



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:29 PM BST

PDB ID : 1F16  
Title : SOLUTION STRUCTURE OF A PRO-APOPTOTIC PROTEIN BAX  
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Deposited on : 2000-05-18

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

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

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

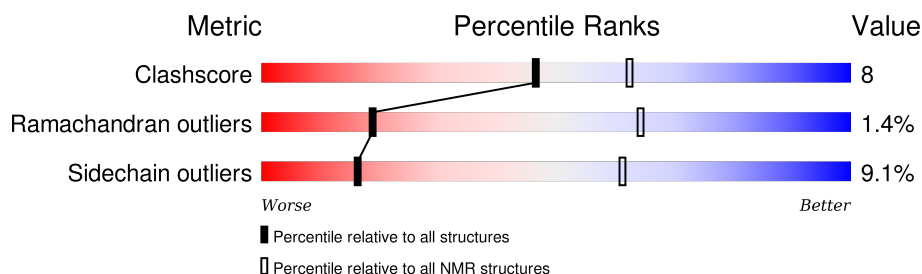
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



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

Mol	Chain	Length	Quality of chain
1	A	192	 66% 7% 27%

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:15-A:35, A:54-A:83, A:88-A:99, A:109-A:166, A:170-A:188 (140)	0.43	8

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

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

The models can be grouped into 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2977 atoms, of which 1489 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA).

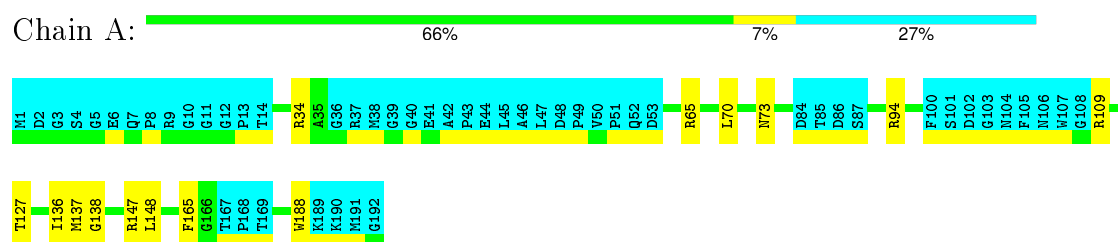
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	192	2977	949	1489	252	277	10	0

## 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: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

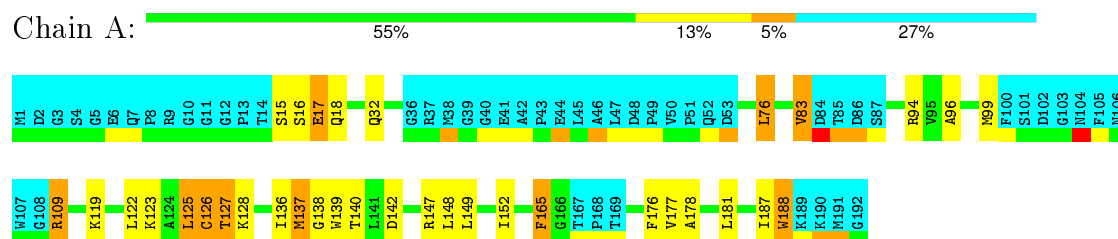


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

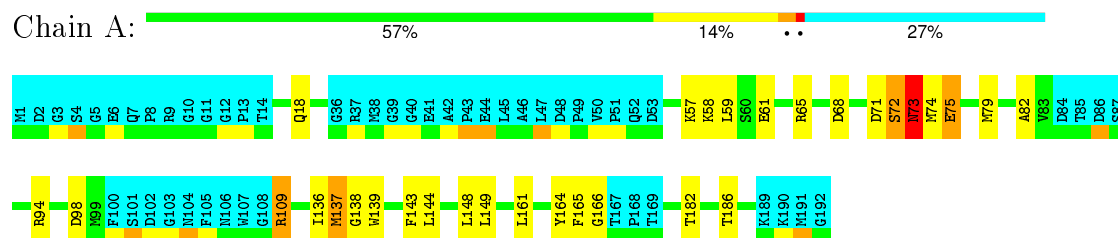
#### 4.2.1 Score per residue for model 1

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



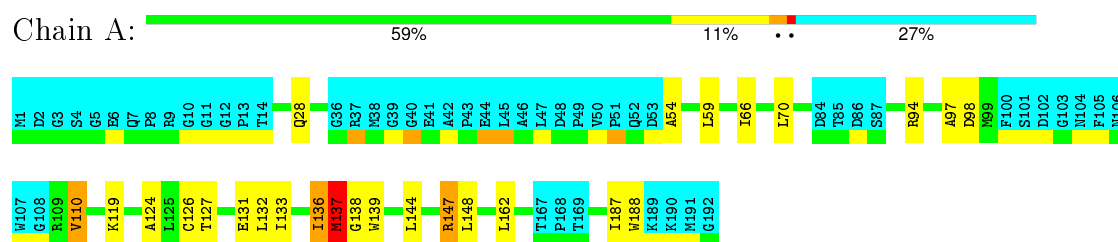
#### 4.2.2 Score per residue for model 2

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



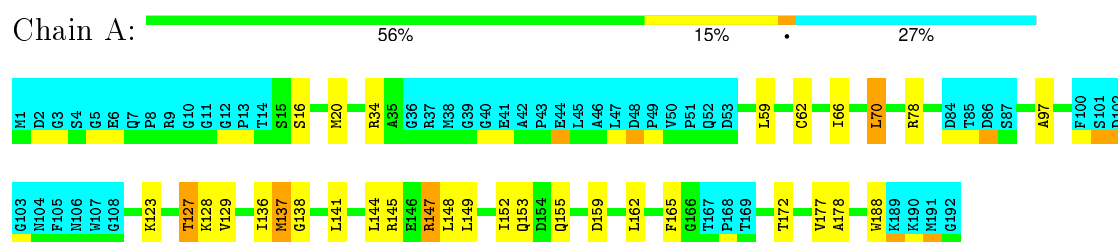
#### 4.2.3 Score per residue for model 3

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



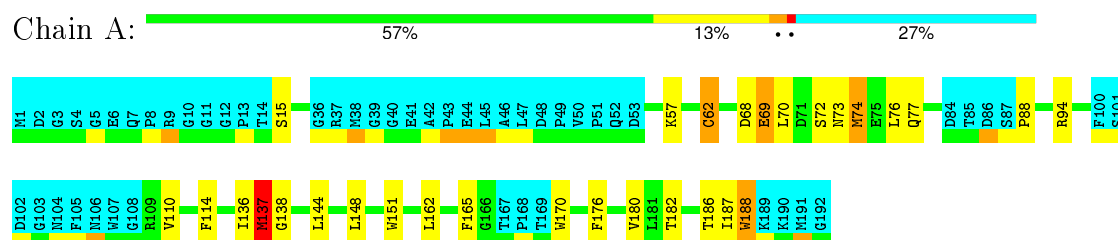
#### 4.2.4 Score per residue for model 4

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



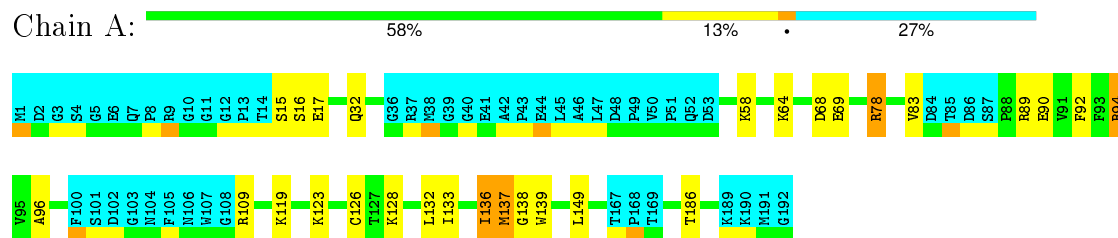
#### 4.2.5 Score per residue for model 5

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



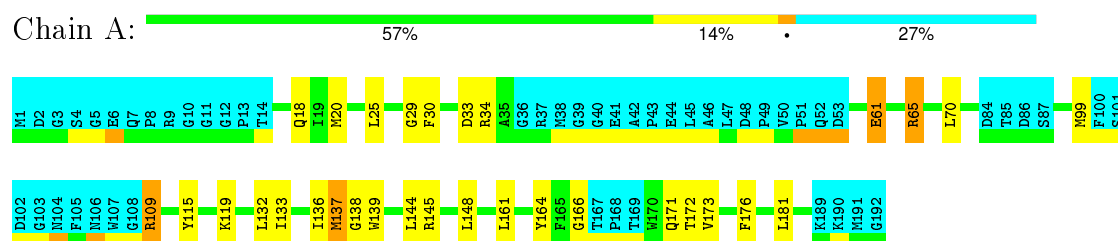
#### 4.2.6 Score per residue for model 6

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



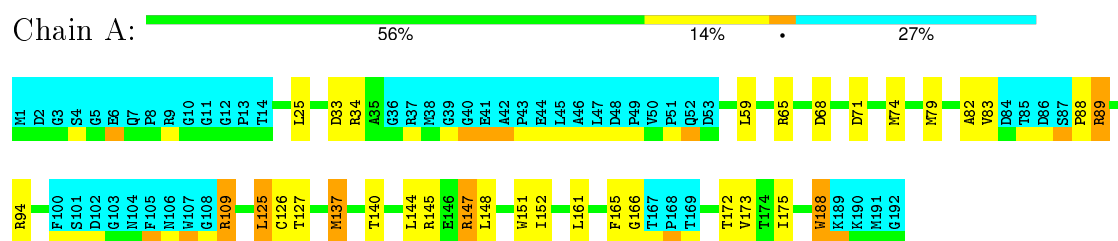
#### 4.2.7 Score per residue for model 7

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



#### 4.2.8 Score per residue for model 8 (medoid)

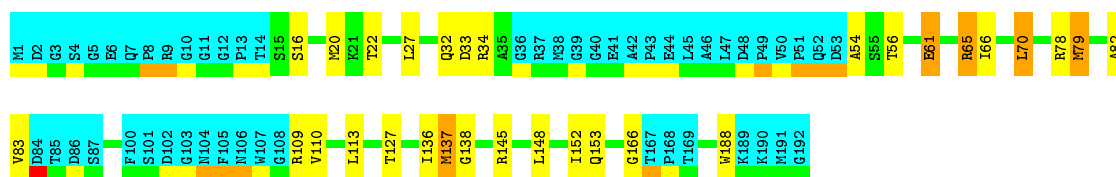
- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



#### 4.2.9 Score per residue for model 9

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

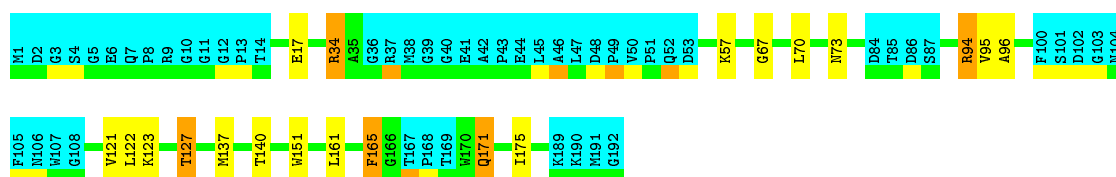




#### 4.2.10 Score per residue for model 10

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

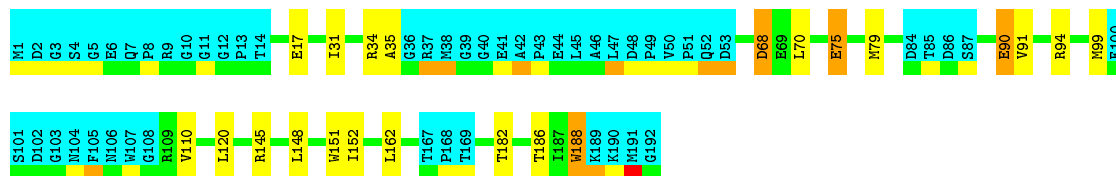
Chain A: 63% 8% 27%



#### 4.2.11 Score per residue for model 11

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

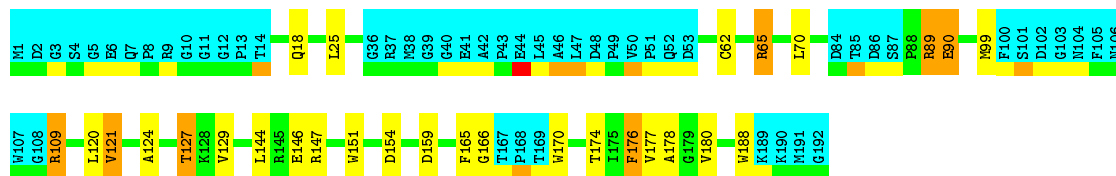
Chain A: 61% 9% 27%



#### 4.2.12 Score per residue for model 12

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

Chain A: 58% 11% 27%





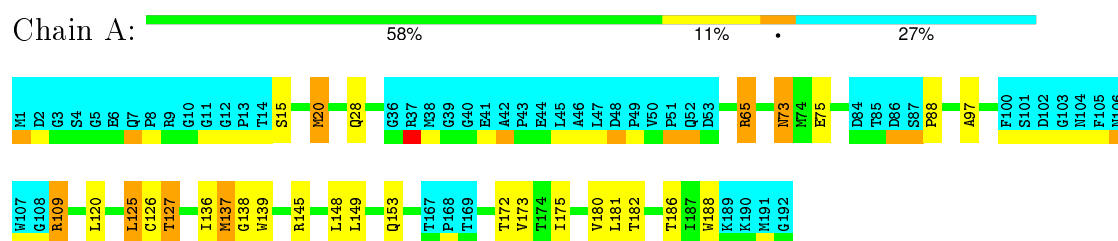
### 4.2.13 Score per residue for model 13

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



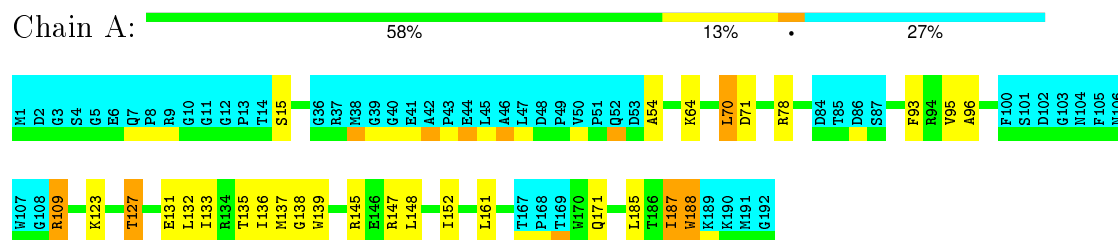
### 4.2.14 Score per residue for model 14

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



### 4.2.15 Score per residue for model 15

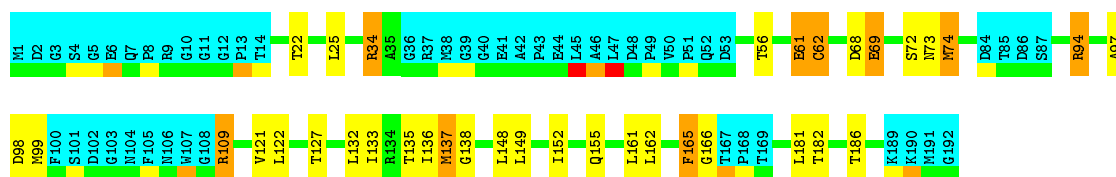
- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



### 4.2.16 Score per residue for model 16

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

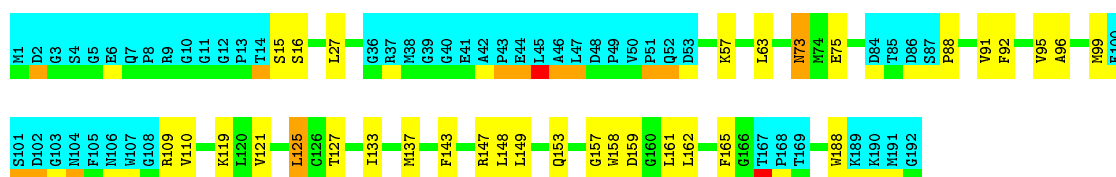




#### 4.2.17 Score per residue for model 17

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

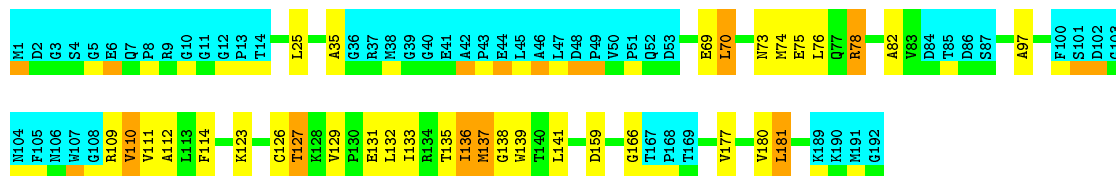
Chain A: 56% 16% 27%



#### 4.2.18 Score per residue for model 18

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

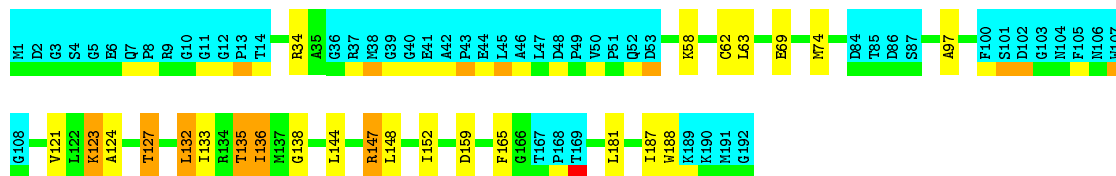
Chain A: 55% 14% 27%



#### 4.2.19 Score per residue for model 19

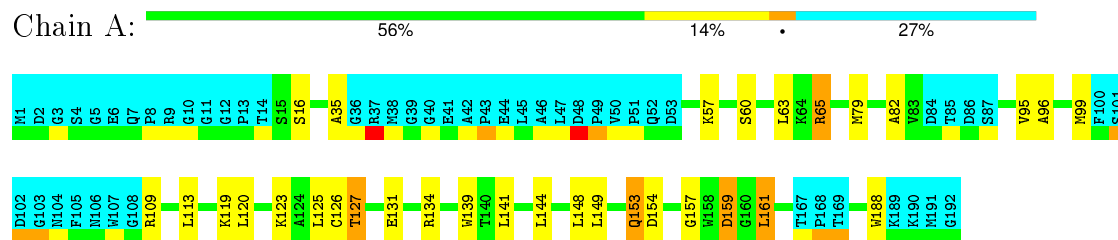
- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)

Chain A: 60% 10% 27%



#### 4.2.20 Score per residue for model 20

- Molecule 1: PROTEIN (APOPTOSIS REGULATOR BAX, MEMBRANE ISOFORM ALPHA)



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *DISTANCE GEOMETRY SIMULATED ANNEALING MOLECULAR DYNAMICS*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *STRUCTURES WITH THE LOWEST ENERGY*.

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

Software name	Classification	Version
X-PLOR	refinement	3.840
NMRPIPE 1.7 REV	structure solution	1999.039.11.31
PIPP	structure solution	4.1.5
UXNMR	structure solution	2.5

No chemical shift data was provided. 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](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.05±0.00	0±0/1135 (0.0±0.0%)	0.93±0.01	0±0/1534 (0.0±0.0%)
All	All	1.05	0/22700 (0.0%)	0.93	2/30680 (0.0%)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	127	THR	CA-CB-CG2	-6.03	103.96	112.40	17	2

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	1113	1151	1151	18±3
All	All	22260	23020	23020	358

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:182:THR:O	1:A:186:THR:HG22	0.75	1.82	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:GLU:O	1:A:135:THR:HG23	0.72	1.84	15	1
1:A:109:ARG:H	1:A:109:ARG:NE	0.69	1.85	2	1
1:A:83:VAL:HG13	1:A:83:VAL:O	0.65	1.90	9	1
1:A:126:CYS:SG	1:A:127:THR:N	0.64	2.70	14	7
1:A:181:LEU:C	1:A:181:LEU:HD13	0.63	2.13	1	2
1:A:129:VAL:HG13	1:A:129:VAL:O	0.61	1.95	18	2
1:A:76:LEU:O	1:A:76:LEU:HD13	0.61	1.96	1	1
1:A:20:MET:SD	1:A:145:ARG:NH2	0.59	2.75	14	2
1:A:62:CYS:SG	1:A:165:PHE:CZ	0.58	2.97	4	4
1:A:62:CYS:SG	1:A:165:PHE:CE1	0.57	2.97	5	2
1:A:73:ASN:HD22	1:A:75:GLU:H	0.56	1.43	17	1
1:A:94:ARG:NH1	1:A:188:TRP:CD1	0.56	2.73	5	1
1:A:136:ILE:O	1:A:138:GLY:N	0.56	2.39	1	13
1:A:115:TYR:CE2	1:A:119:LYS:NZ	0.55	2.72	7	1
1:A:144:LEU:C	1:A:144:LEU:HD23	0.55	2.22	19	1
1:A:73:ASN:O	1:A:75:GLU:N	0.55	2.40	18	1
1:A:187:ILE:HD12	1:A:188:TRP:N	0.55	2.16	15	1
1:A:94:ARG:NH1	1:A:188:TRP:NE1	0.55	2.55	5	1
1:A:109:ARG:CD	1:A:109:ARG:H	0.54	2.13	16	1
1:A:62:CYS:SG	1:A:165:PHE:CD2	0.54	3.00	16	2
1:A:89:ARG:CG	1:A:89:ARG:NH1	0.54	2.70	8	2
1:A:33:ASP:OD1	1:A:34:ARG:N	0.54	2.41	7	1
1:A:144:LEU:HD12	1:A:148:LEU:HB2	0.54	1.80	13	2
1:A:74:MET:N	1:A:74:MET:SD	0.53	2.81	19	3
1:A:15:SER:O	1:A:17:GLU:N	0.53	2.41	6	3
1:A:73:ASN:OD1	1:A:73:ASN:O	0.53	2.27	10	1
1:A:62:CYS:SG	1:A:165:PHE:CE2	0.53	3.02	16	2
1:A:136:ILE:O	1:A:139:TRP:N	0.53	2.41	14	8
1:A:65:ARG:HH11	1:A:65:ARG:CG	0.52	2.18	13	2
1:A:65:ARG:NH1	1:A:65:ARG:CG	0.52	2.72	20	4
1:A:89:ARG:CG	1:A:89:ARG:HH11	0.52	2.17	8	1
1:A:72:SER:O	1:A:73:ASN:C	0.52	2.48	2	2
1:A:145:ARG:CG	1:A:145:ARG:NH1	0.52	2.73	11	2
1:A:121:VAL:CG2	1:A:136:ILE:HG21	0.52	2.34	19	1
1:A:68:ASP:OD1	1:A:69:GLU:N	0.52	2.42	6	3
1:A:34:ARG:CG	1:A:34:ARG:NH1	0.52	2.71	16	1
1:A:73:ASN:ND2	1:A:75:GLU:H	0.52	2.02	17	3
1:A:91:VAL:CG1	1:A:92:PHE:N	0.52	2.73	17	1
1:A:147:ARG:CG	1:A:147:ARG:NH1	0.52	2.72	15	4
1:A:34:ARG:NH1	1:A:34:ARG:CG	0.51	2.71	10	3
1:A:176:PHE:O	1:A:180:VAL:HG12	0.51	2.03	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ARG:CG	1:A:65:ARG:HH11	0.51	2.18	12	3
1:A:34:ARG:CG	1:A:34:ARG:HH11	0.51	2.19	16	2
1:A:123:LYS:O	1:A:127:THR:OG1	0.51	2.29	1	8
1:A:78:ARG:CG	1:A:78:ARG:NH1	0.51	2.73	6	1
1:A:73:ASN:O	1:A:74:MET:CB	0.51	2.59	5	1
1:A:61:GLU:OE1	1:A:61:GLU:N	0.51	2.44	7	1
1:A:65:ARG:CG	1:A:65:ARG:NH1	0.51	2.72	14	2
1:A:34:ARG:HH11	1:A:34:ARG:CG	0.50	2.17	10	2
1:A:109:ARG:NH1	1:A:148:LEU:HD22	0.50	2.22	13	1
1:A:90:GLU:OE1	1:A:90:GLU:N	0.50	2.44	12	2
1:A:109:ARG:HH11	1:A:109:ARG:CG	0.50	2.19	16	1
1:A:119:LYS:CG	1:A:120:LEU:N	0.50	2.75	20	1
1:A:78:ARG:HE	1:A:78:ARG:C	0.50	2.09	18	1
1:A:83:VAL:CG1	1:A:83:VAL:O	0.50	2.60	9	1
1:A:62:CYS:SG	1:A:165:PHE:CD1	0.50	3.05	5	2
1:A:17:GLU:OE1	1:A:18:GLN:N	0.50	2.44	1	1
1:A:147:ARG:CG	1:A:147:ARG:HH11	0.50	2.18	8	4
1:A:66:ILE:O	1:A:70:LEU:N	0.50	2.44	4	3
1:A:109:ARG:NH1	1:A:109:ARG:CG	0.49	2.72	16	2
1:A:147:ARG:HH11	1:A:147:ARG:CG	0.49	2.19	3	2
1:A:147:ARG:NH1	1:A:147:ARG:CG	0.49	2.73	4	2
1:A:94:ARG:NH1	1:A:98:ASP:OD2	0.49	2.46	3	2
1:A:61:GLU:N	1:A:61:GLU:OE1	0.49	2.45	9	2
1:A:121:VAL:O	1:A:124:ALA:N	0.49	2.46	12	2
1:A:95:VAL:HG13	1:A:96:ALA:N	0.49	2.23	10	5
1:A:145:ARG:CG	1:A:145:ARG:HH11	0.49	2.21	11	3
1:A:157:GLY:O	1:A:159:ASP:N	0.48	2.46	17	1
1:A:148:LEU:O	1:A:152:ILE:HD12	0.48	2.08	8	5
1:A:17:GLU:OE1	1:A:145:ARG:NH2	0.48	2.46	11	1
1:A:15:SER:C	1:A:17:GLU:H	0.48	2.12	1	1
1:A:182:THR:O	1:A:186:THR:N	0.48	2.44	5	3
1:A:79:MET:O	1:A:82:ALA:N	0.48	2.44	20	4
1:A:20:MET:SD	1:A:141:LEU:HD22	0.48	2.49	4	1
1:A:127:THR:O	1:A:128:LYS:CB	0.48	2.61	13	2
1:A:134:ARG:CG	1:A:134:ARG:NH1	0.47	2.75	20	1
1:A:148:LEU:O	1:A:152:ILE:CD1	0.47	2.62	1	6
1:A:136:ILE:C	1:A:138:GLY:N	0.47	2.67	1	8
1:A:136:ILE:O	1:A:137:MET:C	0.47	2.51	14	12
1:A:95:VAL:CG1	1:A:96:ALA:N	0.47	2.77	13	5
1:A:180:VAL:CG2	1:A:181:LEU:N	0.47	2.77	14	1
1:A:109:ARG:O	1:A:112:ALA:N	0.47	2.47	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:161:LEU:O	1:A:165:PHE:CD1	0.47	2.68	10	1
1:A:16:SER:OG	1:A:153:GLN:NE2	0.47	2.47	17	2
1:A:78:ARG:CG	1:A:78:ARG:HH11	0.47	2.21	6	1
1:A:78:ARG:NE	1:A:78:ARG:C	0.47	2.67	18	1
1:A:20:MET:O	1:A:20:MET:SD	0.47	2.73	4	1
1:A:94:ARG:CG	1:A:94:ARG:NH1	0.46	2.73	6	1
1:A:99:MET:C	1:A:109:ARG:HH12	0.46	2.13	12	1
1:A:61:GLU:OE2	1:A:65:ARG:NH2	0.46	2.49	2	1
1:A:94:ARG:CG	1:A:94:ARG:HH11	0.46	2.23	6	1
1:A:57:LYS:O	1:A:60:SER:OG	0.46	2.33	20	1
1:A:125:LEU:HD23	1:A:125:LEU:O	0.45	2.11	14	2
1:A:134:ARG:CG	1:A:134:ARG:HH11	0.45	2.24	20	1
1:A:141:LEU:CD2	1:A:141:LEU:N	0.45	2.79	18	2
1:A:144:LEU:HG	1:A:148:LEU:HD12	0.45	1.88	5	1
1:A:34:ARG:NH2	1:A:67:GLY:O	0.45	2.49	10	1
1:A:15:SER:C	1:A:17:GLU:N	0.45	2.68	1	2
1:A:177:VAL:HG23	1:A:178:ALA:N	0.45	2.25	1	3
1:A:171:GLN:H	1:A:171:GLN:CD	0.45	2.15	7	1
1:A:145:ARG:HG2	1:A:145:ARG:HH11	0.45	1.72	11	3
1:A:31:ILE:O	1:A:35:ALA:N	0.45	2.48	11	1
1:A:132:LEU:O	1:A:135:THR:N	0.45	2.49	19	2
1:A:70:LEU:O	1:A:73:ASN:CG	0.45	2.55	10	1
1:A:63:LEU:N	1:A:63:LEU:CD1	0.44	2.80	19	2
1:A:127:THR:HG23	1:A:129:VAL:HG23	0.44	1.89	12	1
1:A:28:GLN:O	1:A:28:GLN:NE2	0.44	2.50	14	1
1:A:78:ARG:NE	1:A:78:ARG:O	0.44	2.50	18	1
1:A:137:MET:O	1:A:140:THR:OG1	0.44	2.34	10	3
1:A:181:LEU:C	1:A:181:LEU:CD1	0.44	2.86	14	2
1:A:157:GLY:C	1:A:159:ASP:N	0.44	2.69	17	2
1:A:148:LEU:O	1:A:149:LEU:CB	0.44	2.65	14	4
1:A:112:ALA:HB2	1:A:177:VAL:HG13	0.44	1.89	18	1
1:A:109:ARG:HG2	1:A:109:ARG:HH11	0.44	1.73	15	1
1:A:34:ARG:HH11	1:A:34:ARG:HG2	0.44	1.72	7	1
1:A:125:LEU:O	1:A:125:LEU:HD23	0.44	2.13	8	2
1:A:123:LYS:NZ	1:A:123:LYS:CB	0.44	2.81	10	1
1:A:127:THR:O	1:A:128:LYS:HB2	0.43	2.12	13	1
1:A:134:ARG:HG2	1:A:134:ARG:HH11	0.43	1.74	20	1
1:A:73:ASN:C	1:A:75:GLU:N	0.43	2.71	18	1
1:A:114:PHE:CD1	1:A:114:PHE:N	0.43	2.85	18	1
1:A:151:TRP:CD1	1:A:151:TRP:N	0.43	2.86	12	1
1:A:145:ARG:HH11	1:A:145:ARG:HG2	0.43	1.72	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:109:ARG:O	1:A:112:ALA:HB3	0.43	2.14	18	1
1:A:187:ILE:O	1:A:188:TRP:C	0.43	2.57	3	3
1:A:63:LEU:N	1:A:63:LEU:HD12	0.43	2.26	19	3
1:A:131:GLU:N	1:A:131:GLU:CD	0.43	2.72	3	1
1:A:30:PHE:O	1:A:33:ASP:OD1	0.43	2.36	7	1
1:A:73:ASN:O	1:A:76:LEU:N	0.43	2.51	18	1
1:A:75:GLU:OE1	1:A:79:MET:SD	0.43	2.77	11	1
1:A:34:ARG:NH1	1:A:68:ASP:CG	0.43	2.71	11	1
1:A:177:VAL:CG2	1:A:178:ALA:N	0.43	2.82	12	2
1:A:182:THR:O	1:A:186:THR:OG1	0.43	2.33	13	1
1:A:96:ALA:O	1:A:99:MET:N	0.43	2.51	1	1
1:A:147:ARG:HH11	1:A:147:ARG:HG2	0.43	1.73	17	1
1:A:187:ILE:CG2	1:A:188:TRP:N	0.43	2.82	3	1
1:A:181:LEU:HD13	1:A:181:LEU:O	0.43	2.12	18	1
1:A:132:LEU:O	1:A:133:ILE:C	0.43	2.55	16	7
1:A:30:PHE:C	1:A:33:ASP:OD1	0.43	2.56	7	1
1:A:99:MET:O	1:A:109:ARG:NH1	0.43	2.52	12	1
1:A:70:LEU:HG	1:A:71:ASP:N	0.43	2.29	15	1
1:A:181:LEU:O	1:A:181:LEU:HD13	0.42	2.14	1	1
1:A:62:CYS:SG	1:A:165:PHE:CG	0.42	3.12	5	1
1:A:164:TYR:C	1:A:166:GLY:H	0.42	2.17	2	1
1:A:68:ASP:O	1:A:71:ASP:OD2	0.42	2.37	2	1
1:A:143:PHE:CD1	1:A:143:PHE:C	0.42	2.92	17	2
1:A:171:GLN:HE22	1:A:175:ILE:HD11	0.42	1.74	10	1
1:A:63:LEU:CD1	1:A:63:LEU:N	0.42	2.82	17	1
1:A:124:ALA:O	1:A:127:THR:OG1	0.42	2.31	3	1
1:A:121:VAL:HG23	1:A:136:ILE:HG21	0.42	1.89	19	1
1:A:188:TRP:O	1:A:188:TRP:CG	0.42	2.72	17	1
1:A:187:ILE:C	1:A:187:ILE:CD1	0.42	2.88	15	1
1:A:159:ASP:OD1	1:A:159:ASP:N	0.42	2.52	12	1
1:A:171:GLN:CD	1:A:171:GLN:N	0.42	2.73	15	1
1:A:139:TRP:N	1:A:139:TRP:CD1	0.42	2.85	20	1
1:A:17:GLU:CD	1:A:17:GLU:N	0.42	2.73	10	1
1:A:170:TRP:O	1:A:174:THR:HG23	0.42	2.15	12	1
1:A:24:ALA:O	1:A:28:GLN:NE2	0.42	2.53	13	1
1:A:64:LYS:O	1:A:68:ASP:OD2	0.42	2.37	6	1
1:A:89:ARG:HH11	1:A:89:ARG:HG2	0.41	1.74	8	1
1:A:145:ARG:NH1	1:A:145:ARG:CG	0.41	2.78	4	1
1:A:99:MET:C	1:A:109:ARG:NH1	0.41	2.74	12	1
1:A:109:ARG:HG3	1:A:109:ARG:HH11	0.41	1.75	8	1
1:A:135:THR:O	1:A:136:ILE:C	0.41	2.57	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:147:ARG:HG2	1:A:147:ARG:HH11	0.41	1.76	19	2
1:A:131:GLU:H	1:A:131:GLU:CD	0.41	2.18	3	1
1:A:110:VAL:CG1	1:A:114:PHE:CE1	0.41	3.04	5	1
1:A:70:LEU:O	1:A:73:ASN:OD1	0.41	2.38	10	1
1:A:138:GLY:O	1:A:142:ASP:OD1	0.41	2.38	1	1
1:A:25:LEU:HD23	1:A:56:THR:HG21	0.41	1.91	16	1
1:A:126:CYS:C	1:A:128:LYS:N	0.41	2.72	6	1
1:A:70:LEU:O	1:A:70:LEU:HD23	0.41	2.15	18	1
1:A:172:THR:O	1:A:173:VAL:C	0.41	2.58	8	3
1:A:76:LEU:O	1:A:77:GLN:C	0.41	2.58	5	1
1:A:109:ARG:CD	1:A:109:ARG:N	0.41	2.84	2	1
1:A:65:ARG:HG2	1:A:65:ARG:HH11	0.41	1.76	9	1
1:A:157:GLY:C	1:A:159:ASP:H	0.41	2.19	17	1
1:A:172:THR:O	1:A:175:ILE:N	0.41	2.54	8	2
1:A:119:LYS:O	1:A:123:LYS:N	0.41	2.47	6	1
1:A:146:GLU:CG	1:A:147:ARG:N	0.41	2.84	12	1
1:A:94:ARG:HH11	1:A:94:ARG:HG3	0.41	1.76	10	1
1:A:73:ASN:HD22	1:A:75:GLU:N	0.41	2.12	17	1
1:A:65:ARG:O	1:A:68:ASP:OD1	0.41	2.39	8	1
1:A:89:ARG:CG	1:A:90:GLU:N	0.41	2.83	6	1
1:A:69:GLU:OE1	1:A:69:GLU:O	0.41	2.38	19	1
1:A:90:GLU:CD	1:A:90:GLU:N	0.41	2.73	12	1
1:A:57:LYS:C	1:A:57:LYS:CD	0.41	2.88	2	1
1:A:110:VAL:O	1:A:113:LEU:N	0.41	2.52	9	1
1:A:25:LEU:O	1:A:29:GLY:N	0.41	2.49	7	1
1:A:72:SER:O	1:A:73:ASN:OD1	0.41	2.39	16	1
1:A:90:GLU:N	1:A:90:GLU:CD	0.40	2.75	11	1
1:A:34:ARG:HG2	1:A:34:ARG:HH11	0.40	1.74	4	1
1:A:153:GLN:NE2	1:A:153:GLN:O	0.40	2.54	20	1
1:A:154:ASP:N	1:A:154:ASP:OD1	0.40	2.54	20	1
1:A:94:ARG:HG2	1:A:94:ARG:HH11	0.40	1.75	6	1
1:A:92:PHE:CD1	1:A:92:PHE:C	0.40	2.95	6	1
1:A:131:GLU:O	1:A:131:GLU:CD	0.40	2.60	18	1
1:A:115:TYR:CD2	1:A:119:LYS:NZ	0.40	2.88	7	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	140/192 (73%)	127±4 (91±3%)	11±3 (8±2%)	2±1 (1±1%)	19	64
All	All	2800/3840 (73%)	2548 (91%)	214 (8%)	38 (1%)	19	64

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	137	MET	10
1	A	166	GLY	6
1	A	136	ILE	4
1	A	165	PHE	3
1	A	88	PRO	3
1	A	188	TRP	3
1	A	83	VAL	2
1	A	16	SER	2
1	A	74	MET	2
1	A	73	ASN	1
1	A	72	SER	1
1	A	158	TRP	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	118/157 (75%)	107±3 (91±2%)	11±3 (9±2%)	16	61
All	All	2360/3140 (75%)	2146 (91%)	214 (9%)	16	61

All 74 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	109	ARG	11
1	A	127	THR	11
1	A	70	LEU	8
1	A	161	LEU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	188	TRP	7
1	A	94	ARG	7
1	A	125	LEU	6
1	A	65	ARG	6
1	A	144	LEU	6
1	A	162	LEU	6
1	A	59	LEU	5
1	A	147	ARG	5
1	A	149	LEU	5
1	A	181	LEU	5
1	A	121	VAL	5
1	A	78	ARG	5
1	A	99	MET	5
1	A	34	ARG	5
1	A	159	ASP	4
1	A	137	MET	4
1	A	122	LEU	3
1	A	69	GLU	3
1	A	73	ASN	3
1	A	58	LYS	3
1	A	15	SER	3
1	A	25	LEU	3
1	A	119	LYS	3
1	A	153	GLN	3
1	A	120	LEU	3
1	A	61	GLU	3
1	A	18	GLN	3
1	A	176	PHE	2
1	A	185	LEU	2
1	A	32	GLN	2
1	A	22	THR	2
1	A	110	VAL	2
1	A	62	CYS	2
1	A	165	PHE	2
1	A	89	ARG	2
1	A	27	LEU	2
1	A	113	LEU	2
1	A	74	MET	2
1	A	90	GLU	2
1	A	33	ASP	2
1	A	20	MET	2
1	A	75	GLU	2

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Mol	Chain	Res	Type	Models (Total)
1	A	171	GLN	1
1	A	71	ASP	1
1	A	56	THR	1
1	A	172	THR	1
1	A	64	LYS	1
1	A	128	LYS	1
1	A	76	LEU	1
1	A	83	VAL	1
1	A	148	LEU	1
1	A	131	GLU	1
1	A	154	ASP	1
1	A	145	ARG	1
1	A	17	GLU	1
1	A	126	CYS	1
1	A	180	VAL	1
1	A	28	GLN	1
1	A	123	LYS	1
1	A	186	THR	1
1	A	68	ASP	1
1	A	91	VAL	1
1	A	132	LEU	1
1	A	135	THR	1
1	A	187	ILE	1
1	A	93	PHE	1
1	A	57	LYS	1
1	A	79	MET	1
1	A	16	SER	1
1	A	155	GLN	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

No chemical shift data were provided