



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 21, 2021 – 08:04 AM EDT

PDB ID : 7K3S  
Title : Solution NMR Structure of the Coiled-coil BRCA1-PALB2 Heterodimer  
Authors : Daigham, N.S.; Liu, G.; Bunting, S.F.; Montelione, G.T.  
Deposited on : 2020-09-13

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:

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 : 2.23.1  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

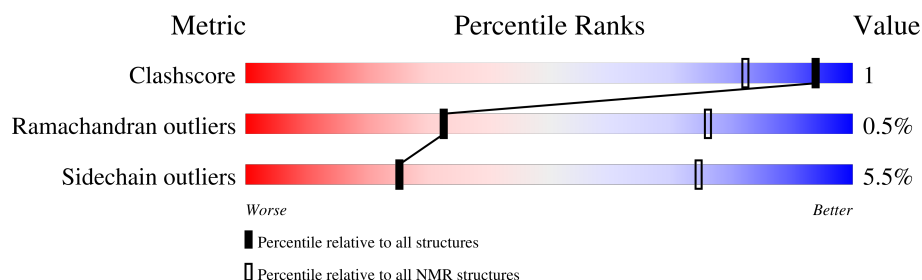
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 75%.

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	60	
2	B	68	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 8 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:12-A:45, B:110-B:143 (68)	0.66	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 3 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2090 atoms, of which 1047 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Breast cancer type 1 susceptibility protein homolog.

Mol	Chain	Residues	Atoms						Trace
1	A	60	Total	C	H	N	O	S	0
			949	291	465	94	95	4	

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P48754
A	54	GLU	-	expression tag	UNP P48754
A	55	HIS	-	expression tag	UNP P48754
A	56	HIS	-	expression tag	UNP P48754
A	57	HIS	-	expression tag	UNP P48754
A	58	HIS	-	expression tag	UNP P48754
A	59	HIS	-	expression tag	UNP P48754
A	60	HIS	-	expression tag	UNP P48754

- Molecule 2 is a protein called Partner and localizer of BRCA2.

Mol	Chain	Residues	Atoms						Trace
2	B	68	Total	C	H	N	O	S	0
			1141	350	582	107	101	1	

There are 8 discrepancies between the modelled and reference sequences:

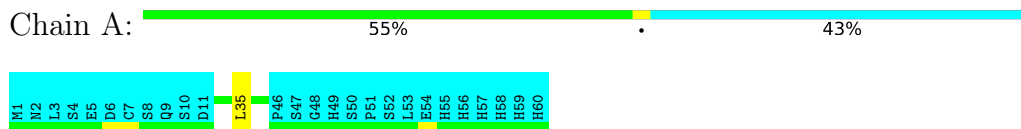
Chain	Residue	Modelled	Actual	Comment	Reference
B	161	LEU	-	expression tag	UNP Q3U0P1
B	162	GLU	-	expression tag	UNP Q3U0P1
B	163	HIS	-	expression tag	UNP Q3U0P1
B	164	HIS	-	expression tag	UNP Q3U0P1
B	165	HIS	-	expression tag	UNP Q3U0P1
B	166	HIS	-	expression tag	UNP Q3U0P1
B	167	HIS	-	expression tag	UNP Q3U0P1
B	168	HIS	-	expression tag	UNP Q3U0P1

## 4 Residue-property plots

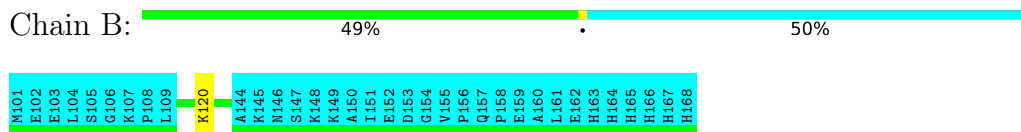
### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: Breast cancer type 1 susceptibility protein homolog



- Molecule 2: Partner and localizer of BRCA2

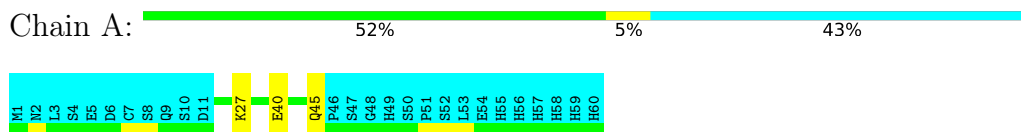


### 4.2 Scores per residue for each member of the ensemble

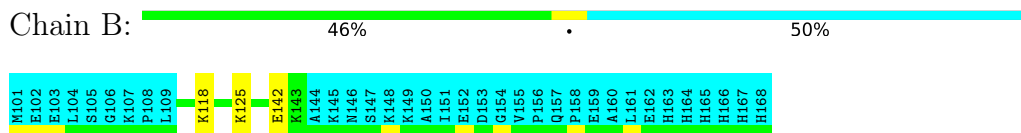
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

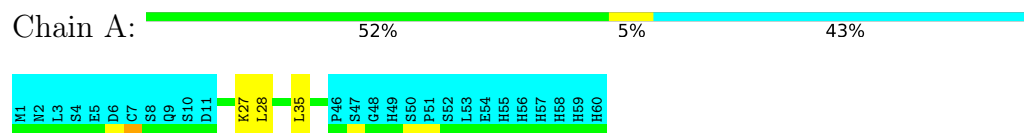


- Molecule 2: Partner and localizer of BRCA2

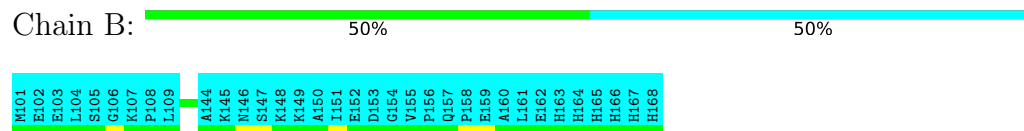


### 4.2.2 Score per residue for model 2

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

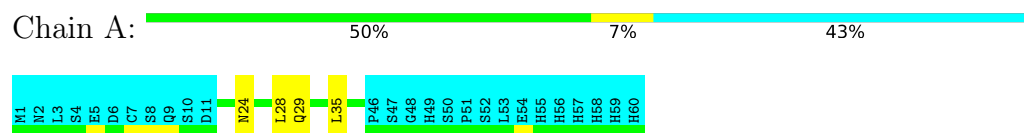


- Molecule 2: Partner and localizer of BRCA2

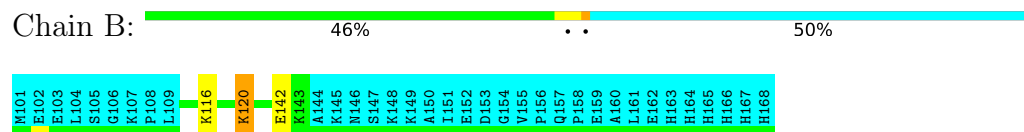


### 4.2.3 Score per residue for model 3

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

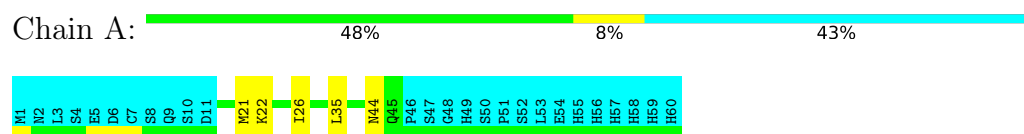


- Molecule 2: Partner and localizer of BRCA2

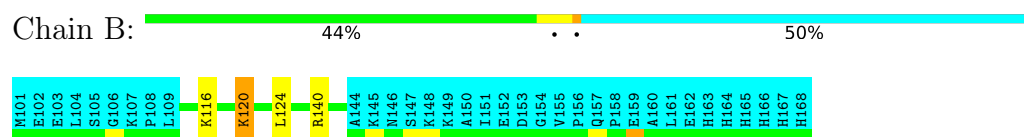


### 4.2.4 Score per residue for model 4

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

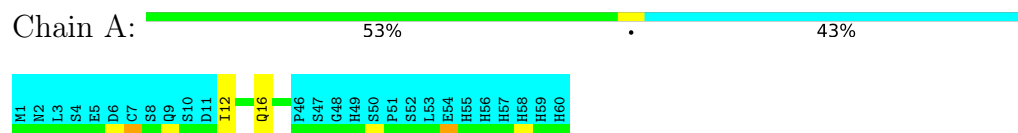


- Molecule 2: Partner and localizer of BRCA2

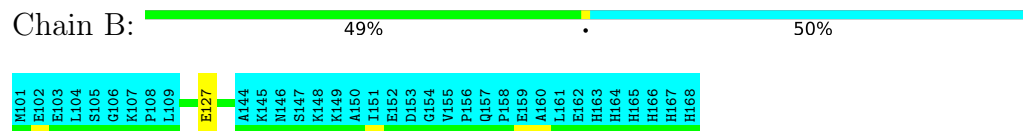


### 4.2.5 Score per residue for model 5

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

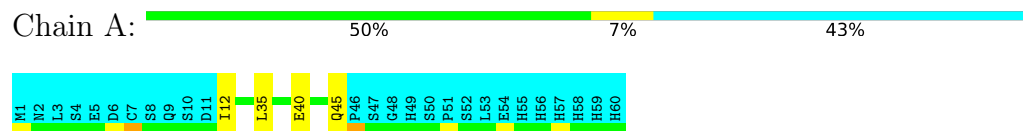


- Molecule 2: Partner and localizer of BRCA2

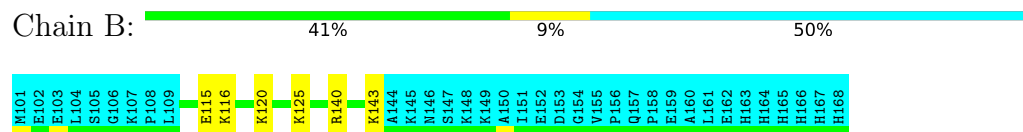


### 4.2.6 Score per residue for model 6

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

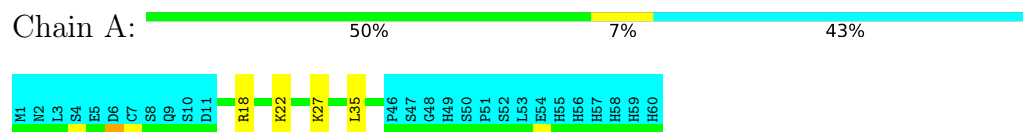


- Molecule 2: Partner and localizer of BRCA2

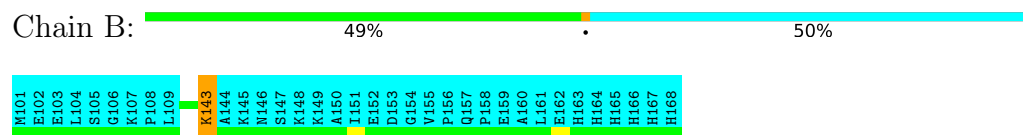


### 4.2.7 Score per residue for model 7

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

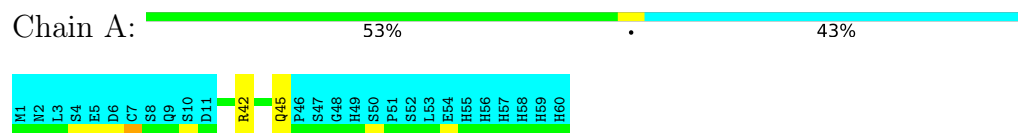


- Molecule 2: Partner and localizer of BRCA2

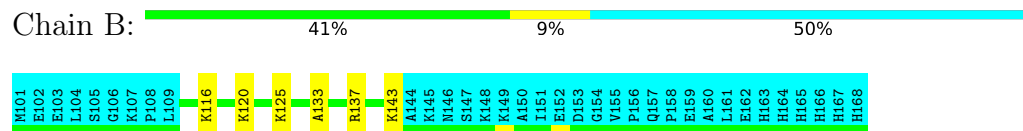


### 4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

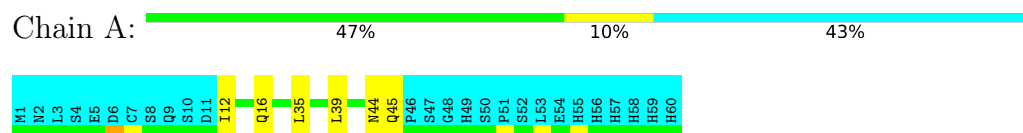


- Molecule 2: Partner and localizer of BRCA2

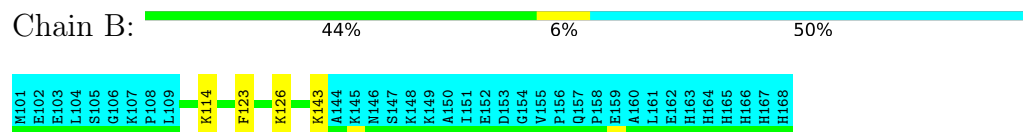


### 4.2.9 Score per residue for model 9

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

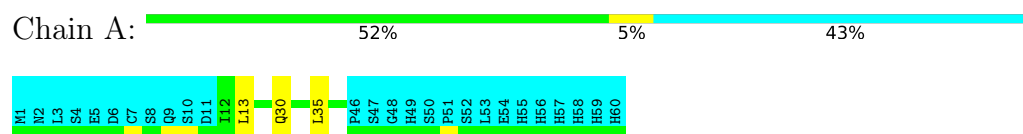


- Molecule 2: Partner and localizer of BRCA2

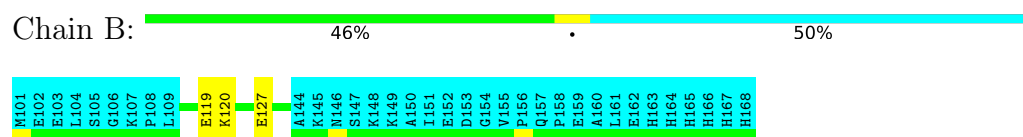


### 4.2.10 Score per residue for model 10

- Molecule 1: Breast cancer type 1 susceptibility protein homolog



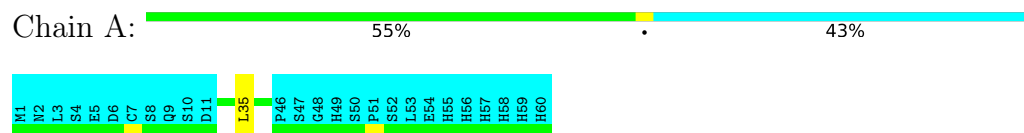
- Molecule 2: Partner and localizer of BRCA2



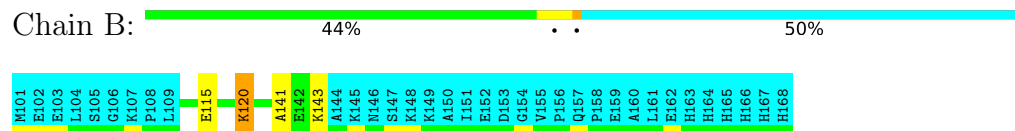


### 4.2.11 Score per residue for model 11

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

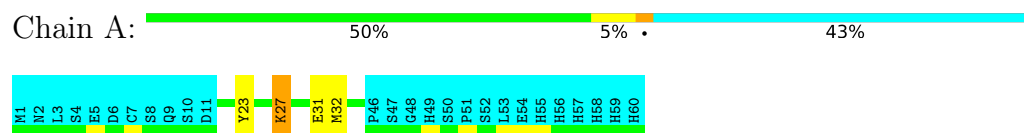


- Molecule 2: Partner and localizer of BRCA2

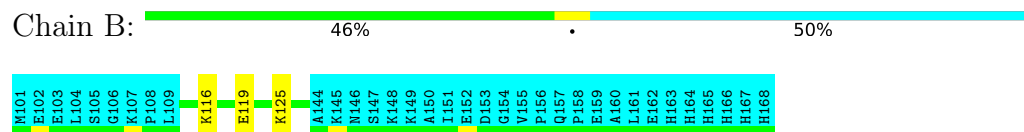


### 4.2.12 Score per residue for model 12

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

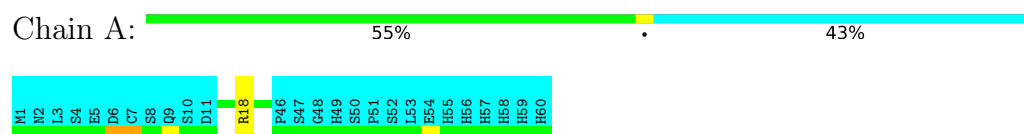


- Molecule 2: Partner and localizer of BRCA2

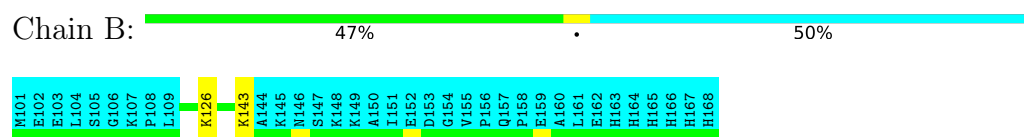


### 4.2.13 Score per residue for model 13

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

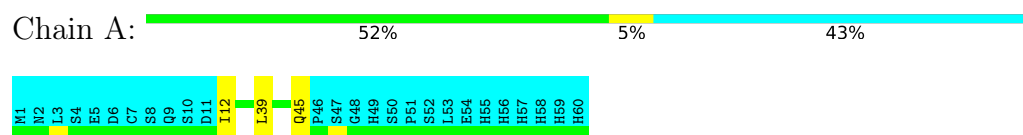


- Molecule 2: Partner and localizer of BRCA2

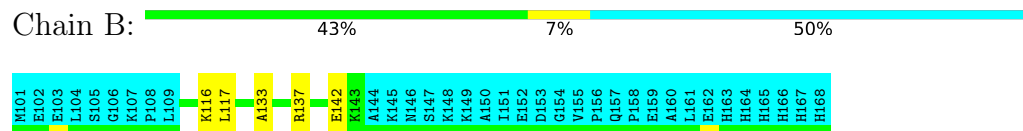


#### 4.2.14 Score per residue for model 14

- Molecule 1: Breast cancer type 1 susceptibility protein homolog

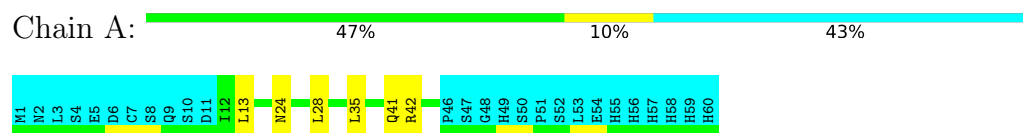


- Molecule 2: Partner and localizer of BRCA2

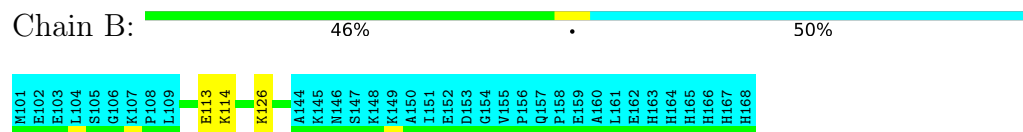


#### 4.2.15 Score per residue for model 15

- Molecule 1: Breast cancer type 1 susceptibility protein homolog



- Molecule 2: Partner and localizer of BRCA2



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 200 calculated structures, 15 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 calculation	
CNS	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)	working_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)	75%

## 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	278	290	289	1±1
2	B	289	318	318	1±1
All	All	8505	9120	9105	21

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:LEU:HG	2:B:120:LYS:HG3	0.61	1.71	3	1
1:A:39:LEU:HG	1:A:44:ASN:HB2	0.55	1.77	9	1
1:A:41:GLN:HG3	1:A:42:ARG:HG3	0.54	1.79	15	1
1:A:21:MET:SD	1:A:22:LYS:N	0.49	2.85	4	1
2:B:140:ARG:HH11	2:B:143:LYS:HD2	0.48	1.68	6	1
1:A:27:LYS:HG3	1:A:28:LEU:N	0.47	2.25	2	1
1:A:39:LEU:HD22	2:B:117:LEU:HD13	0.47	1.87	14	1
2:B:133:ALA:HB1	2:B:137:ARG:HE	0.46	1.71	8	1
1:A:35:LEU:HD21	2:B:120:LYS:HB3	0.46	1.86	11	1
1:A:18:ARG:O	1:A:22:LYS:HG2	0.46	2.10	7	1
1:A:35:LEU:HD13	2:B:120:LYS:HB3	0.45	1.87	4	1
1:A:35:LEU:HD22	2:B:120:LYS:HB2	0.45	1.88	10	1
2:B:115:GLU:HG3	2:B:116:LYS:HD2	0.45	1.87	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:119:GLU:HG3	2:B:120:LYS:HG3	0.45	1.88	10	1
1:A:24:ASN:O	1:A:28:LEU:HG	0.45	2.12	3	2
1:A:32:MET:SD	2:B:125:LYS:HG3	0.43	2.53	12	1
1:A:22:LYS:O	1:A:26:ILE:HG12	0.42	2.15	4	1
2:B:116:LYS:O	2:B:120:LYS:HG2	0.41	2.14	4	1
1:A:23:TYR:O	1:A:27:LYS:HG3	0.40	2.16	12	1
2:B:133:ALA:O	2:B:137:ARG:HD3	0.40	2.17	14	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	34/60 (57%)	31±1 (91±3%)	3±1 (8±4%)	0±0 (1±1%)	20	68
2	B	34/68 (50%)	33±1 (96±3%)	1±1 (4±3%)	0±0 (0±0%)	100	100
All	All	1020/1920 (53%)	955 (94%)	60 (6%)	5 (0%)	32	76

All 2 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	12	ILE	4
1	A	44	ASN	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	30/55 (55%)	29±1 (95±3%)	1±1 (5±3%)	29	78
2	B	29/58 (50%)	27±1 (94±4%)	2±1 (6±4%)	22	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	885/1695 (52%)	836 (94%)	49 (6%)	25 74

All 24 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	45	GLN	4
2	B	120	LYS	4
1	A	35	LEU	4
1	A	27	LYS	3
2	B	125	LYS	3
2	B	116	LYS	3
2	B	143	LYS	3
2	B	126	LYS	3
1	A	40	GLU	2
2	B	142	GLU	2
1	A	16	GLN	2
2	B	127	GLU	2
2	B	114	LYS	2
1	A	13	LEU	2
2	B	118	LYS	1
1	A	29	GLN	1
2	B	124	LEU	1
1	A	42	ARG	1
2	B	123	PHE	1
1	A	30	GLN	1
2	B	115	GLU	1
1	A	31	GLU	1
1	A	18	ARG	1
2	B	113	GLU	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 monosaccharides in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

## 7 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 75% for the well-defined parts and 67% for the entire structure.

### 7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *het.bmrB*

#### 7.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	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)	0

#### 7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	108	$-0.34 \pm 0.06$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	102	$0.14 \pm 0.04$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
$^{15}\text{N}$	108	$-1.23 \pm 0.09$	Should be applied

#### 7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 75%, i.e. 711 atoms were assigned a chemical shift out of a possible 942. 11 out of 11 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	268/340 (79%)	134/136 (99%)	66/136 (49%)	68/68 (100%)
Sidechain	430/561 (77%)	271/331 (82%)	158/193 (82%)	1/37 (3%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	13/41 (32%)	7/21 (33%)	6/18 (33%)	0/2 (0%)
Overall	711/942 (75%)	412/488 (84%)	230/347 (66%)	69/107 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 67%, i.e. 1128 atoms were assigned a chemical shift out of a possible 1676. 16 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	432/630 (69%)	216/251 (86%)	108/256 (42%)	108/123 (88%)
Sidechain	683/901 (76%)	432/537 (80%)	248/319 (78%)	3/45 (7%)
Aromatic	13/145 (9%)	7/73 (10%)	6/44 (14%)	0/28 (0%)
Overall	1128/1676 (67%)	655/861 (76%)	362/619 (58%)	111/196 (57%)

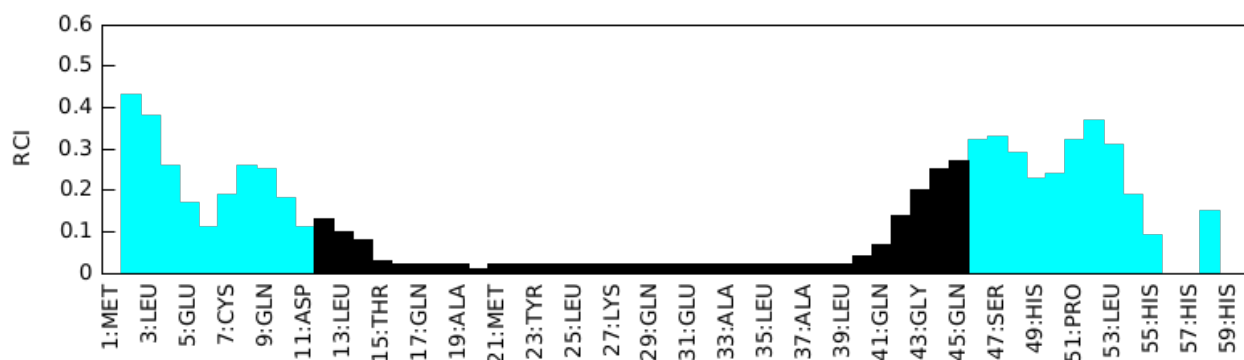
#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:

