



# Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 12:04 am BST

PDB ID : 2MEJ  
Title : Solution Structure of the Complex Between BCL-xL and the p53 Core Domain determined with PRE restraints  
Authors : Viacava Follis, A.; Grace, C.R.; Kriwacki, R.W.  
Deposited on : 2013-09-25

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

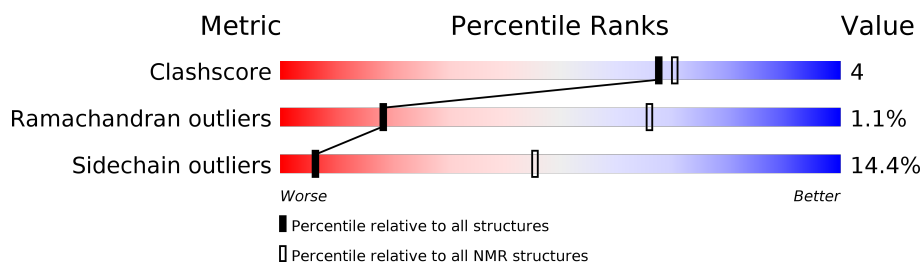
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 19%.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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

Mol	Chain	Length	Quality of chain
1	A	212	
2	B	217	

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:5-A:31, A:86-A:201, B:96-B:290 (338)	0.17	15

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 16 single-model clusters were found.

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

### 3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3336 atoms, of which 633 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Bcl-2-like protein 1.

Mol	Chain	Residues	Atoms						Trace
1	A	144	Total	C	H	N	O	S	0
			1426	746	258	197	220	5	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q07817
A	2	HIS	-	EXPRESSION TAG	UNP Q07817
A	3	SER	-	EXPRESSION TAG	UNP Q07817

- Molecule 2 is a protein called Cellular tumor antigen p53.

Mol	Chain	Residues	Atoms						Trace
2	B	195	Total	C	H	N	O	S	0
			1909	945	375	285	288	16	

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

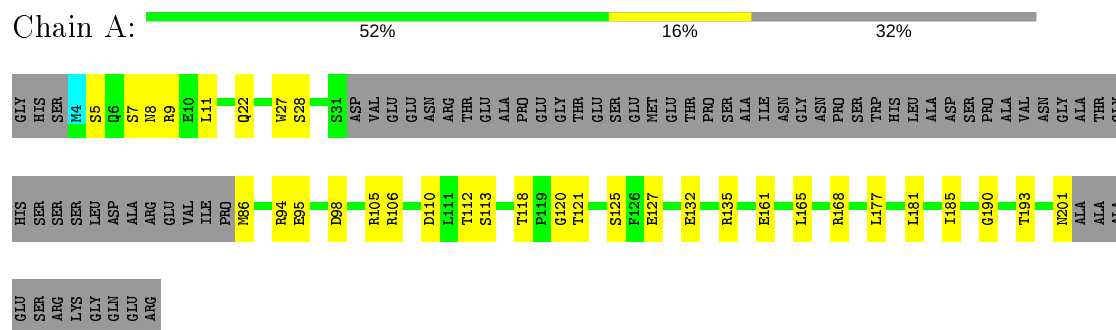
Mol	Chain	Residues	Atoms	
3	B	1	Total	Zn
			1	1

## 4 Residue-property plots [i](#)

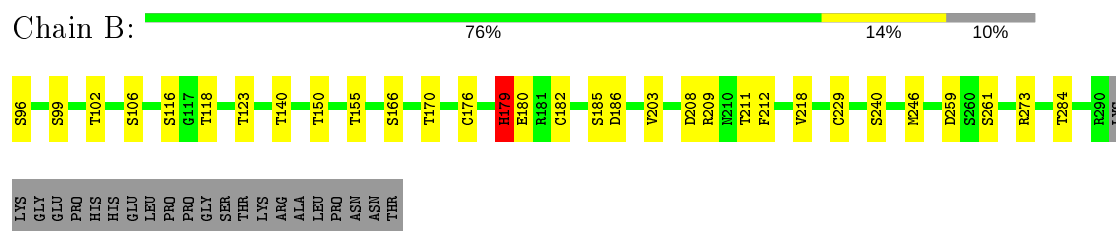
### 4.1 Average score per residue in the NMR ensemble

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: Bcl-2-like protein 1



- Molecule 2: Cellular tumor antigen p53



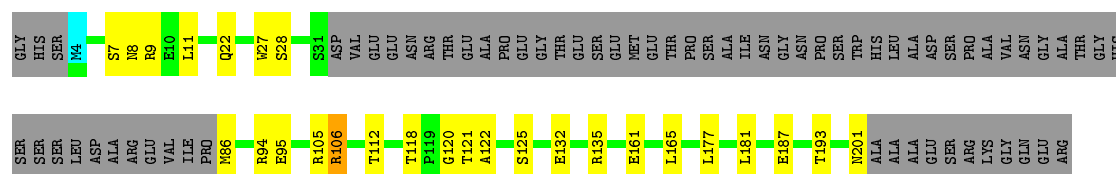
### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

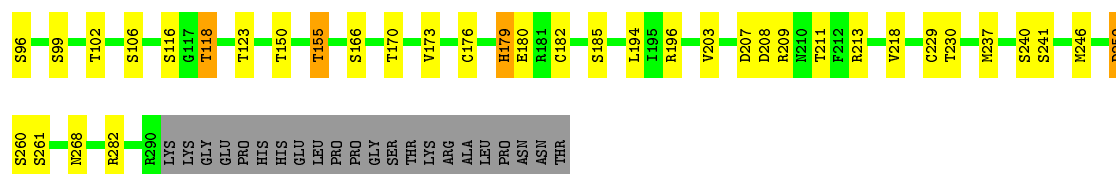
- Molecule 1: Bcl-2-like protein 1





### • Molecule 2: Cellular tumor antigen p53

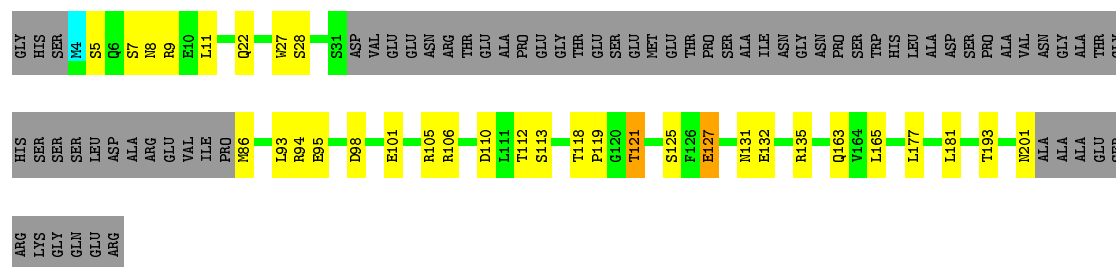
Chain B: 73% 15% 10%



## 4.2.2 Score per residue for model 2

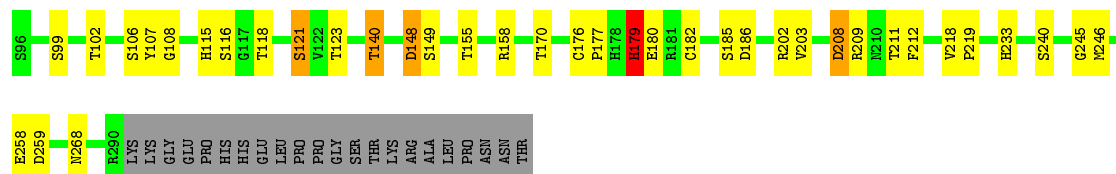
### • Molecule 1: Bcl-2-like protein 1

Chain A: 52% 15% 32%



### • Molecule 2: Cellular tumor antigen p53

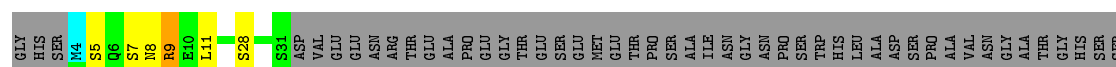
Chain B: 72% 15% 10%

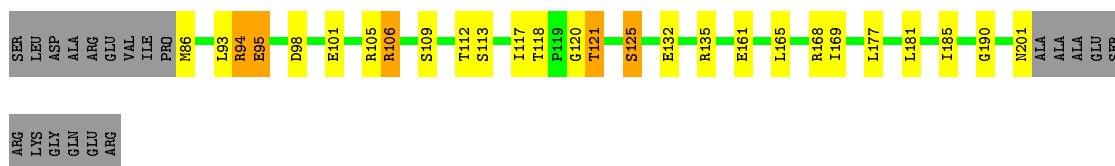


## 4.2.3 Score per residue for model 3

### • Molecule 1: Bcl-2-like protein 1

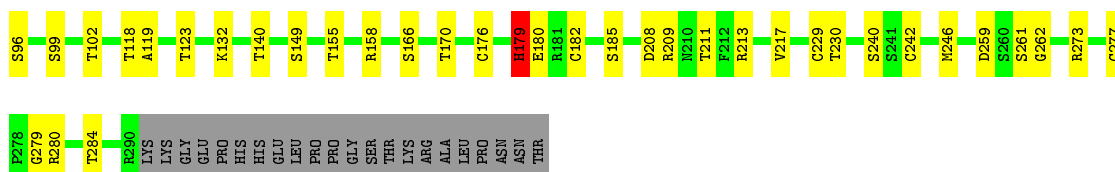
Chain A: 52% 13% 32%





- Molecule 2: Cellular tumor antigen p53

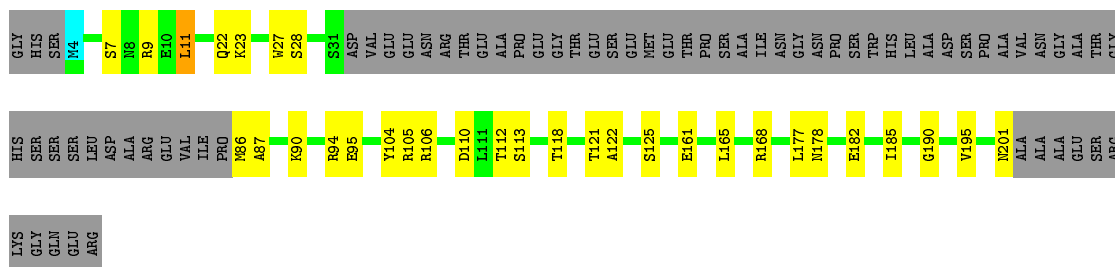
Chain B: 73% 16% 10%



#### 4.2.4 Score per residue for model 4

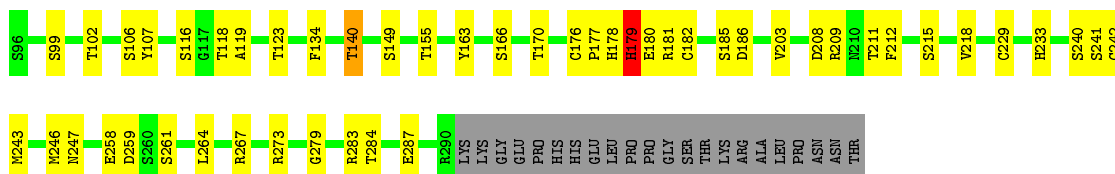
- Molecule 1: Bcl-2-like protein 1

Chain A: 52% 15% 32%



- Molecule 2: Cellular tumor antigen p53

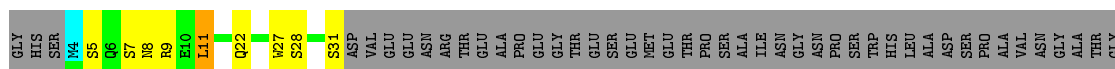
Chain B: 67% 22% 10%

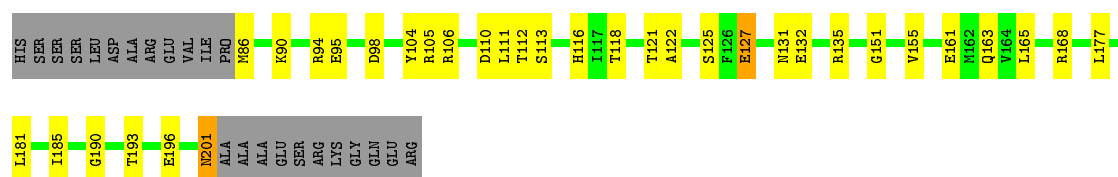


#### 4.2.5 Score per residue for model 5

- Molecule 1: Bcl-2-like protein 1

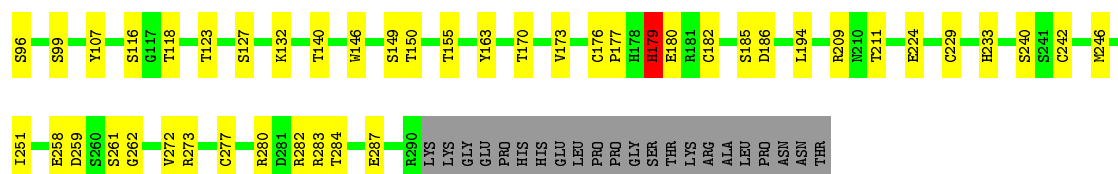
Chain A: 47% 19% 32%





- Molecule 2: Cellular tumor antigen p53

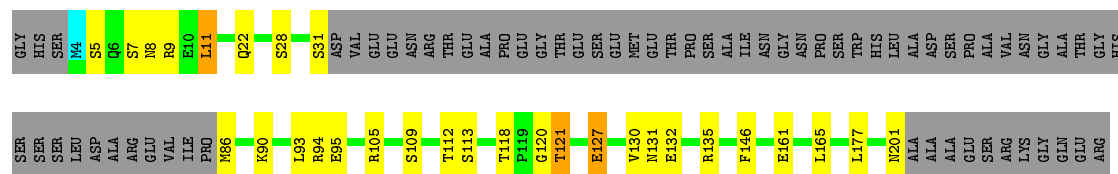
Chain B: 69% 20% 10%



#### 4.2.6 Score per residue for model 6

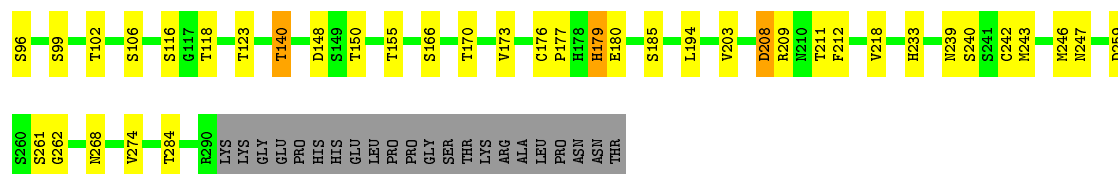
- Molecule 1: Bcl-2-like protein 1

Chain A: 53% 13% 32%



- Molecule 2: Cellular tumor antigen p53

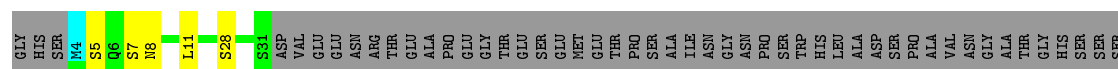
Chain B: 72% 17% 10%



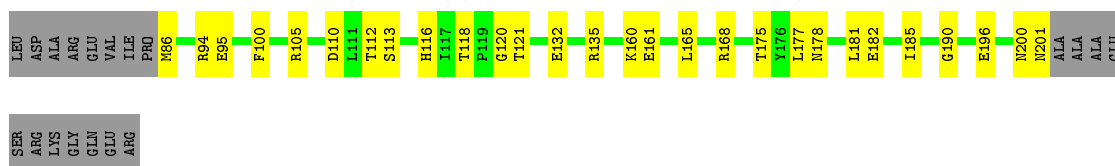
#### 4.2.7 Score per residue for model 7

- Molecule 1: Bcl-2-like protein 1

Chain A: 52% 16% 32%

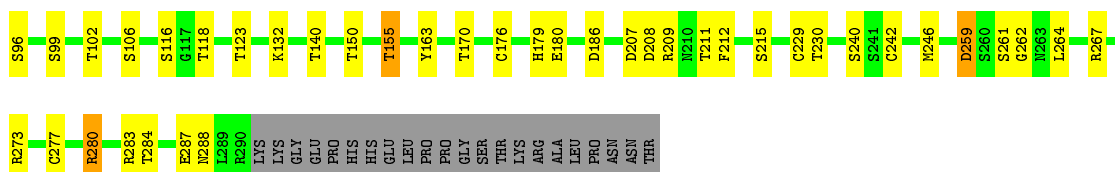






### • Molecule 2: Cellular tumor antigen p53

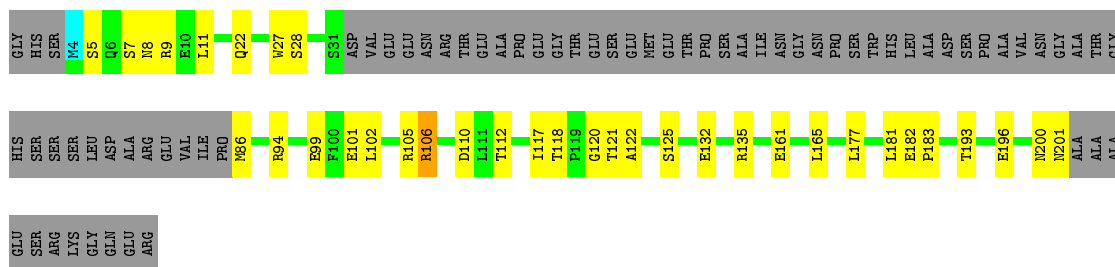
Chain B: 71% 17% 10%



## 4.2.8 Score per residue for model 8

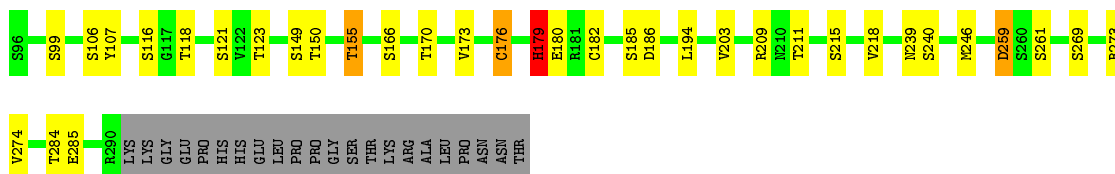
### • Molecule 1: Bcl-2-like protein 1

Chain A: 51% 16% 32%



### • Molecule 2: Cellular tumor antigen p53

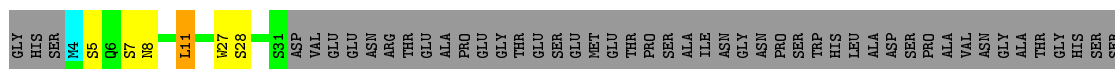
Chain B: 74% 14% 10%

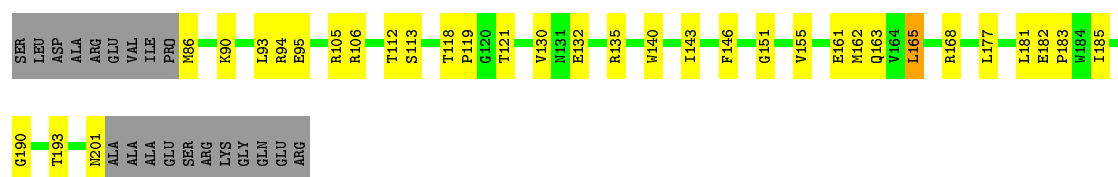


## 4.2.9 Score per residue for model 9

### • Molecule 1: Bcl-2-like protein 1

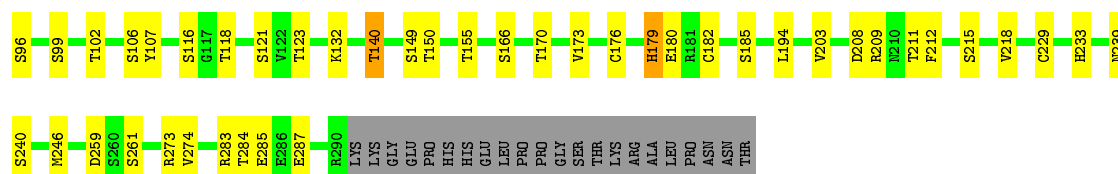
Chain A: 49% 17% 32%





#### • Molecule 2: Cellular tumor antigen p53

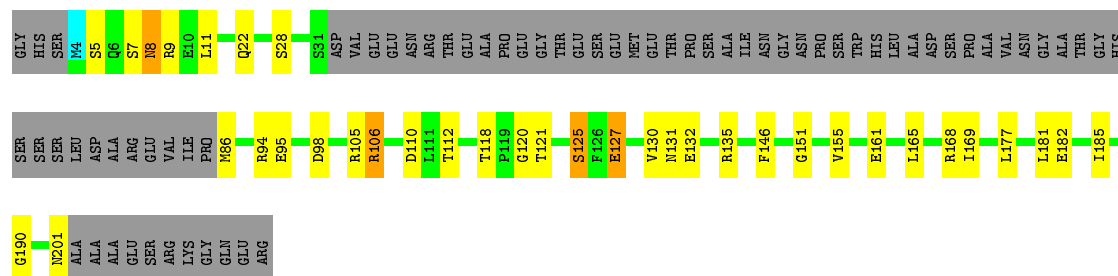
Chain B: 70% 19% 10%



### 4.2.10 Score per residue for model 10

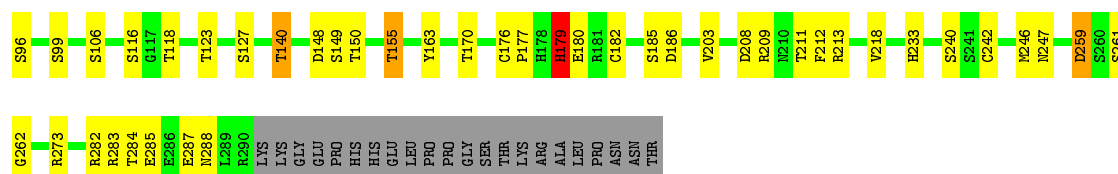
#### • Molecule 1: Bcl-2-like protein 1

Chain A: 50% 16% 32%



#### • Molecule 2: Cellular tumor antigen p53

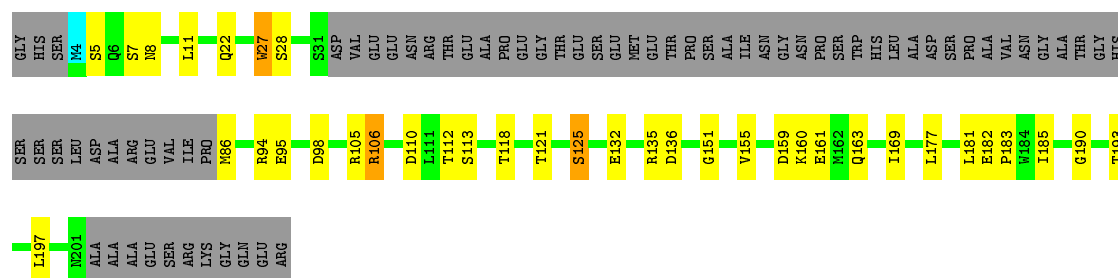
Chain B: 70% 18% 10%



### 4.2.11 Score per residue for model 11

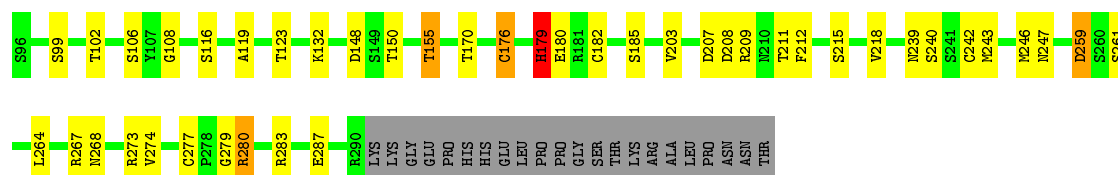
#### • Molecule 1: Bcl-2-like protein 1

Chain A: 50% 16% 32%



- Molecule 2: Cellular tumor antigen p53

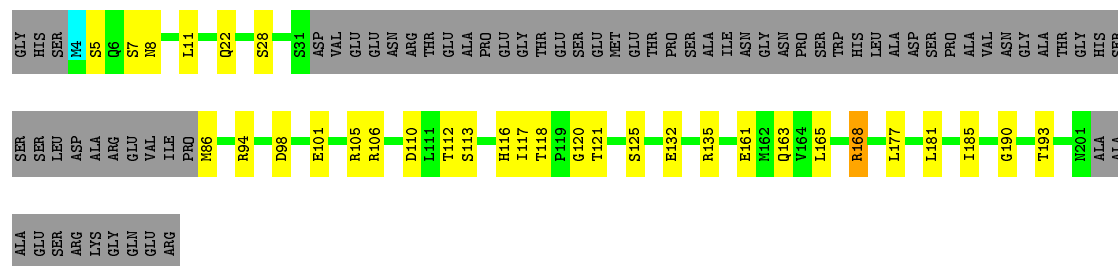
Chain B: 



#### 4.2.12 Score per residue for model 12

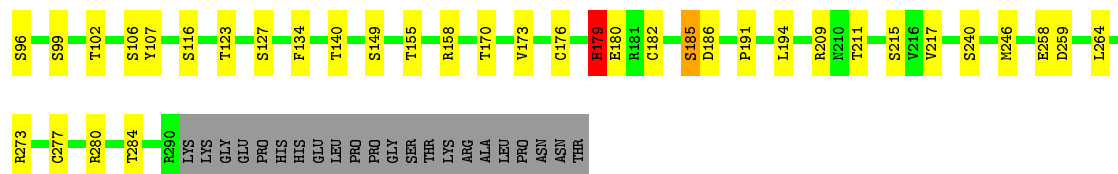
- Molecule 1: Bcl-2-like protein 1

Chain A: 



- Molecule 2: Cellular tumor antigen p53

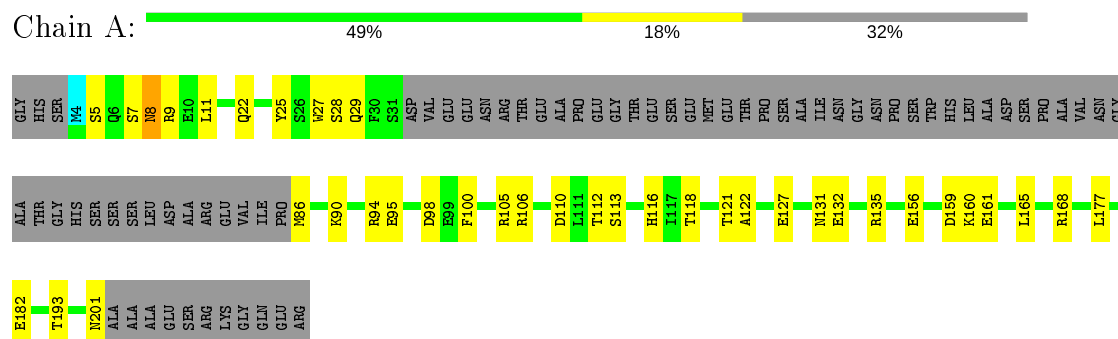
Chain B: 



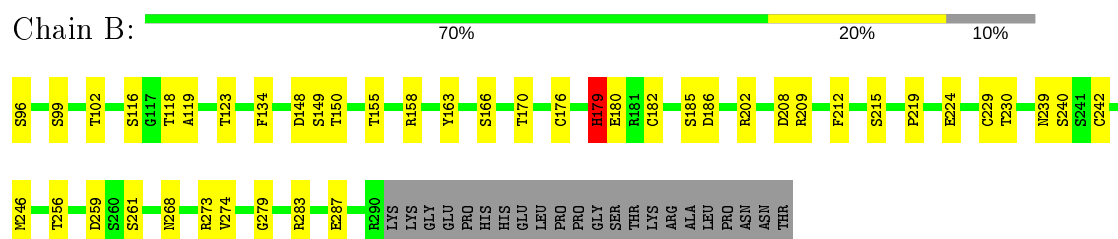
#### 4.2.13 Score per residue for model 13

- Molecule 1: Bcl-2-like protein 1



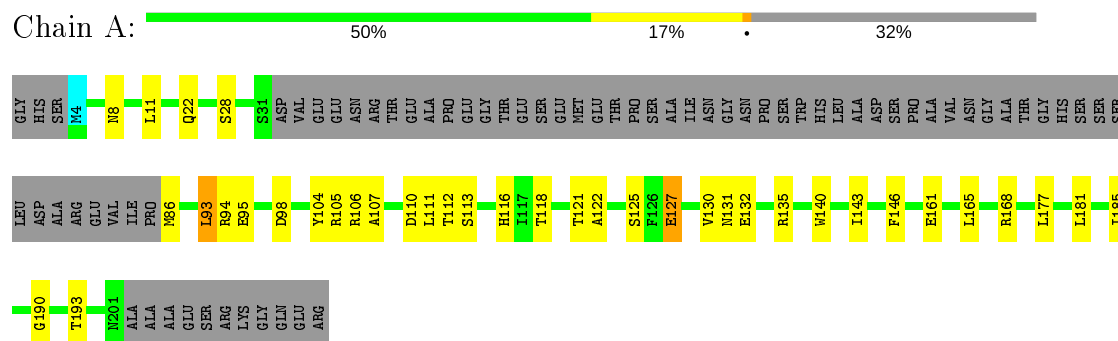


- Molecule 2: Cellular tumor antigen p53

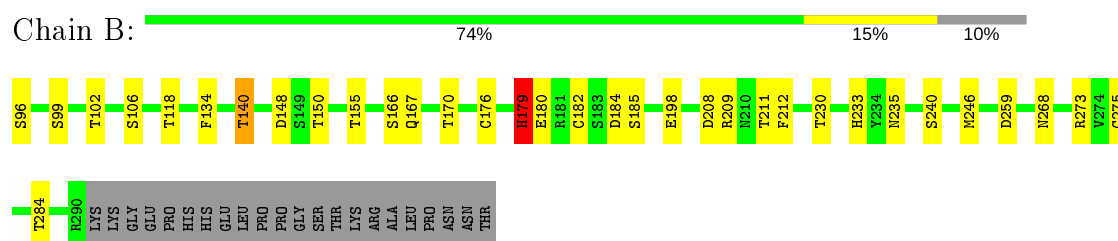


#### 4.2.16 Score per residue for model 16

- Molecule 1: Bcl-2-like protein 1

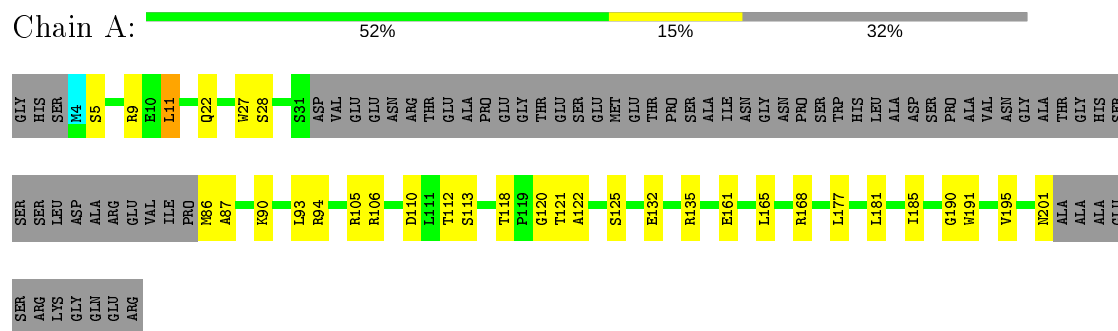


- Molecule 2: Cellular tumor antigen p53

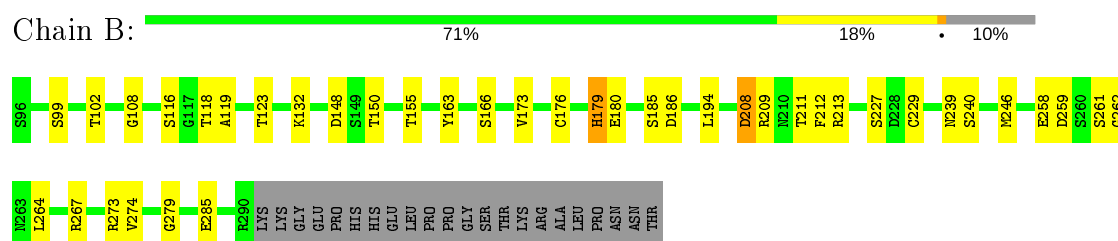


## 4.2.17 Score per residue for model 17

- Molecule 1: Bcl-2-like protein 1

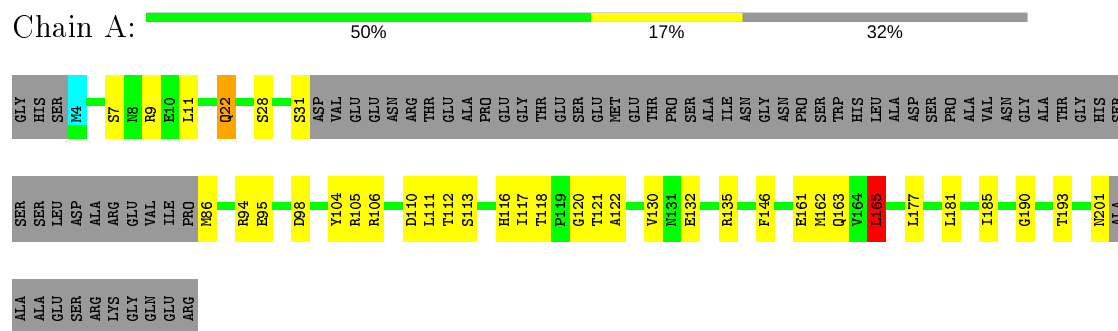


- Molecule 2: Cellular tumor antigen p53

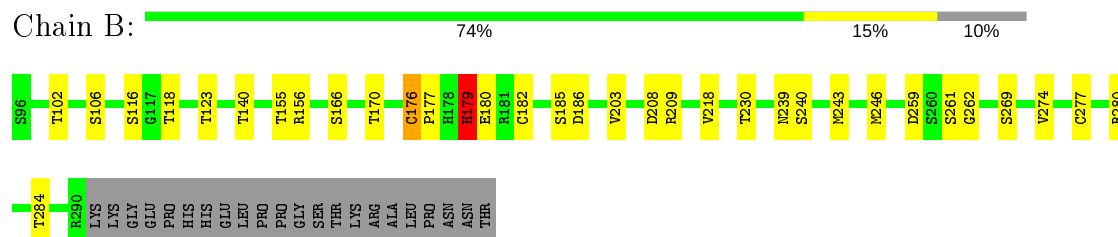


## 4.2.18 Score per residue for model 18

- Molecule 1: Bcl-2-like protein 1

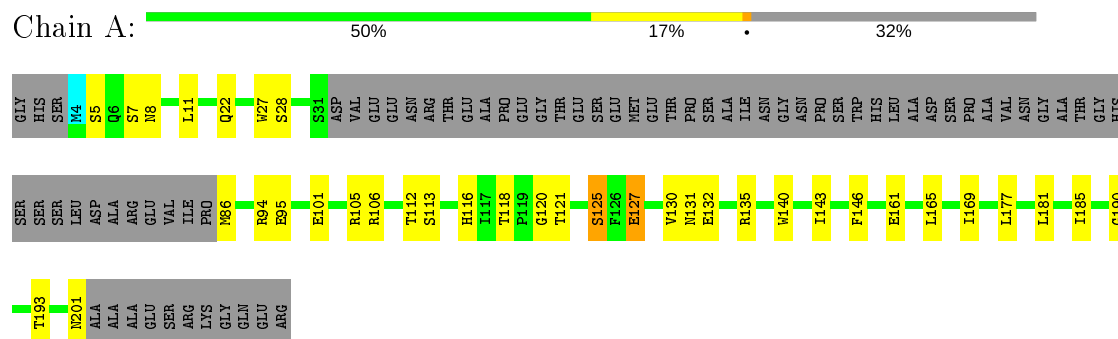


- Molecule 2: Cellular tumor antigen p53

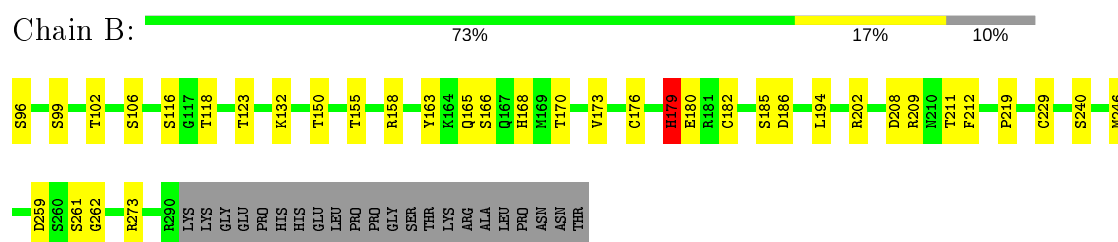


## 4.2.19 Score per residue for model 19

- Molecule 1: Bcl-2-like protein 1

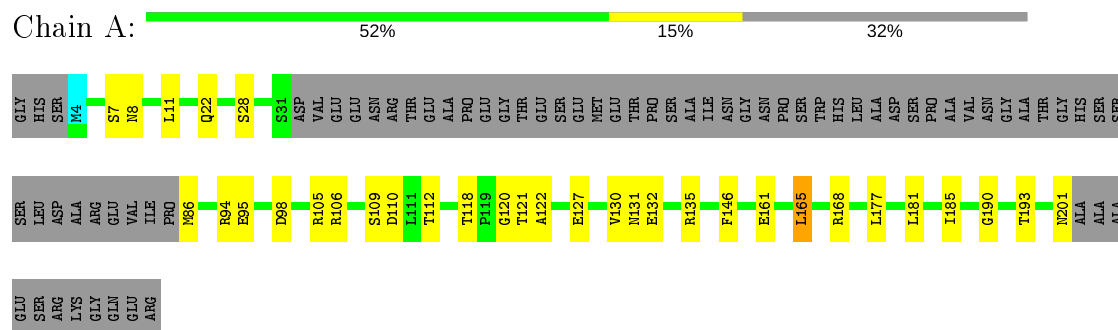


- Molecule 2: Cellular tumor antigen p53

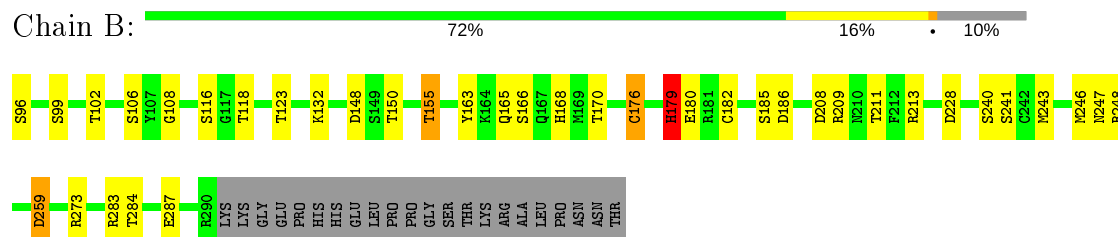


## 4.2.20 Score per residue for model 20

- Molecule 1: Bcl-2-like protein 1



- Molecule 2: Cellular tumor antigen p53



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
HADDOCK	structure solution	
AMBER	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1254
Number of shifts mapped to atoms	1254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	19%

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

COVALENT-GEOMETRY INFOmissingINFO

### 5.1 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	1160	257	1097	9±2
2	B	1534	375	1496	13±3
3	B	1	0	0	1±1
All	All	53900	12640	51848	414

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 4.



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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:176:CYS:SG	3:B:401:ZN:ZN	1.44	1.03	20	19
2:B:176:CYS:HG	3:B:401:ZN:ZN	0.94	0.72	8	8
2:B:240:SER:HA	2:B:246:MET:SD	0.77	2.20	14	20
2:B:155:THR:HG22	2:B:259:ASP:HA	0.73	1.58	20	6
1:A:132:GLU:HA	1:A:135:ARG:HD2	0.71	1.62	1	18
2:B:132:LYS:HE2	2:B:273:ARG:HB2	0.69	1.65	14	10
2:B:283:ARG:HA	2:B:287:GLU:HB3	0.69	1.65	11	7
2:B:243:MET:HA	2:B:247:ASN:HA	0.69	1.63	6	3
1:A:177:LEU:HA	1:A:181:LEU:HB2	0.68	1.66	2	12
2:B:176:CYS:SG	2:B:179:HIS:HB2	0.68	2.28	15	1
1:A:11:LEU:HD11	1:A:93:LEU:HG	0.67	1.67	3	3
2:B:176:CYS:HB3	2:B:242:CYS:HB3	0.66	1.67	15	6
2:B:140:THR:HG22	2:B:233:HIS:HB3	0.62	1.70	14	7
1:A:168:ARG:HE	1:A:168:ARG:HA	0.61	1.56	5	6
2:B:107:TYR:HA	2:B:149:SER:HB2	0.59	1.74	12	6
1:A:168:ARG:NE	1:A:168:ARG:HA	0.58	2.13	17	8
2:B:163:TYR:HE2	2:B:246:MET:HA	0.58	1.59	10	7
1:A:121:THR:HB	1:A:165:LEU:HG	0.57	1.77	20	1
1:A:177:LEU:HD12	1:A:181:LEU:HB2	0.56	1.77	5	6
1:A:185:ILE:HG23	1:A:190:GLY:HA3	0.56	1.77	5	14
2:B:208:ASP:HB3	2:B:213:ARG:HB2	0.56	1.75	10	5
1:A:130:VAL:HA	1:A:146:PHE:HE1	0.56	1.60	6	8
2:B:239:ASN:HA	2:B:274:VAL:HB	0.56	1.78	17	7
2:B:283:ARG:HA	2:B:287:GLU:CB	0.55	2.31	11	9
2:B:273:ARG:HG2	2:B:275:CYS:SG	0.55	2.42	16	1
1:A:9:ARG:HA	1:A:177:LEU:HD21	0.55	1.78	18	8
2:B:108:GLY:HA3	2:B:148:ASP:HB2	0.55	1.78	2	5
1:A:9:ARG:HG2	1:A:177:LEU:HD23	0.55	1.79	5	4
2:B:203:VAL:HA	2:B:218:VAL:HG12	0.54	1.79	9	11
1:A:168:ARG:HA	1:A:168:ARG:HE	0.54	1.61	4	3
2:B:134:PHE:CE2	2:B:273:ARG:HD3	0.53	2.38	12	4
2:B:185:SER:HB3	2:B:191:PRO:HD3	0.53	1.80	12	1
1:A:125:SER:HB2	1:A:169:ILE:HD11	0.53	1.81	19	4
1:A:196:GLU:HA	1:A:200:ASN:HB3	0.52	1.80	13	3
1:A:182:GLU:HB2	1:A:183:PRO:HD3	0.52	1.80	13	4
1:A:9:ARG:HA	1:A:177:LEU:CD2	0.52	2.35	1	3
2:B:208:ASP:O	2:B:212:PHE:HA	0.52	2.05	2	13
2:B:119:ALA:O	2:B:279:GLY:HA3	0.52	2.04	13	6
2:B:173:VAL:HG12	2:B:194:LEU:HD13	0.51	1.81	8	8
1:A:168:ARG:HA	1:A:168:ARG:NE	0.51	2.19	20	4
1:A:127:GLU:O	1:A:131:ASN:HB2	0.51	2.05	19	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:104:TYR:CE2	1:A:110:ASP:HB2	0.51	2.40	18	1
2:B:179:HIS:HA	2:B:182:CYS:SG	0.51	2.46	18	15
2:B:158:ARG:HG2	2:B:217:VAL:HB	0.50	1.83	12	2
1:A:161:GLU:HG3	2:B:243:MET:HB2	0.50	1.81	11	1
2:B:273:ARG:HD2	2:B:285:GLU:OE2	0.50	2.07	9	4
2:B:163:TYR:HE1	2:B:246:MET:HA	0.49	1.66	5	2
1:A:178:ASN:HA	1:A:182:GLU:HG3	0.49	1.82	4	2
1:A:26:SER:HB3	2:B:243:MET:SD	0.49	2.48	13	1
2:B:264:LEU:HD11	2:B:267:ARG:HB2	0.49	1.85	13	5
1:A:159:ASP:OD2	2:B:176:CYS:SG	0.48	2.60	15	1
2:B:198:GLU:HB2	2:B:235:ASN:OD1	0.48	2.09	16	2
2:B:176:CYS:HB2	2:B:177:PRO:HD2	0.48	1.84	6	5
1:A:99:GLU:O	1:A:102:LEU:HG	0.48	2.09	8	1
2:B:202:ARG:HD2	2:B:219:PRO:HG2	0.48	1.85	15	3
1:A:23:LYS:HB3	2:B:178:HIS:HB2	0.48	1.85	4	1
1:A:11:LEU:HD11	1:A:90:LYS:HA	0.48	1.86	9	7
1:A:119:PRO:HG3	2:B:121:SER:HA	0.47	1.87	9	2
2:B:241:SER:HA	2:B:248:ARG:HA	0.47	1.87	20	1
1:A:22:GLN:NE2	2:B:181:ARG:HH22	0.46	2.08	4	1
2:B:258:GLU:HG3	2:B:264:LEU:HA	0.46	1.86	12	1
2:B:277:CYS:HB2	2:B:280:ARG:HB3	0.46	1.88	18	6
1:A:106:ARG:HA	2:B:182:CYS:O	0.46	2.10	1	5
2:B:140:THR:CG2	2:B:233:HIS:HB3	0.46	2.40	6	7
1:A:104:TYR:HE1	1:A:110:ASP:HB2	0.46	1.71	14	2
1:A:161:GLU:HB2	2:B:241:SER:O	0.45	2.11	1	4
1:A:140:TRP:O	1:A:143:ILE:HG22	0.45	2.11	9	3
2:B:251:ILE:HG13	2:B:272:VAL:HB	0.44	1.89	5	2
1:A:8:ASN:HB2	1:A:182:GLU:HG2	0.43	1.90	15	4
2:B:127:SER:HA	2:B:282:ARG:NH2	0.43	2.29	5	2
1:A:156:GLU:HG3	1:A:160:LYS:HE3	0.42	1.91	15	1
1:A:107:ALA:HB3	2:B:184:ASP:HB3	0.42	1.90	16	1
1:A:25:TYR:CD2	1:A:29:GLN:HB2	0.42	2.49	15	1
2:B:163:TYR:CE1	2:B:246:MET:HA	0.42	2.49	5	1
1:A:160:LYS:HA	2:B:242:CYS:HA	0.42	1.92	11	2
2:B:165:GLN:HB2	2:B:168:HIS:HB2	0.42	1.90	19	2
1:A:104:TYR:CE1	1:A:110:ASP:HB2	0.42	2.50	14	1
2:B:158:ARG:HB3	2:B:256:THR:CG2	0.42	2.45	15	1
2:B:166:SER:HA	2:B:169:MET:SD	0.42	2.55	14	1
2:B:146:TRP:HA	2:B:229:CYS:SG	0.42	2.55	5	1
2:B:196:ARG:NH1	2:B:237:MET:HG3	0.41	2.30	1	1
1:A:196:GLU:O	1:A:201:ASN:HB2	0.41	2.15	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:ARG:HD3	1:A:95:GLU:OE1	0.41	2.15	3	1
1:A:162:MET:SD	1:A:165:LEU:HD12	0.41	2.55	9	2
2:B:239:ASN:HD22	2:B:274:VAL:HG12	0.41	1.75	15	1
1:A:27:TRP:CH2	1:A:163:GLN:HA	0.41	2.49	11	1
1:A:87:ALA:HB1	1:A:195:VAL:HG21	0.41	1.93	4	1
1:A:104:TYR:HD2	1:A:111:LEU:HB2	0.41	1.74	16	2
2:B:177:PRO:HD3	2:B:243:MET:O	0.41	2.15	18	1
1:A:151:GLY:O	1:A:155:VAL:HG23	0.41	2.15	9	4
1:A:191:TRP:O	1:A:195:VAL:HG23	0.40	2.15	17	1
1:A:87:ALA:O	1:A:195:VAL:HG11	0.40	2.15	17	1
1:A:159:ASP:OD1	2:B:176:CYS:HB2	0.40	2.16	11	1
2:B:118:THR:HG23	2:B:282:ARG:HD3	0.40	1.94	1	1
2:B:158:ARG:HB3	2:B:256:THR:HG23	0.40	1.92	15	1

## 5.2 Torsion angles ⓘ

### 5.2.1 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	140/212 (66%)	122±2 (87±1%)	16±3 (11±2%)	2±1 (2±1%)	14	59
2	B	193/217 (89%)	181±2 (94±1%)	11±2 (5±1%)	1±1 (1±0%)	26	73
All	All	6660/8580 (78%)	6057 (91%)	533 (8%)	70 (1%)	18	66

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	179	HIS	18
1	A	120	GLY	13
1	A	122	ALA	10
2	B	262	GLY	8
1	A	163	GLN	5
1	A	22	GLN	5
1	A	117	ILE	4
1	A	121	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	165	LEU	2
1	A	187	GLU	1
2	B	245	GLY	1

### 5.2.2 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	122/176 (69%)	101±2 (83±2%)	21±2 (17±2%)	5	40
2	B	175/194 (90%)	153±2 (87±1%)	22±2 (13±1%)	8	50
All	All	5940/7400 (80%)	5086 (86%)	854 (14%)	6	45

All 84 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)
2	B	259	ASP	20
2	B	179	HIS	20
2	B	180	GLU	20
2	B	155	THR	20
1	A	118	THR	20
1	A	28	SER	20
2	B	209	ARG	20
1	A	105	ARG	20
1	A	94	ARG	19
1	A	86	MET	19
1	A	121	THR	19
1	A	112	THR	19
2	B	170	THR	19
2	B	116	SER	18
2	B	123	THR	18
2	B	211	THR	18
1	A	165	LEU	18
2	B	185	SER	18
2	B	99	SER	18
2	B	118	THR	18
1	A	7	SER	18

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Mol	Chain	Res	Type	Models (Total)
1	A	11	LEU	17
1	A	95	GLU	17
2	B	102	THR	17
1	A	106	ARG	17
2	B	261	SER	16
1	A	201	ASN	16
1	A	113	SER	16
2	B	106	SER	16
2	B	150	THR	15
1	A	8	ASN	15
2	B	186	ASP	14
1	A	193	THR	14
2	B	166	SER	14
1	A	125	SER	14
2	B	284	THR	14
2	B	96	SER	14
1	A	161	GLU	14
1	A	5	SER	14
1	A	110	ASP	12
2	B	140	THR	12
1	A	98	ASP	11
1	A	27	TRP	11
1	A	22	GLN	11
2	B	229	CYS	10
1	A	116	HIS	8
2	B	215	SER	8
2	B	268	ASN	7
1	A	127	GLU	6
2	B	230	THR	6
1	A	93	LEU	5
2	B	176	CYS	5
2	B	148	ASP	5
1	A	101	GLU	5
2	B	208	ASP	5
2	B	121	SER	4
2	B	288	ASN	4
2	B	258	GLU	4
1	A	31	SER	3
1	A	109	SER	3
2	B	149	SER	3
2	B	207	ASP	3
2	B	260	SER	2

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Mol	Chain	Res	Type	Models (Total)
2	B	269	SER	2
2	B	158	ARG	2
1	A	100	PHE	2
1	A	168	ARG	2
2	B	247	ASN	2
2	B	224	GLU	2
2	B	280	ARG	2
1	A	175	THR	1
2	B	227	SER	1
2	B	127	SER	1
1	A	90	LYS	1
2	B	228	ASP	1
1	A	111	LEU	1
1	A	9	ARG	1
2	B	156	ARG	1
2	B	241	SER	1
1	A	176	TYR	1
2	B	115	HIS	1
2	B	167	GLN	1
1	A	197	LEU	1
1	A	136	ASP	1

### 5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.5 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

## 5.6 Other polymers [i](#)

There are no such molecules in this entry.

## 5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 19% for the well-defined parts and 19% for the entire structure.

### 6.1 Chemical shift list 1

File name: input\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 6.1.1 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	1254
Number of shifts mapped to atoms	1254
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

#### 6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	203	$0.13 \pm 0.25$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	188	$1.75 \pm 0.09$	Should be applied
$^{13}\text{C}'$	192	$-0.15 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	203	$1.05 \pm 0.27$	Should be applied

#### 6.1.3 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 19%, i.e. 810 atoms were assigned a chemical shift out of a possible 4189. 25 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	561/1658 (34%)	141/660 (21%)	279/676 (41%)	141/322 (44%)
Sidechain	239/2149 (11%)	54/1269 (4%)	185/761 (24%)	0/119 (0%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	10/382 (3%)	5/203 (2%)	0/164 (0%)	5/15 (33%)
Overall	810/4189 (19%)	200/2132 (9%)	464/1601 (29%)	146/456 (32%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 19%, i.e. 815 atoms were assigned a chemical shift out of a possible 4202. 25 out of 54 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	565/1663 (34%)	142/662 (21%)	281/678 (41%)	142/323 (44%)
Sidechain	240/2157 (11%)	54/1274 (4%)	186/764 (24%)	0/119 (0%)
Aromatic	10/382 (3%)	5/203 (2%)	0/164 (0%)	5/15 (33%)
Overall	815/4202 (19%)	201/2139 (9%)	467/1606 (29%)	147/457 (32%)

#### 6.1.4 Statistically unusual chemical shifts ⓘ

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	138	VAL	HG23	-0.75	2.20 – -0.60	-5.5
1	A	138	VAL	HG22	-0.75	2.20 – -0.60	-5.5
1	A	138	VAL	HG21	-0.75	2.20 – -0.60	-5.5

#### 6.1.5 Random Coil Index (RCI) plots ⓘ

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:

