1:A:111:PHE:CE2	0.41	2.51	11	1
1:A:133:ASP:C	1:A:135:THR:N	0.41	2.74	18	1
1:A:123:LEU:CB	1:A:127:ILE:HD13	0.41	2.36	17	1
1:A:100:ASP:OD1	1:A:102:VAL:CG2	0.41	2.68	17	2
1:A:100:ASP:CG	1:A:102:VAL:HG22	0.41	2.36	11	1
1:A:134:GLU:C	1:A:136:LEU:N	0.41	2.74	19	1
1:A:73:ILE:HD11	1:A:96:TYR:CD2	0.41	2.51	13	1
1:A:97:GLN:HG2	1:A:162:THR:CG2	0.41	2.46	18	1
1:A:90:VAL:HG21	1:A:127:ILE:HG12	0.41	1.92	14	1
1:A:163:ARG:HB3	1:A:163:ARG:CZ	0.41	2.46	14	1
1:A:116:VAL:HG23	1:A:117:LYS:N	0.41	2.29	4	1
1:A:115:ILE:C	1:A:117:LYS:N	0.41	2.74	20	1
1:A:93:VAL:CG2	1:A:165:GLU:HB2	0.41	2.46	20	1
1:A:81:ILE:O	1:A:82:CYS:O	0.41	2.39	7	2
1:A:87:VAL:O	1:A:87:VAL:CG1	0.41	2.69	2	1
1:A:136:LEU:HD12	1:A:137:SER:N	0.41	2.31	1	1
1:A:78:GLN:OE1	1:A:80:VAL:CG1	0.41	2.68	11	1
1:A:145:ARG:O	1:A:146:LEU:C	0.40	2.60	10	1
1:A:139:ARG:CZ	1:A:139:ARG:CB	0.40	2.99	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ARG:CZ	1:A:156:ARG:CB	0.40	2.99	16	1
1:A:139:ARG:C	1:A:139:ARG:CD	0.40	2.90	12	1
1:A:141:ILE:HD12	1:A:141:ILE:H	0.40	1.77	5	1
1:A:151:ASP:OD1	1:A:151:ASP:O	0.40	2.40	15	1
1:A:111:PHE:CE2	1:A:115:ILE:CG1	0.40	3.04	17	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	104/113 (92%)	84±3 (81±3%)	17±3 (16±3%)	4±1 (3±1%)	8	38
All	All	2080/2260 (92%)	1679 (81%)	331 (16%)	70 (3%)	8	38

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	132	LEU	20
1	A	82	CYS	19
1	A	105	VAL	6
1	A	98	VAL	6
1	A	108	VAL	4
1	A	138	GLY	4
1	A	168	ARG	3
1	A	135	THR	3
1	A	69	ARG	3
1	A	102	VAL	2

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	95/103 (92%)	86±2 (91±3%)	9±2 (9±3%)	16	61
All	All	1900/2060 (92%)	1729 (91%)	171 (9%)	16	61

All 33 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	130	MET	19
1	A	111	PHE	17
1	A	74	ASP	15
1	A	160	LYS	14
1	A	151	ASP	13
1	A	162	THR	10
1	A	70	GLU	10
1	A	110	ASP	7
1	A	91	ASP	7
1	A	148	GLU	5
1	A	133	ASP	5
1	A	156	ARG	4
1	A	152	LYS	4
1	A	85	ASN	4
1	A	84	ASP	3
1	A	164	VAL	3
1	A	69	ARG	3
1	A	145	ARG	3
1	A	155	ASP	3
1	A	163	ARG	3
1	A	168	ARG	2
1	A	140	ASP	2
1	A	117	LYS	2
1	A	136	LEU	2
1	A	143	ASN	2
1	A	135	THR	2
1	A	159	VAL	1
1	A	82	CYS	1
1	A	150	LEU	1
1	A	107	ASN	1
1	A	93	VAL	1
1	A	139	ARG	1
1	A	99	ILE	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 ⓘ

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 11060

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	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	101	-0.43 ± 0.30	None needed (< 0.5 ppm)
$^{13}C_\beta$	109	0.19 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	0	—	—
^{15}N	106	1.02 ± 0.47	Should be applied

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 83%, i.e. 1092 atoms were assigned a chemical shift out of a possible 1323. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	396/510 (78%)	203/203 (100%)	94/208 (45%)	99/99 (100%)
Sidechain	647/760 (85%)	392/437 (90%)	247/286 (86%)	8/37 (22%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	49/53 (92%)	25/27 (93%)	23/23 (100%)	1/3 (33%)
Overall	1092/1323 (83%)	620/667 (93%)	364/517 (70%)	108/139 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1167 atoms were assigned a chemical shift out of a possible 1422. 0 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	425/555 (77%)	218/221 (99%)	101/226 (45%)	106/108 (98%)
Sidechain	689/806 (85%)	418/463 (90%)	263/305 (86%)	8/38 (21%)
Aromatic	53/61 (87%)	27/31 (87%)	25/25 (100%)	1/5 (20%)
Overall	1167/1422 (82%)	663/715 (93%)	389/556 (70%)	115/151 (76%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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: