



Full wwPDB NMR Structure Validation Report ⓘ

Feb 17, 2018 – 09:00 pm GMT

PDB ID : 2M03
Title : Solution structure of BCL-xL determined with selective isotope labelling of I,L,V sidechains
Authors : Viacava Follis, A.; Royappa, G.; Kriwacki, R.W.
Deposited on : 2012-10-19

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk30686
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

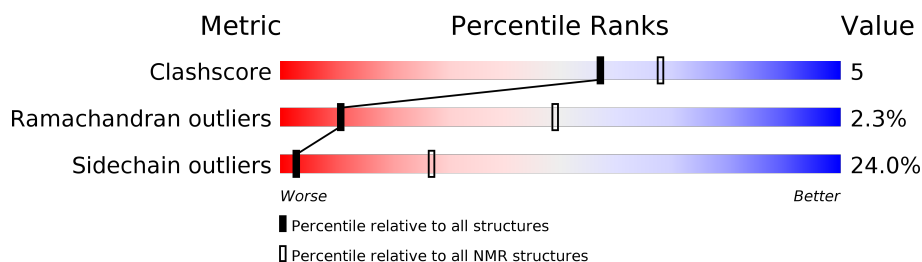
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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	136279	12091
Ramachandran outliers	132675	10835
Sidechain outliers	132484	10811

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

Mol	Chain	Length	Quality of chain
1	A	181	

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

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:26, A:47-A:78, A:83-A:159 (131)	0.78	1

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2764 atoms, of which 1338 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	177	Total	C	H	N	O	S	0
			2764	894	1338	246	280	6	

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q07817
A	2	SER	-	EXPRESSION TAG	UNP Q07817
A	3	MET	-	EXPRESSION TAG	UNP Q07817
A	4	ALA	-	EXPRESSION TAG	UNP Q07817
A	?	-	MET	DELETION	UNP Q07817
A	?	-	GLU	DELETION	UNP Q07817
A	?	-	THR	DELETION	UNP Q07817
A	?	-	PRO	DELETION	UNP Q07817
A	?	-	SER	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	?	-	ILE	DELETION	UNP Q07817
A	?	-	ASN	DELETION	UNP Q07817
A	?	-	GLY	DELETION	UNP Q07817
A	?	-	ASN	DELETION	UNP Q07817
A	?	-	PRO	DELETION	UNP Q07817
A	?	-	SER	DELETION	UNP Q07817
A	?	-	TRP	DELETION	UNP Q07817
A	?	-	HIS	DELETION	UNP Q07817
A	?	-	LEU	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	?	-	ASP	DELETION	UNP Q07817
A	?	-	SER	DELETION	UNP Q07817
A	?	-	PRO	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	?	-	VAL	DELETION	UNP Q07817
A	?	-	ASN	DELETION	UNP Q07817
A	?	-	GLY	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	?	-	THR	DELETION	UNP Q07817
A	?	-	GLY	DELETION	UNP Q07817
A	?	-	HIS	DELETION	UNP Q07817

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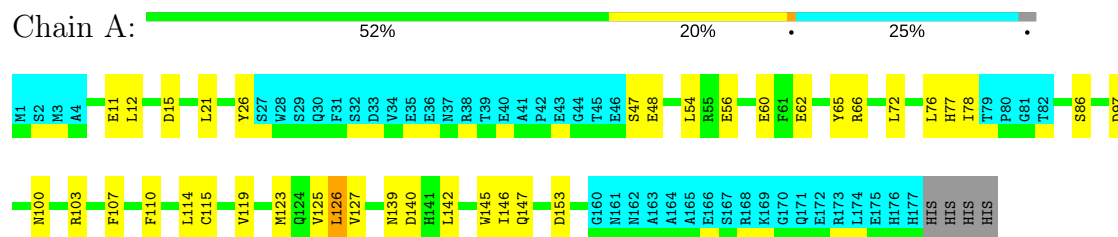
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	DELETION	UNP Q07817
A	?	-	SER	DELETION	UNP Q07817
A	?	-	SER	DELETION	UNP Q07817
A	?	-	LEU	DELETION	UNP Q07817
A	?	-	ASP	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	?	-	ARG	DELETION	UNP Q07817
A	?	-	GLU	DELETION	UNP Q07817
A	?	-	VAL	DELETION	UNP Q07817
A	?	-	ILE	DELETION	UNP Q07817
A	?	-	PRO	DELETION	UNP Q07817
A	?	-	MET	DELETION	UNP Q07817
A	?	-	ALA	DELETION	UNP Q07817
A	174	LEU	-	EXPRESSION TAG	UNP Q07817
A	175	GLU	-	EXPRESSION TAG	UNP Q07817
A	176	HIS	-	EXPRESSION TAG	UNP Q07817
A	177	HIS	-	EXPRESSION TAG	UNP Q07817
A	178	HIS	-	EXPRESSION TAG	UNP Q07817
A	179	HIS	-	EXPRESSION TAG	UNP Q07817
A	180	HIS	-	EXPRESSION TAG	UNP Q07817
A	181	HIS	-	EXPRESSION TAG	UNP Q07817

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: Bcl-2-like protein 1

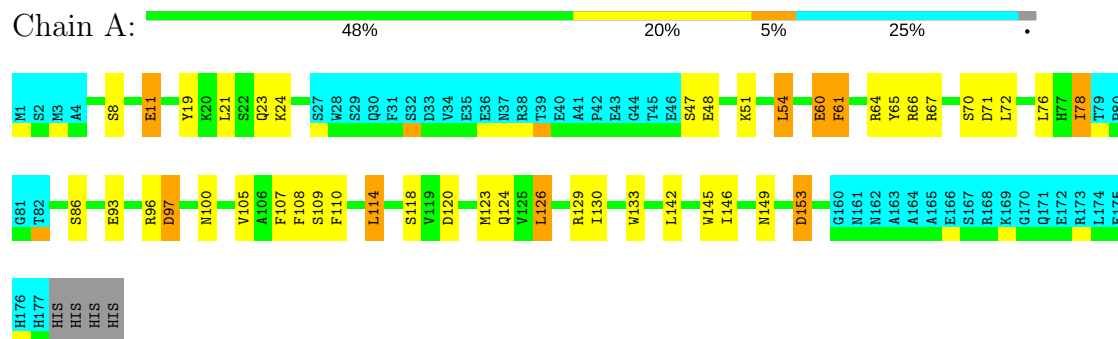


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Bcl-2-like protein 1



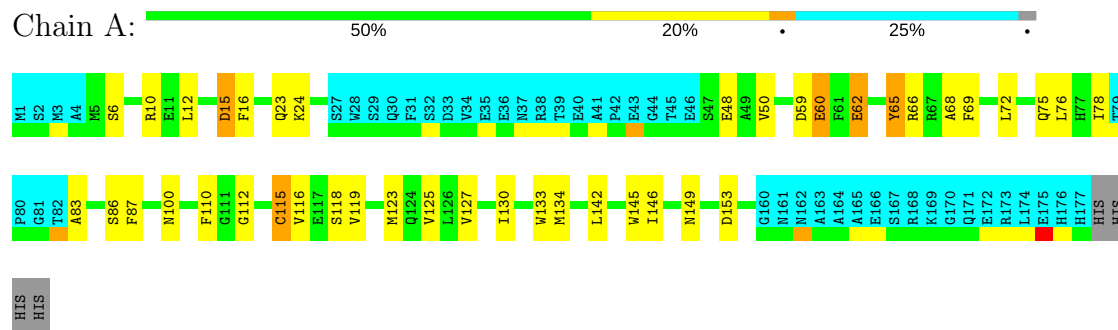
4.2.2 Score per residue for model 2

- Molecule 1: Bcl-2-like protein 1



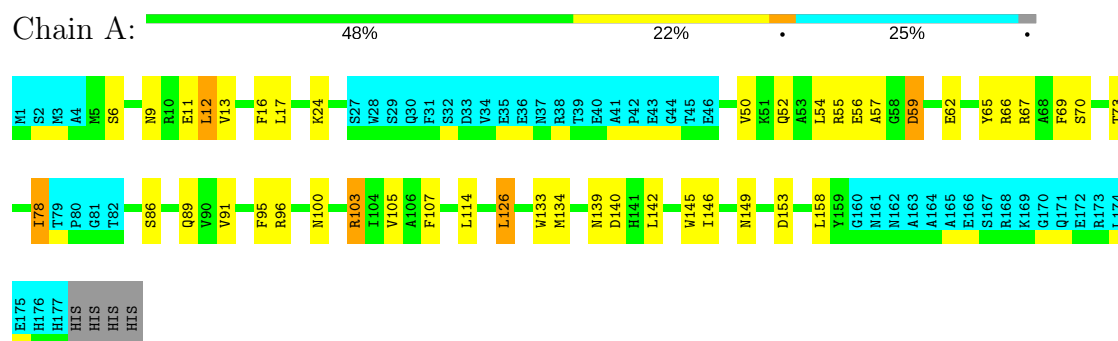
4.2.6 Score per residue for model 6

- Molecule 1: Bcl-2-like protein 1



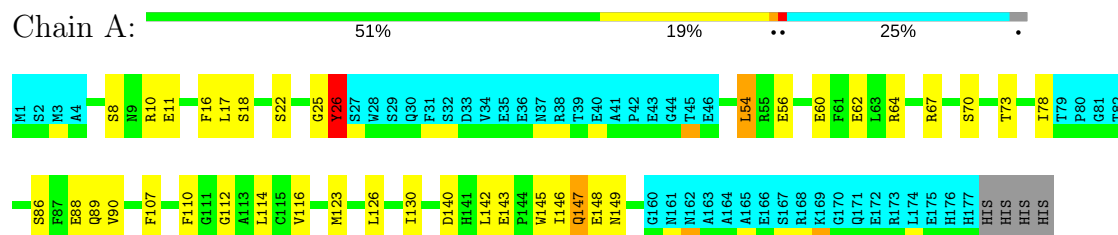
4.2.7 Score per residue for model 7

- Molecule 1: Bcl-2-like protein 1



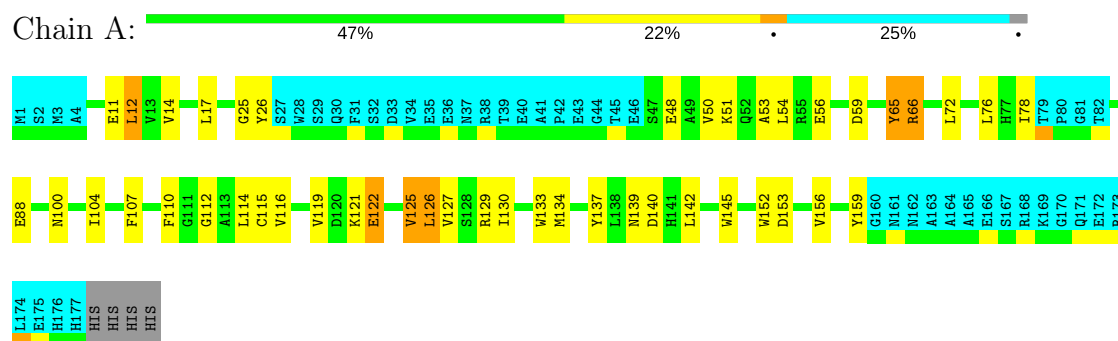
4.2.8 Score per residue for model 8

- Molecule 1: Bcl-2-like protein 1



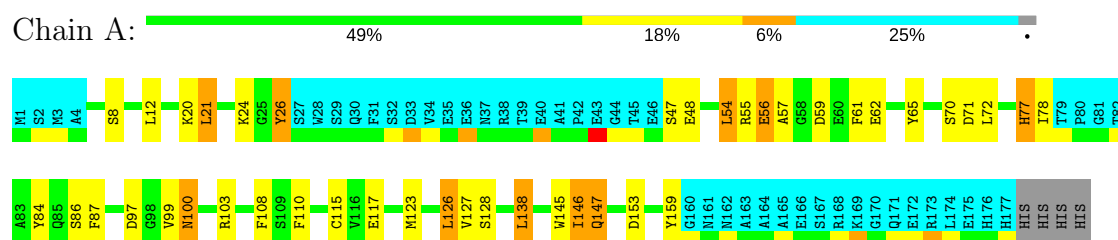
4.2.9 Score per residue for model 9

- Molecule 1: Bcl-2-like protein 1



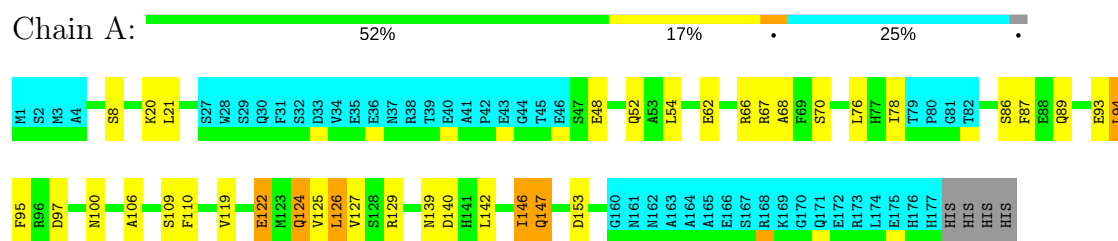
4.2.10 Score per residue for model 10

- Molecule 1: Bcl-2-like protein 1



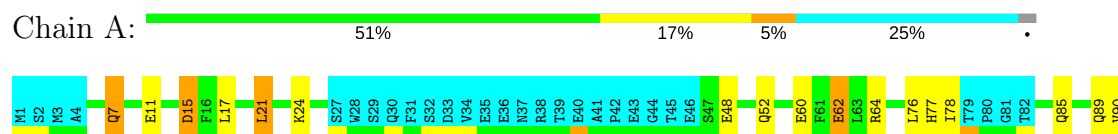
4.2.11 Score per residue for model 11

- Molecule 1: Bcl-2-like protein 1



4.2.12 Score per residue for model 12

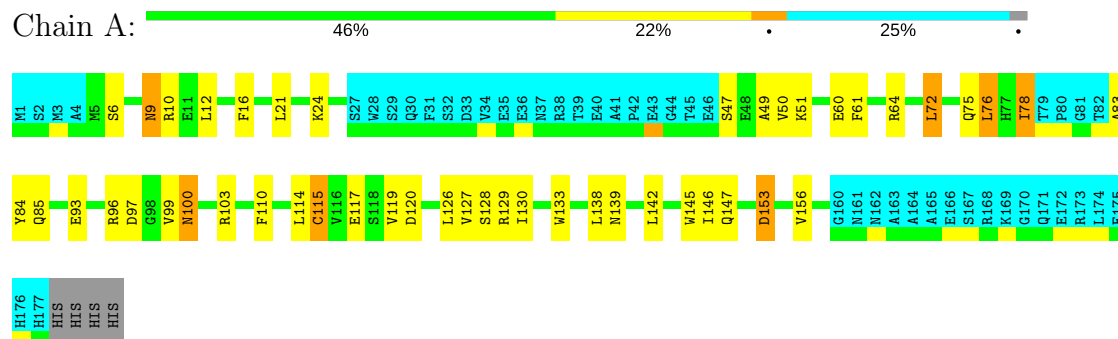
- Molecule 1: Bcl-2-like protein 1





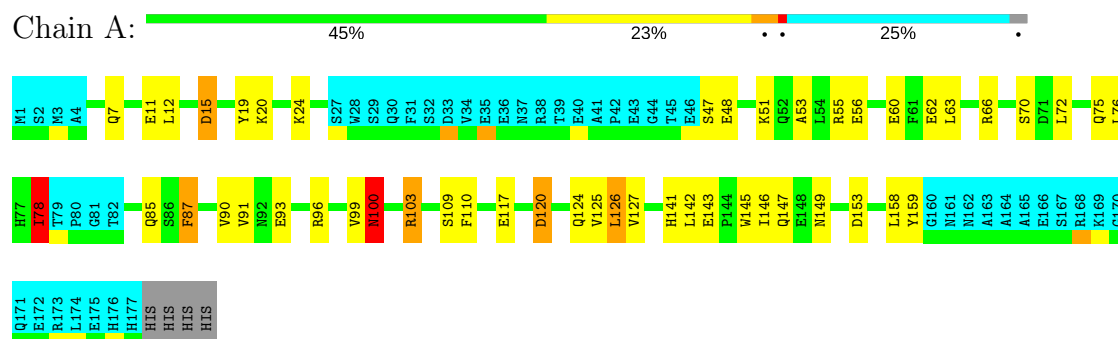
4.2.13 Score per residue for model 13

- Molecule 1: Bcl-2-like protein 1



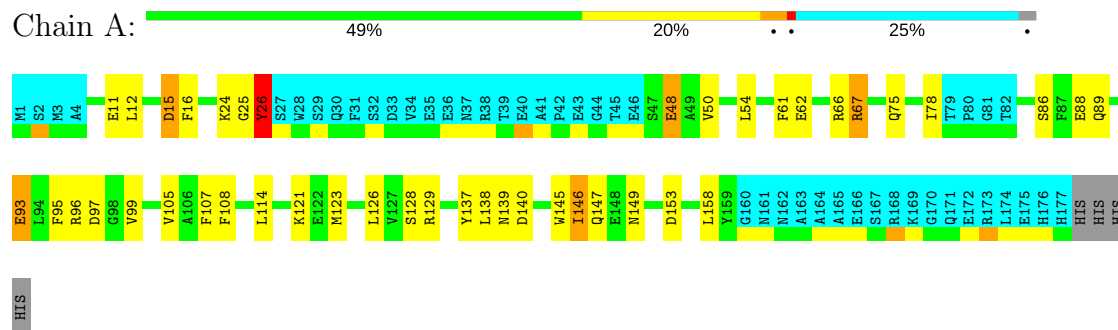
4.2.14 Score per residue for model 14

- Molecule 1: Bcl-2-like protein 1



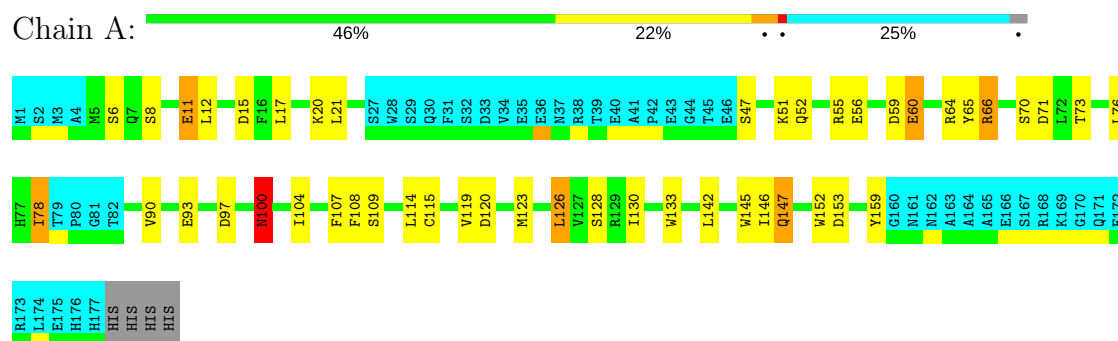
4.2.15 Score per residue for model 15

- Molecule 1: Bcl-2-like protein 1



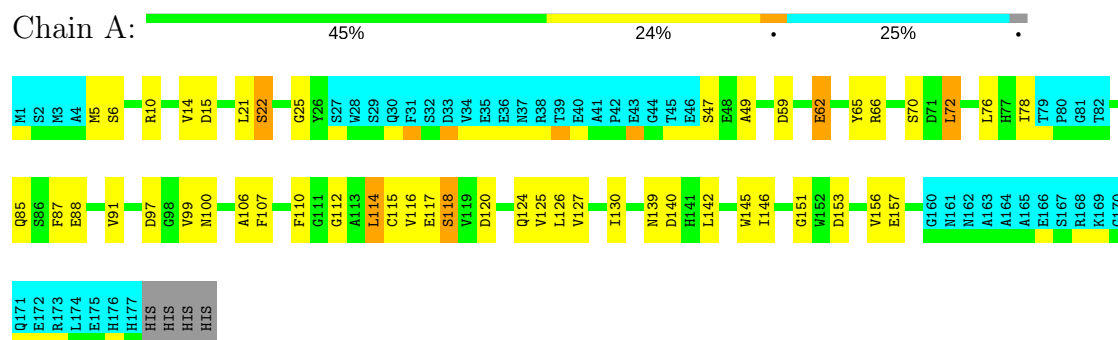
4.2.16 Score per residue for model 16

- Molecule 1: Bcl-2-like protein 1



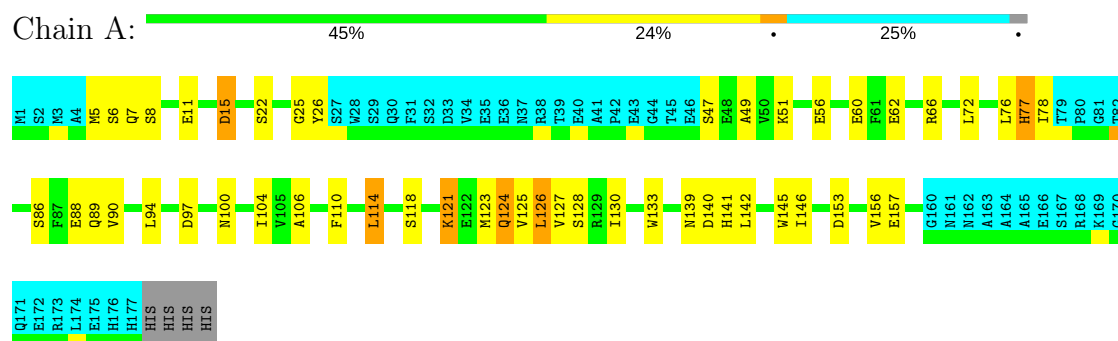
4.2.17 Score per residue for model 17

- Molecule 1: Bcl-2-like protein 1



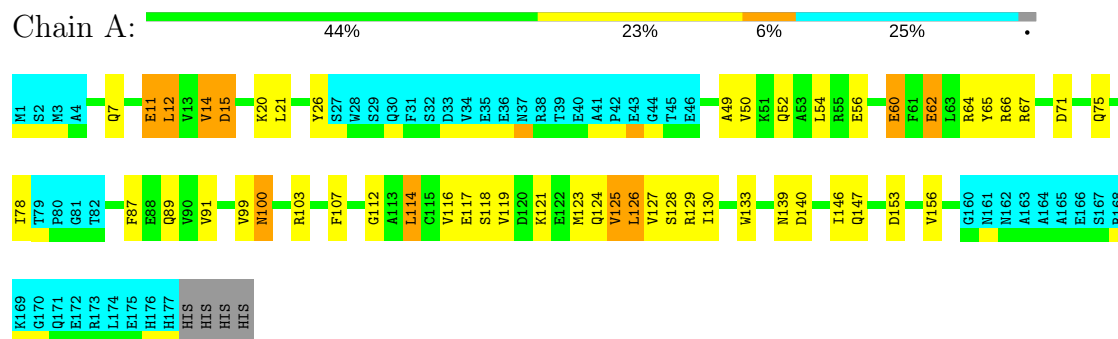
4.2.18 Score per residue for model 18

- Molecule 1: Bcl-2-like protein 1



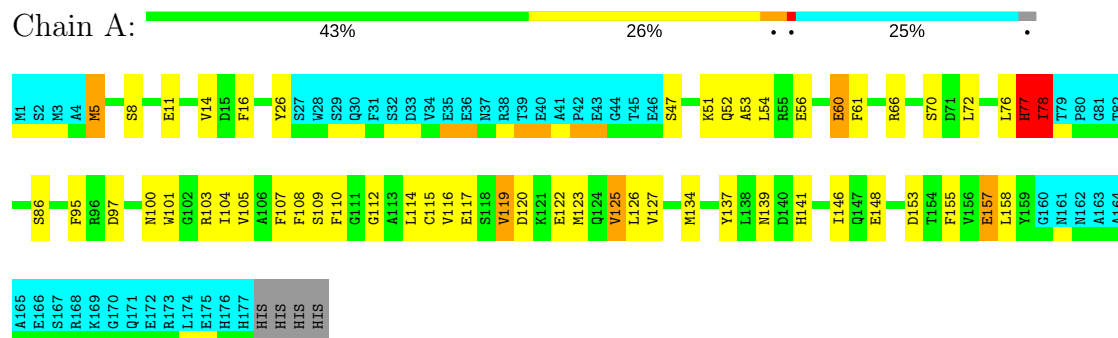
4.2.19 Score per residue for model 19

- Molecule 1: Bcl-2-like protein 1



4.2.20 Score per residue for model 20

- Molecule 1: Bcl-2-like protein 1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle simulated annealing, molecular dynamics*.

Of the 100 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
CYANA	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 7 of this report.

Chemical shift file(s)	2m03_cs.str
Number of chemical shift lists	1
Total number of shifts	1050
Number of shifts mapped to atoms	1050
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

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

6 Model quality

6.1 Standard geometry

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	0.72±0.03	1±1/1099 (0.0±0.1%)	0.87±0.02	1±1/1487 (0.0±0.1%)
All	All	0.72	10/21980 (0.0%)	0.88	14/29740 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	6.0±1.9
All	All	0	120

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	93	GLU	CD-OE1	7.45	1.33	1.25	15	1
1	A	117	GLU	CD-OE2	6.68	1.32	1.25	10	1
1	A	93	GLU	CD-OE2	-6.58	1.18	1.25	15	1
1	A	143	GLU	CD-OE2	-5.89	1.19	1.25	12	1
1	A	117	GLU	CD-OE1	-5.86	1.19	1.25	10	1
1	A	143	GLU	CD-OE1	-5.68	1.19	1.25	5	2
1	A	48	GLU	CD-OE1	5.13	1.31	1.25	15	1
1	A	48	GLU	CD-OE2	-5.08	1.20	1.25	15	1
1	A	157	GLU	CD-OE1	-5.06	1.20	1.25	18	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	15	ASP	CB-CG-OD2	-10.49	108.86	118.30	12	7

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	ASP	CB-CG-OD1	-7.14	111.87	118.30	7	2
1	A	59	ASP	CB-CG-OD2	-6.83	112.15	118.30	17	2
1	A	120	ASP	CB-CG-OD1	-6.43	112.51	118.30	14	1
1	A	103	ARG	NE-CZ-NH1	5.31	122.95	120.30	14	1
1	A	65	TYR	CB-CG-CD2	-5.01	117.99	121.00	2	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	11	GLU	Mainchain,Sidechain	13
1	A	100	ASN	Mainchain	13
1	A	62	GLU	Sidechain	11
1	A	60	GLU	Sidechain	10
1	A	15	ASP	Sidechain,Mainchain	10
1	A	56	GLU	Sidechain,Mainchain	5
1	A	59	ASP	Sidechain,Mainchain	5
1	A	65	TYR	Sidechain,Mainchain	4
1	A	153	ASP	Mainchain,Sidechain	4
1	A	26	TYR	Sidechain,Mainchain	4
1	A	48	GLU	Sidechain	3
1	A	120	ASP	Sidechain	3
1	A	66	ARG	Mainchain	3
1	A	97	ASP	Sidechain	3
1	A	7	GLN	Mainchain	2
1	A	157	GLU	Sidechain	2
1	A	121	LYS	Mainchain	2
1	A	64	ARG	Mainchain	1
1	A	25	GLY	Mainchain	1
1	A	67	ARG	Mainchain	1
1	A	147	GLN	Sidechain	1
1	A	124	GLN	Mainchain	1
1	A	119	VAL	Mainchain	1
1	A	122	GLU	Sidechain	1
1	A	159	TYR	Sidechain	1
1	A	140	ASP	Sidechain	1
1	A	18	SER	Mainchain	1
1	A	5	MET	Mainchain	1
1	A	52	GLN	Mainchain	1
1	A	71	ASP	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	84	TYR	Mainchain	1
1	A	21	LEU	Mainchain	1
1	A	117	GLU	Sidechain	1
1	A	93	GLU	Sidechain	1

6.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1073	1023	1023	12±4
All	All	21460	20460	20460	230

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:HD21	1:A:130:ILE:HD12	0.86	1.45	18	1
1:A:76:LEU:HD21	1:A:114:LEU:HD23	0.83	1.48	3	1
1:A:114:LEU:HD21	1:A:130:ILE:HD13	0.81	1.50	17	2
1:A:78:ILE:HD11	1:A:126:LEU:HD11	0.80	1.52	5	5
1:A:107:PHE:CE2	1:A:138:LEU:HD13	0.71	2.20	15	1
1:A:78:ILE:HD11	1:A:126:LEU:HD12	0.69	1.64	20	1
1:A:78:ILE:HD11	1:A:126:LEU:HD21	0.68	1.64	19	6
1:A:114:LEU:HD23	1:A:130:ILE:HD13	0.68	1.65	1	1
1:A:114:LEU:HD12	1:A:130:ILE:CD1	0.67	2.19	3	1
1:A:49:ALA:HB1	1:A:156:VAL:HG22	0.67	1.66	18	1
1:A:124:GLN:HB3	1:A:126:LEU:HD22	0.65	1.66	11	2
1:A:106:ALA:HB1	1:A:110:PHE:CE2	0.64	2.28	11	1
1:A:16:PHE:CE2	1:A:54:LEU:HD22	0.63	2.28	3	2
1:A:126:LEU:HD13	1:A:127:VAL:N	0.63	2.09	10	1
1:A:53:ALA:HB1	1:A:155:PHE:CD1	0.63	2.29	20	1
1:A:100:ASN:HA	1:A:104:ILE:HD12	0.62	1.70	20	4
1:A:76:LEU:HD22	1:A:110:PHE:CE1	0.62	2.29	3	1
1:A:78:ILE:HD11	1:A:126:LEU:HD13	0.61	1.71	15	1
1:A:90:VAL:HG21	1:A:110:PHE:CD2	0.60	2.31	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:VAL:HG21	1:A:110:PHE:CE2	0.59	2.32	8	1
1:A:119:VAL:HG13	1:A:127:VAL:HG21	0.59	1.75	13	1
1:A:21:LEU:HD12	1:A:115:CYS:HB3	0.59	1.74	17	1
1:A:78:ILE:CD1	1:A:114:LEU:HD11	0.59	2.28	3	2
1:A:12:LEU:HD21	1:A:50:VAL:HG11	0.59	1.74	7	1
1:A:114:LEU:HD12	1:A:130:ILE:HD13	0.57	1.74	3	1
1:A:78:ILE:HB	1:A:114:LEU:HD11	0.57	1.76	8	2
1:A:114:LEU:CD1	1:A:130:ILE:HD12	0.57	2.29	13	1
1:A:26:TYR:CE1	1:A:119:VAL:HG11	0.57	2.35	9	2
1:A:78:ILE:HD11	1:A:126:LEU:HD22	0.57	1.76	17	2
1:A:68:ALA:HB3	1:A:110:PHE:CZ	0.57	2.35	11	1
1:A:104:ILE:HD11	1:A:142:LEU:CD1	0.56	2.31	5	2
1:A:90:VAL:HG11	1:A:110:PHE:CD2	0.56	2.35	18	1
1:A:123:MET:HB3	1:A:126:LEU:HD23	0.56	1.77	1	3
1:A:12:LEU:HD21	1:A:50:VAL:HG12	0.56	1.77	6	1
1:A:95:PHE:CE1	1:A:99:VAL:HG23	0.56	2.36	15	1
1:A:94:LEU:HD22	1:A:106:ALA:CB	0.55	2.32	18	1
1:A:12:LEU:HD13	1:A:50:VAL:HG12	0.55	1.77	15	1
1:A:126:LEU:HD22	1:A:126:LEU:C	0.54	2.21	10	1
1:A:78:ILE:HG22	1:A:114:LEU:HD11	0.54	1.79	5	1
1:A:146:ILE:HD12	1:A:147:GLN:N	0.54	2.17	12	1
1:A:114:LEU:HD23	1:A:115:CYS:N	0.54	2.18	17	1
1:A:114:LEU:CD2	1:A:130:ILE:HD13	0.54	2.33	19	3
1:A:110:PHE:CZ	1:A:114:LEU:HD11	0.54	2.38	12	2
1:A:53:ALA:HB2	1:A:159:TYR:HB2	0.54	1.80	14	2
1:A:78:ILE:HD11	1:A:126:LEU:CD1	0.54	2.33	15	5
1:A:126:LEU:O	1:A:126:LEU:HD22	0.53	2.04	10	1
1:A:104:ILE:HD11	1:A:142:LEU:HD12	0.53	1.81	5	1
1:A:77:HIS:O	1:A:114:LEU:HD23	0.53	2.03	20	1
1:A:78:ILE:CD1	1:A:126:LEU:HD21	0.53	2.34	14	2
1:A:114:LEU:CD2	1:A:130:ILE:HD12	0.53	2.29	18	1
1:A:61:PHE:CG	1:A:105:VAL:HG11	0.53	2.39	5	3
1:A:76:LEU:HD21	1:A:114:LEU:CD2	0.53	2.29	3	1
1:A:72:LEU:HD13	1:A:110:PHE:HB2	0.53	1.80	6	1
1:A:78:ILE:HD13	1:A:114:LEU:HD11	0.52	1.80	3	2
1:A:76:LEU:HD13	1:A:110:PHE:CE1	0.52	2.39	20	2
1:A:72:LEU:HD22	1:A:110:PHE:CD1	0.52	2.39	17	1
1:A:115:CYS:SG	1:A:127:VAL:HG13	0.52	2.44	9	1
1:A:78:ILE:CG2	1:A:114:LEU:HD11	0.52	2.34	5	1
1:A:61:PHE:CD2	1:A:105:VAL:HG11	0.52	2.40	3	1
1:A:124:GLN:HB2	1:A:126:LEU:HD22	0.52	1.81	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:ALA:HB3	1:A:156:VAL:HG22	0.52	1.80	13	1
1:A:12:LEU:HD11	1:A:54:LEU:HD22	0.51	1.81	15	1
1:A:12:LEU:HD21	1:A:50:VAL:CG1	0.51	2.36	6	3
1:A:54:LEU:HD21	1:A:108:PHE:CE2	0.51	2.41	1	1
1:A:78:ILE:HD13	1:A:126:LEU:HD21	0.51	1.82	10	1
1:A:90:VAL:HG21	1:A:110:PHE:CE1	0.50	2.40	3	1
1:A:87:PHE:O	1:A:91:VAL:HG23	0.50	2.06	14	4
1:A:21:LEU:HD11	1:A:119:VAL:HG21	0.50	1.84	19	1
1:A:126:LEU:HD12	1:A:127:VAL:N	0.50	2.22	4	1
1:A:110:PHE:CE1	1:A:114:LEU:HD11	0.50	2.42	9	1
1:A:112:GLY:O	1:A:116:VAL:HG23	0.49	2.07	12	7
1:A:16:PHE:CD2	1:A:54:LEU:HD13	0.49	2.42	3	1
1:A:72:LEU:HD22	1:A:110:PHE:CG	0.49	2.42	13	2
1:A:78:ILE:HD13	1:A:118:SER:HB3	0.49	1.83	19	1
1:A:126:LEU:HD23	1:A:127:VAL:N	0.49	2.23	18	4
1:A:118:SER:CB	1:A:127:VAL:HG13	0.49	2.38	17	1
1:A:21:LEU:HD11	1:A:127:VAL:HG11	0.48	1.83	13	1
1:A:76:LEU:HD11	1:A:90:VAL:HG21	0.48	1.85	16	1
1:A:65:TYR:CE1	1:A:68:ALA:HB2	0.48	2.44	6	1
1:A:78:ILE:HD11	1:A:130:ILE:HD13	0.48	1.85	6	1
1:A:49:ALA:CB	1:A:156:VAL:HG22	0.48	2.38	13	3
1:A:78:ILE:HD11	1:A:126:LEU:CD2	0.48	2.38	17	1
1:A:17:LEU:HD22	1:A:107:PHE:CZ	0.48	2.43	16	1
1:A:49:ALA:HB1	1:A:156:VAL:HA	0.47	1.86	17	1
1:A:78:ILE:CG1	1:A:126:LEU:HD11	0.47	2.39	18	2
1:A:119:VAL:HG23	1:A:127:VAL:HG21	0.47	1.87	6	1
1:A:12:LEU:HD13	1:A:152:TRP:CZ3	0.47	2.44	9	1
1:A:115:CYS:HB2	1:A:127:VAL:HG13	0.47	1.86	13	1
1:A:126:LEU:O	1:A:130:ILE:HD12	0.47	2.09	9	1
1:A:115:CYS:O	1:A:119:VAL:HG23	0.47	2.09	3	3
1:A:16:PHE:CD1	1:A:54:LEU:HD23	0.47	2.44	20	1
1:A:78:ILE:HD11	1:A:130:ILE:HD11	0.47	1.87	8	1
1:A:78:ILE:HG13	1:A:114:LEU:HD22	0.47	1.87	12	1
1:A:72:LEU:HD13	1:A:110:PHE:CE2	0.46	2.45	13	1
1:A:16:PHE:CD2	1:A:54:LEU:HD23	0.46	2.45	7	1
1:A:12:LEU:HD11	1:A:50:VAL:CG1	0.46	2.40	19	2
1:A:94:LEU:HD11	1:A:95:PHE:CZ	0.46	2.46	11	1
1:A:72:LEU:HD11	1:A:90:VAL:HG13	0.46	1.86	18	1
1:A:78:ILE:CD1	1:A:114:LEU:HD22	0.46	2.40	12	1
1:A:78:ILE:CD1	1:A:126:LEU:HD11	0.46	2.41	11	4
1:A:124:GLN:HG3	1:A:127:VAL:HG23	0.46	1.86	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:HD22	1:A:152:TRP:CH2	0.45	2.46	16	1
1:A:83:ALA:HB1	1:A:87:PHE:CE2	0.45	2.46	6	1
1:A:61:PHE:CB	1:A:105:VAL:HG11	0.45	2.41	20	1
1:A:146:ILE:HD12	1:A:147:GLN:H	0.45	1.72	8	6
1:A:21:LEU:HD12	1:A:115:CYS:SG	0.45	2.52	12	1
1:A:124:GLN:H	1:A:124:GLN:NE2	0.45	2.10	18	1
1:A:114:LEU:HD23	1:A:130:ILE:HD12	0.45	1.87	16	1
1:A:69:PHE:HA	1:A:72:LEU:HD12	0.45	1.88	6	1
1:A:118:SER:HB2	1:A:127:VAL:HG13	0.45	1.89	17	1
1:A:21:LEU:HD13	1:A:115:CYS:SG	0.44	2.52	10	3
1:A:21:LEU:HD23	1:A:22:SER:N	0.44	2.27	17	1
1:A:86:SER:O	1:A:90:VAL:HG23	0.44	2.12	3	3
1:A:115:CYS:SG	1:A:127:VAL:HG22	0.44	2.53	6	1
1:A:126:LEU:C	1:A:130:ILE:HD12	0.44	2.33	9	1
1:A:118:SER:OG	1:A:127:VAL:HG22	0.44	2.13	19	1
1:A:114:LEU:HD12	1:A:115:CYS:N	0.44	2.28	13	1
1:A:78:ILE:HB	1:A:114:LEU:HD21	0.44	1.90	15	2
1:A:16:PHE:CD2	1:A:54:LEU:HD22	0.43	2.48	8	1
1:A:100:ASN:CA	1:A:104:ILE:HD12	0.43	2.43	9	1
1:A:110:PHE:CE1	1:A:114:LEU:HD13	0.43	2.48	1	1
1:A:50:VAL:HG22	1:A:156:VAL:CG2	0.43	2.43	9	1
1:A:57:ALA:HB1	1:A:105:VAL:HG13	0.43	1.90	7	1
1:A:17:LEU:HD11	1:A:107:PHE:CZ	0.43	2.48	9	1
1:A:100:ASN:HB2	1:A:146:ILE:HD13	0.43	1.90	12	1
1:A:115:CYS:HA	1:A:127:VAL:HG22	0.43	1.88	20	1
1:A:95:PHE:CE1	1:A:106:ALA:HB3	0.43	2.48	11	1
1:A:118:SER:OG	1:A:127:VAL:HG23	0.43	2.14	6	1
1:A:78:ILE:HD12	1:A:126:LEU:HD11	0.43	1.90	16	1
1:A:118:SER:CB	1:A:127:VAL:HG23	0.43	2.44	6	1
1:A:119:VAL:HB	1:A:127:VAL:HG21	0.43	1.91	11	1
1:A:11:GLU:HA	1:A:14:VAL:HG12	0.42	1.91	19	1
1:A:106:ALA:HB1	1:A:110:PHE:CZ	0.42	2.49	17	1
1:A:100:ASN:CB	1:A:146:ILE:HD13	0.42	2.44	12	1
1:A:126:LEU:HD13	1:A:126:LEU:C	0.42	2.35	20	1
1:A:123:MET:O	1:A:126:LEU:HD12	0.42	2.15	10	1
1:A:72:LEU:HD12	1:A:110:PHE:CG	0.41	2.50	18	1
1:A:78:ILE:CG1	1:A:126:LEU:HD21	0.41	2.44	1	1
1:A:100:ASN:HA	1:A:104:ILE:HD13	0.41	1.91	16	1
1:A:12:LEU:HD11	1:A:54:LEU:HD12	0.41	1.91	2	1
1:A:87:PHE:CZ	1:A:130:ILE:HG23	0.41	2.49	17	1
1:A:87:PHE:O	1:A:91:VAL:HG13	0.41	2.15	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:LEU:C	1:A:12:LEU:HD23	0.41	2.36	16	1
1:A:123:MET:CB	1:A:126:LEU:HD23	0.41	2.46	15	1
1:A:69:PHE:CE1	1:A:113:ALA:HB2	0.41	2.51	4	1
1:A:138:LEU:HD23	1:A:139:ASN:N	0.41	2.31	13	1
1:A:75:GLN:C	1:A:76:LEU:HD22	0.41	2.36	14	1
1:A:91:VAL:HG13	1:A:103:ARG:HH11	0.41	1.75	7	1
1:A:104:ILE:HG22	1:A:108:PHE:CE2	0.41	2.51	20	1
1:A:115:CYS:HB3	1:A:127:VAL:HG13	0.41	1.93	4	1
1:A:90:VAL:HG11	1:A:110:PHE:CE2	0.41	2.51	14	1
1:A:9:ASN:ND2	1:A:138:LEU:HD21	0.40	2.31	13	1
1:A:12:LEU:CD1	1:A:54:LEU:HD22	0.40	2.46	10	1
1:A:69:PHE:O	1:A:73:THR:HG22	0.40	2.16	7	1
1:A:126:LEU:HD12	1:A:130:ILE:HG12	0.40	1.93	1	1
1:A:13:VAL:HG12	1:A:17:LEU:HD12	0.40	1.93	7	1
1:A:72:LEU:HD22	1:A:110:PHE:CD2	0.40	2.52	10	1
1:A:94:LEU:HD11	1:A:95:PHE:CE1	0.40	2.52	11	1
1:A:104:ILE:HD12	1:A:104:ILE:N	0.40	2.32	16	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	131/181 (72%)	114±2 (87±2%)	14±2 (10±2%)	3±1 (2±1%)	11	49
All	All	2620/3620 (72%)	2287 (87%)	273 (10%)	60 (2%)	11	49

All 16 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	125	VAL	9
1	A	77	HIS	6
1	A	78	ILE	6
1	A	99	VAL	6
1	A	100	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	25	GLY	5
1	A	83	ALA	4
1	A	97	ASP	3
1	A	122	GLU	3
1	A	47	SER	3
1	A	26	TYR	2
1	A	148	GLU	2
1	A	151	GLY	2
1	A	66	ARG	1
1	A	138	LEU	1
1	A	159	TYR	1

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/154 (73%)	86±4 (76±3%)	27±4 (24±3%)	3	27
All	All	2260/3080 (73%)	1718 (76%)	542 (24%)	3	27

All 90 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	153	ASP	18
1	A	145	TRP	16
1	A	146	ILE	15
1	A	126	LEU	14
1	A	66	ARG	13
1	A	142	LEU	13
1	A	140	ASP	12
1	A	76	LEU	11
1	A	62	GLU	10
1	A	139	ASN	10
1	A	8	SER	10
1	A	51	LYS	10
1	A	129	ARG	9
1	A	133	TRP	9

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Mol	Chain	Res	Type	Models (Total)
1	A	70	SER	9
1	A	86	SER	9
1	A	103	ARG	9
1	A	54	LEU	9
1	A	89	GLN	9
1	A	72	LEU	8
1	A	24	LYS	8
1	A	109	SER	8
1	A	117	GLU	8
1	A	147	GLN	8
1	A	123	MET	8
1	A	47	SER	8
1	A	107	PHE	8
1	A	52	GLN	7
1	A	64	ARG	7
1	A	6	SER	7
1	A	93	GLU	7
1	A	20	LYS	7
1	A	60	GLU	7
1	A	128	SER	7
1	A	56	GLU	6
1	A	149	ASN	6
1	A	96	ARG	6
1	A	67	ARG	6
1	A	5	MET	6
1	A	121	LYS	6
1	A	48	GLU	6
1	A	97	ASP	6
1	A	71	ASP	6
1	A	85	GLN	6
1	A	10	ARG	5
1	A	134	MET	5
1	A	21	LEU	5
1	A	88	GLU	5
1	A	26	TYR	5
1	A	114	LEU	5
1	A	12	LEU	5
1	A	14	VAL	5
1	A	19	TYR	5
1	A	158	LEU	5
1	A	55	ARG	5
1	A	124	GLN	5

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Mol	Chain	Res	Type	Models (Total)
1	A	65	TYR	5
1	A	120	ASP	4
1	A	75	GLN	4
1	A	73	THR	4
1	A	137	TYR	4
1	A	77	HIS	4
1	A	141	HIS	4
1	A	159	TYR	4
1	A	7	GLN	4
1	A	118	SER	4
1	A	108	PHE	3
1	A	95	PHE	3
1	A	17	LEU	3
1	A	11	GLU	3
1	A	100	ASN	3
1	A	143	GLU	3
1	A	61	PHE	3
1	A	87	PHE	3
1	A	125	VAL	3
1	A	22	SER	3
1	A	16	PHE	3
1	A	115	CYS	2
1	A	157	GLU	2
1	A	122	GLU	2
1	A	78	ILE	2
1	A	23	GLN	2
1	A	63	LEU	2
1	A	9	ASN	2
1	A	148	GLU	1
1	A	101	TRP	1
1	A	138	LEU	1
1	A	94	LEU	1
1	A	84	TYR	1
1	A	99	VAL	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 [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 45% for the well-defined parts and 43% for the entire structure.

7.1 Chemical shift list 1

File name: 2m03_cs.str

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	1050
Number of shifts mapped to atoms	1050
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	164	-0.14 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	151	1.36 ± 0.07	Should be applied
$^{13}\text{C}'$	164	-0.49 ± 0.06	None needed (< 0.5 ppm)
^{15}N	166	0.62 ± 0.12	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 45%, i.e. 741 atoms were assigned a chemical shift out of a possible 1658. 21 out of 25 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	508/653 (78%)	127/261 (49%)	254/262 (97%)	127/130 (98%)
Sidechain	225/812 (28%)	54/474 (11%)	171/297 (58%)	0/41 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	8/193 (4%)	4/101 (4%)	0/84 (0%)	4/8 (50%)
Overall	741/1658 (45%)	185/836 (22%)	425/643 (66%)	131/179 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 43%, i.e. 932 atoms were assigned a chemical shift out of a possible 2190. 22 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	656/879 (75%)	164/351 (47%)	328/354 (93%)	164/174 (94%)
Sidechain	266/1082 (25%)	58/634 (9%)	208/392 (53%)	0/56 (0%)
Aromatic	10/229 (4%)	5/120 (4%)	0/97 (0%)	5/12 (42%)
Overall	932/2190 (43%)	227/1105 (21%)	536/843 (64%)	169/242 (70%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	99	VAL	HG21	-0.82	2.20 – -0.60	-5.8
1	A	99	VAL	HG22	-0.82	2.20 – -0.60	-5.8
1	A	99	VAL	HG23	-0.82	2.20 – -0.60	-5.8

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:

