



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 13, 2024 – 05:50 PM EST

PDB ID : 2N9E  
BMRB ID : 25901  
Title : Structure of SUMO-2 bound to phosphorylated RAP80 SIM  
Authors : Anamika, A.; Spyrapoulos, L.  
Deposited on : 2015-11-15

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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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  
Mogul : 2022.3.0, CSD as543be (2022)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

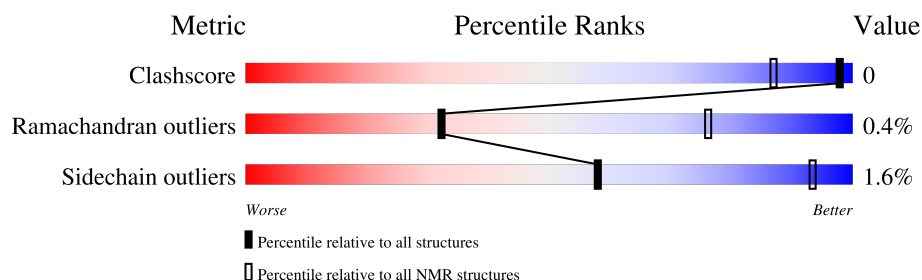
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 29%.

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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	15	
2	B	95	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:38-A:43, A:45-A:45, B:17-B:89 (80)	0.76	7

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1701 atoms, of which 831 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BRCA1-A complex subunit RAP80.

Mol	Chain	Residues	Atoms						Trace
1	A	15	Total	C	H	N	O	P	1
			194	61	85	14	32	2	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	ACE	-	acetylation	UNP Q96RL1
A	50	NH2	-	amidation	UNP Q96RL1

- Molecule 2 is a protein called Small ubiquitin-related modifier 2.

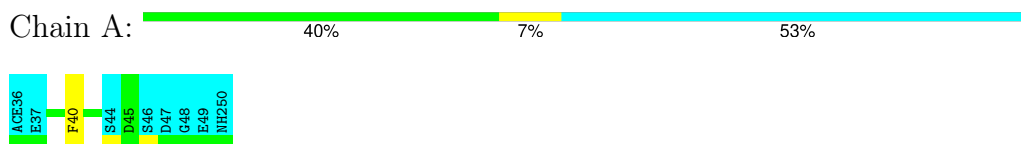
Mol	Chain	Residues	Atoms						Trace
2	B	95	Total	C	H	N	O	S	0
			1507	469	746	135	152	5	

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

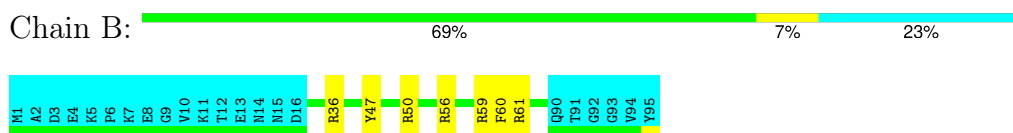
### 4.1 Average score per residue in the NMR ensemble

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: BRCA1-A complex subunit RAP80



- Molecule 2: Small ubiquitin-related modifier 2

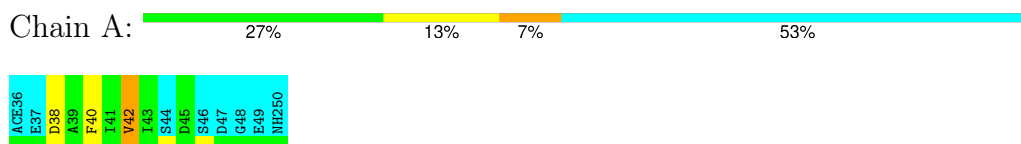


### 4.2 Scores per residue for each member of the ensemble

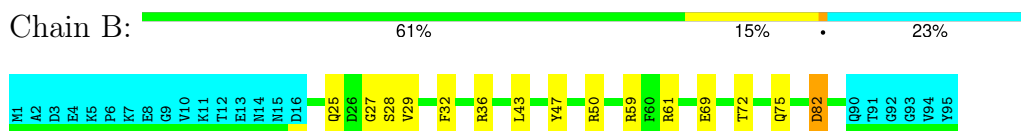
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: BRCA1-A complex subunit RAP80

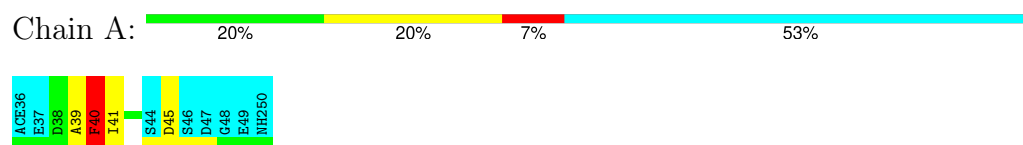


- Molecule 2: Small ubiquitin-related modifier 2

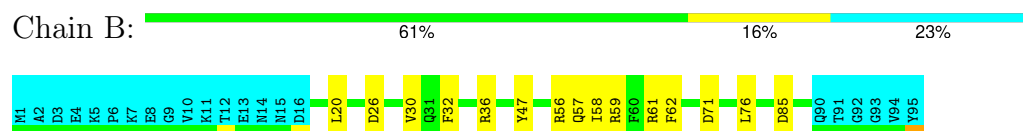


### 4.2.2 Score per residue for model 2

- Molecule 1: BRCA1-A complex subunit RAP80

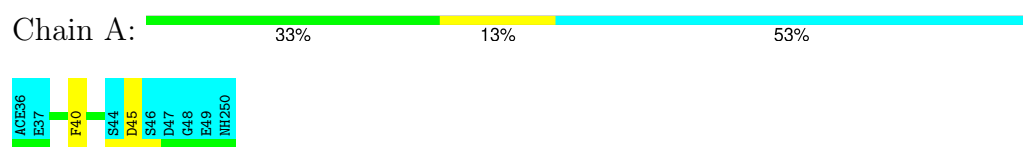


- Molecule 2: Small ubiquitin-related modifier 2

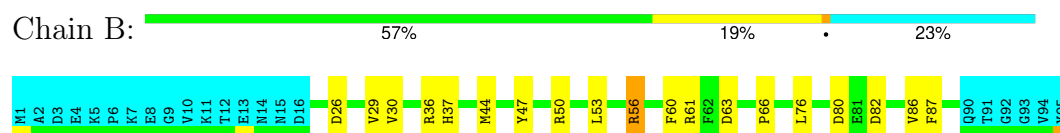


### 4.2.3 Score per residue for model 3

- Molecule 1: BRCA1-A complex subunit RAP80

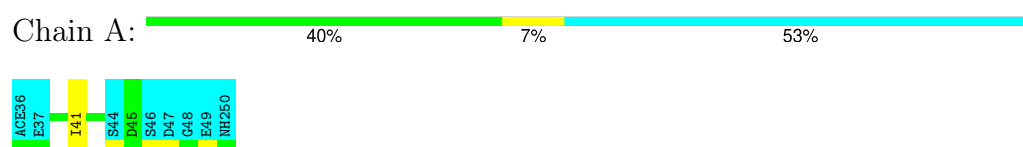


- Molecule 2: Small ubiquitin-related modifier 2

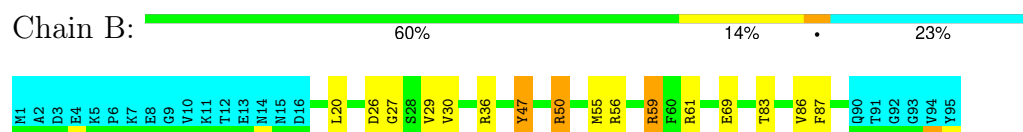


### 4.2.4 Score per residue for model 4

- Molecule 1: BRCA1-A complex subunit RAP80

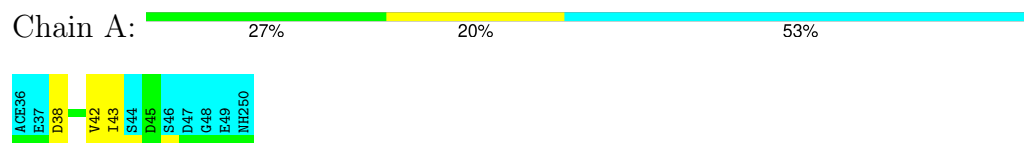


- Molecule 2: Small ubiquitin-related modifier 2

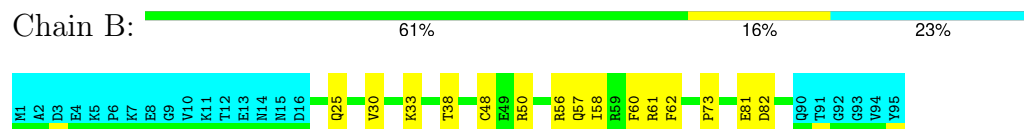


### 4.2.5 Score per residue for model 5

- Molecule 1: BRCA1-A complex subunit RAP80

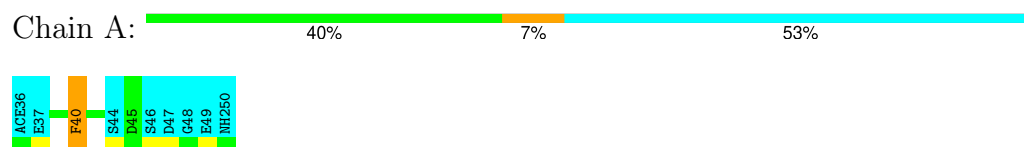


- Molecule 2: Small ubiquitin-related modifier 2

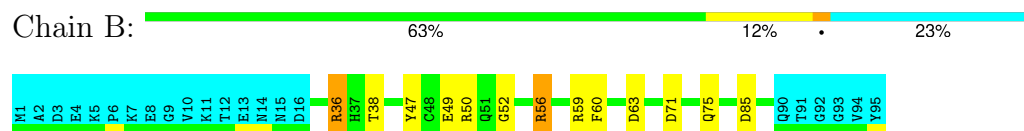


### 4.2.6 Score per residue for model 6

- Molecule 1: BRCA1-A complex subunit RAP80

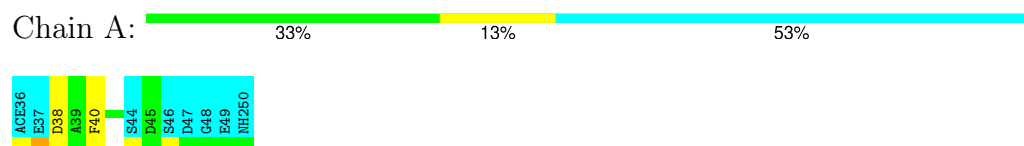


- Molecule 2: Small ubiquitin-related modifier 2

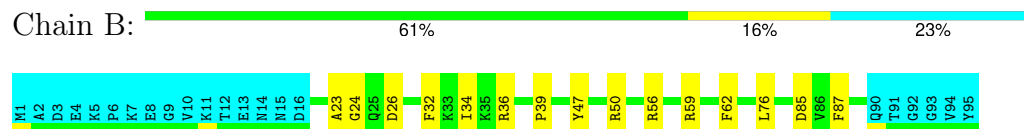


### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: BRCA1-A complex subunit RAP80

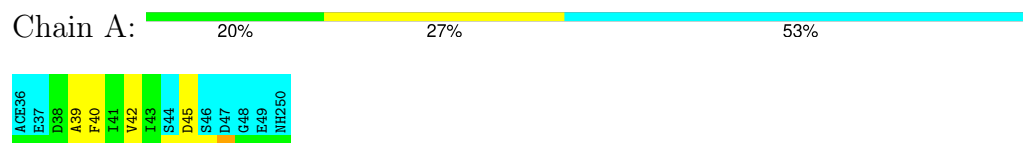


- Molecule 2: Small ubiquitin-related modifier 2

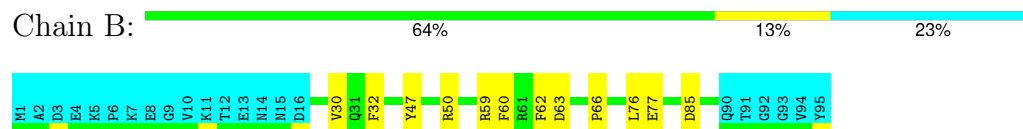


### 4.2.8 Score per residue for model 8

- Molecule 1: BRCA1-A complex subunit RAP80

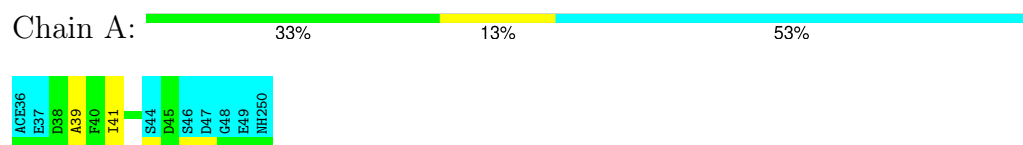


- Molecule 2: Small ubiquitin-related modifier 2

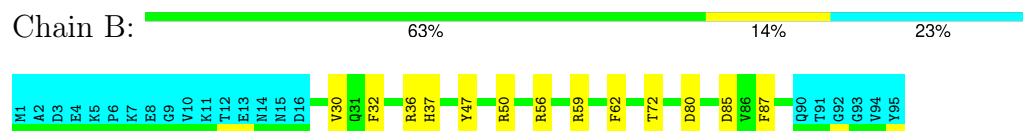


### 4.2.9 Score per residue for model 9

- Molecule 1: BRCA1-A complex subunit RAP80

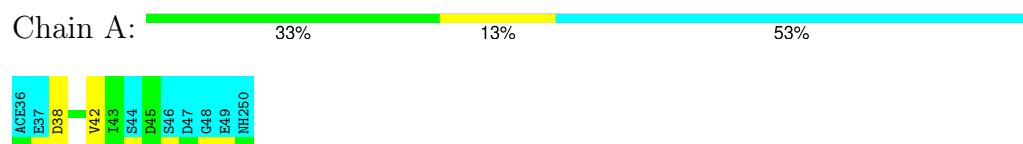


- Molecule 2: Small ubiquitin-related modifier 2

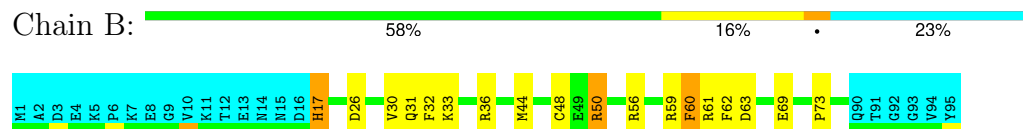


### 4.2.10 Score per residue for model 10

- Molecule 1: BRCA1-A complex subunit RAP80



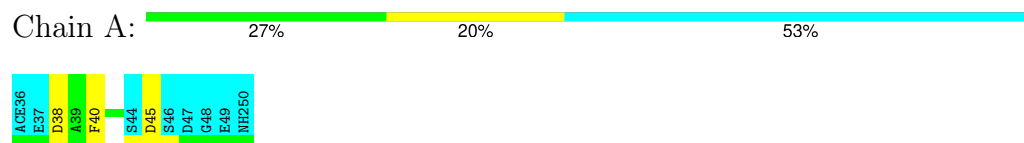
- Molecule 2: Small ubiquitin-related modifier 2



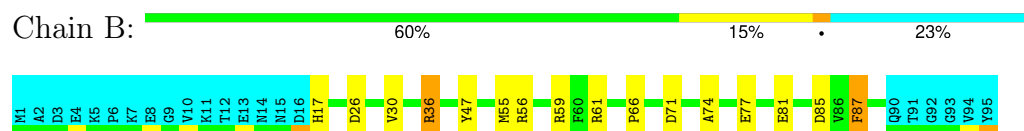


### 4.2.11 Score per residue for model 11

- Molecule 1: BRCA1-A complex subunit RAP80

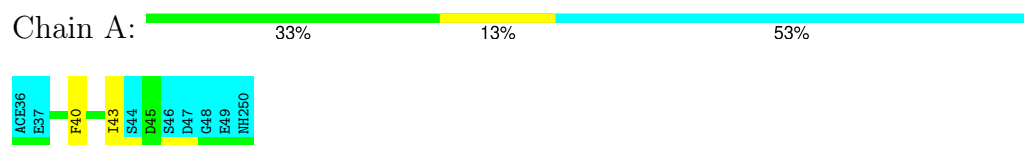


- Molecule 2: Small ubiquitin-related modifier 2

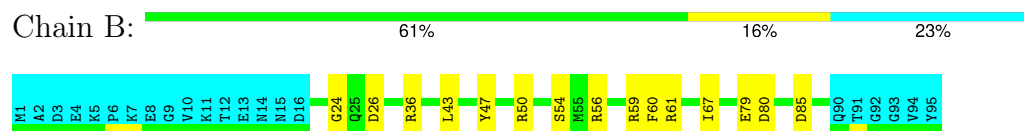


### 4.2.12 Score per residue for model 12

- Molecule 1: BRCA1-A complex subunit RAP80

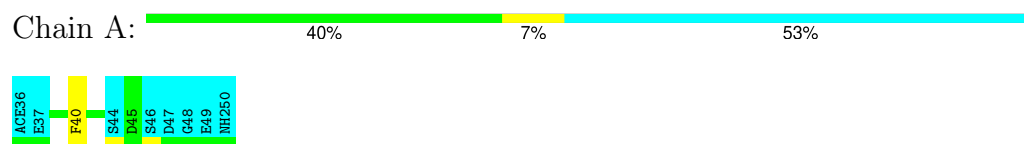


- Molecule 2: Small ubiquitin-related modifier 2

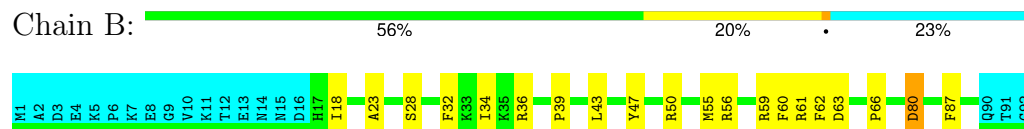


### 4.2.13 Score per residue for model 13

- Molecule 1: BRCA1-A complex subunit RAP80

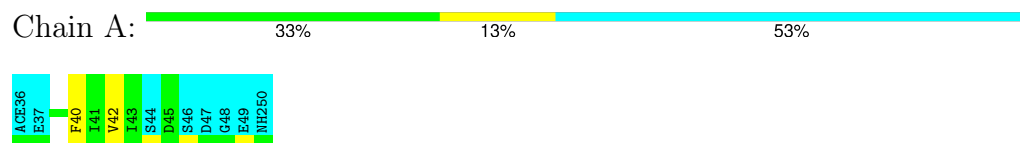


- Molecule 2: Small ubiquitin-related modifier 2

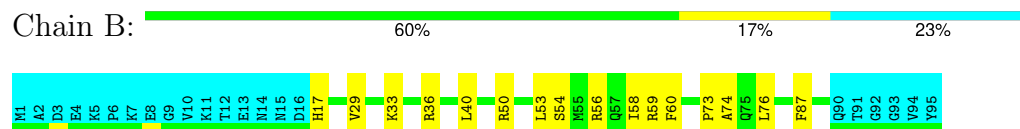


#### 4.2.14 Score per residue for model 14

- Molecule 1: BRCA1-A complex subunit RAP80

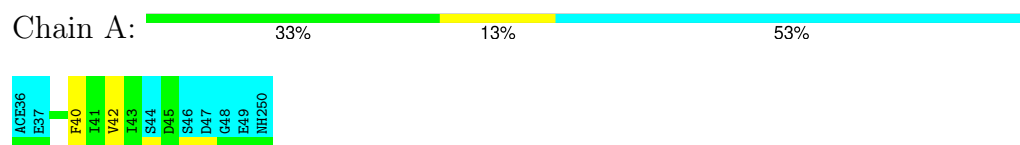


- Molecule 2: Small ubiquitin-related modifier 2

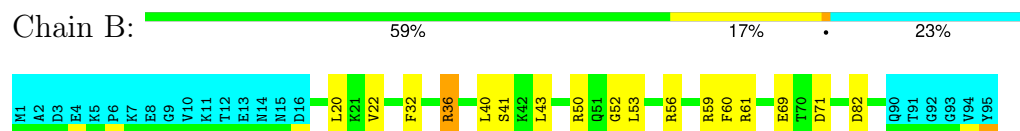


#### 4.2.15 Score per residue for model 15

- Molecule 1: BRCA1-A complex subunit RAP80

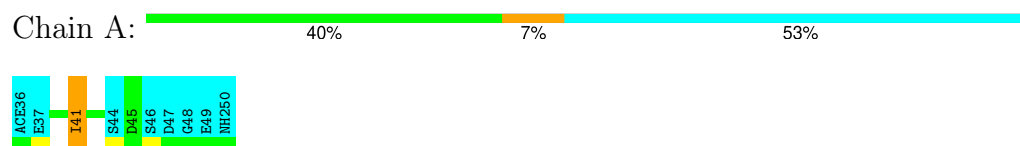


- Molecule 2: Small ubiquitin-related modifier 2

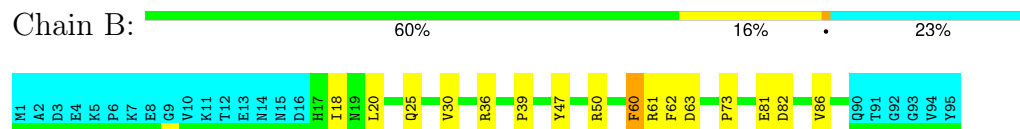


#### 4.2.16 Score per residue for model 16

- Molecule 1: BRCA1-A complex subunit RAP80

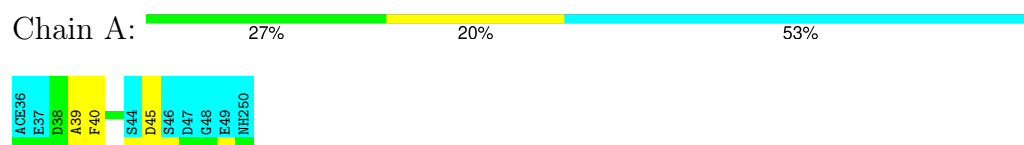


- Molecule 2: Small ubiquitin-related modifier 2

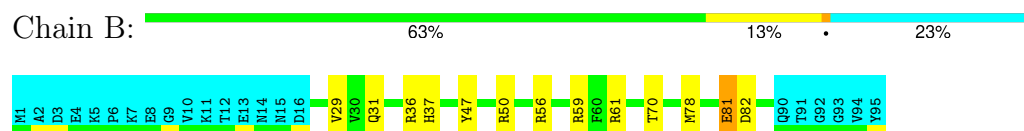


### 4.2.17 Score per residue for model 17

- Molecule 1: BRCA1-A complex subunit RAP80

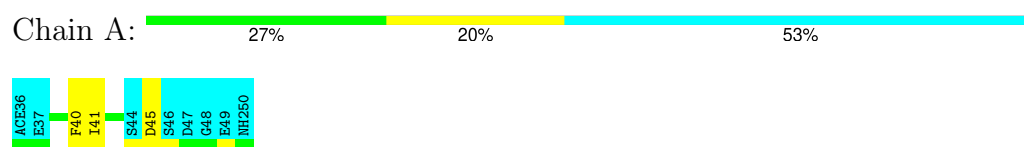


- Molecule 2: Small ubiquitin-related modifier 2

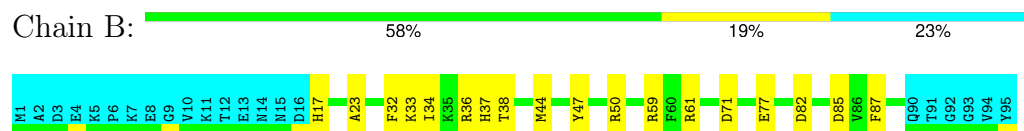


### 4.2.18 Score per residue for model 18

- Molecule 1: BRCA1-A complex subunit RAP80

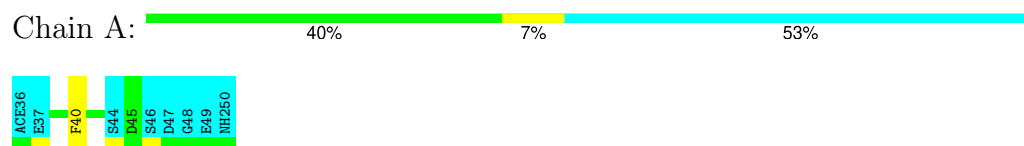


- Molecule 2: Small ubiquitin-related modifier 2

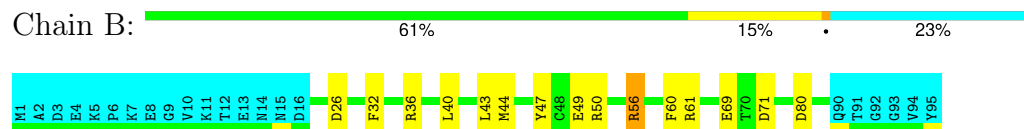


### 4.2.19 Score per residue for model 19

- Molecule 1: BRCA1-A complex subunit RAP80




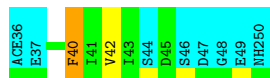
- Molecule 2: Small ubiquitin-related modifier 2



#### 4.2.20 Score per residue for model 20

- Molecule 1: BRCA1-A complex subunit RAP80

Chain A:  33% 7% 7% 53%



- Molecule 2: Small ubiquitin-related modifier 2

Chain B:  62% 14% • 23%



## 5 Refinement protocol and experimental data overview

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

Of the 20 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
Amber	structure solution	14
Amber	refinement	14

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	392
Number of shifts mapped to atoms	392
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	29%

## 6 Model quality (i)

### 6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, NH2, SEP

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	1.48±0.13	0±0/54 ( 0.3± 0.7%)	2.10±0.19	2±1/71 ( 2.7± 1.4%)
2	B	1.50±0.03	2±1/603 ( 0.4± 0.2%)	1.95±0.10	15±4/810 ( 1.8± 0.5%)
All	All	1.50	53/13140 ( 0.4%)	1.96	333/17620 ( 1.9%)

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	0.1±0.4
2	B	0.0±0.0	1.6±1.5
All	All	0	34

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
2	B	50	ARG	CZ-NH2	-7.77	1.23	1.33	20	1
2	B	56	ARG	CZ-NH2	-6.47	1.24	1.33	9	4
2	B	87	PHE	CG-CD1	6.34	1.48	1.38	9	1
2	B	60	PHE	CG-CD1	6.30	1.48	1.38	19	1
2	B	47	TYR	CG-CD2	6.27	1.47	1.39	1	2
2	B	54	SER	CB-OG	6.27	1.50	1.42	14	1
2	B	50	ARG	CZ-NH1	-6.12	1.25	1.33	12	2
2	B	47	TYR	CE1-CZ	6.09	1.46	1.38	13	3
2	B	86	VAL	N-CA	6.09	1.58	1.46	3	1
2	B	48	CYS	CB-SG	-6.03	1.72	1.82	10	1
2	B	58	ILE	N-CA	5.98	1.58	1.46	2	1
2	B	61	ARG	CZ-NH2	-5.96	1.25	1.33	20	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	27	GLY	CA-C	5.93	1.61	1.51	4	1
2	B	73	PRO	N-CD	-5.78	1.39	1.47	16	1
2	B	61	ARG	CZ-NH1	-5.70	1.25	1.33	4	2
1	A	45	ASP	CA-CB	5.64	1.66	1.53	11	1
2	B	62	PHE	CG-CD1	5.50	1.47	1.38	5	1
2	B	28	SER	CA-CB	-5.47	1.44	1.52	13	2
2	B	36	ARG	CZ-NH1	-5.46	1.25	1.33	19	1
2	B	49	GLU	CG-CD	5.44	1.60	1.51	6	1
2	B	59	ARG	CZ-NH2	-5.43	1.25	1.33	6	2
2	B	47	TYR	CB-CG	5.39	1.59	1.51	19	1
2	B	62	PHE	CG-CD2	5.38	1.46	1.38	13	1
2	B	52	GLY	CA-C	5.37	1.60	1.51	20	2
1	A	40	PHE	CE2-CZ	5.33	1.47	1.37	7	1
2	B	26	ASP	N-CA	5.28	1.56	1.46	20	1
2	B	24	GLY	CA-C	5.26	1.60	1.51	12	1
2	B	47	TYR	CD1-CE1	5.26	1.47	1.39	6	2
1	A	40	PHE	CG-CD1	5.24	1.46	1.38	13	1
2	B	38	THR	N-CA	5.17	1.56	1.46	18	1
2	B	69	GLU	CD-OE2	5.14	1.31	1.25	4	1
2	B	59	ARG	CZ-NH1	-5.12	1.26	1.33	8	2
2	B	81	GLU	CD-OE1	-5.09	1.20	1.25	17	1
2	B	61	ARG	CD-NE	5.07	1.55	1.46	2	1
2	B	32	PHE	CG-CD2	5.06	1.46	1.38	10	1
2	B	66	PRO	N-CD	-5.04	1.40	1.47	13	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
2	B	50	ARG	NE-CZ-NH1	20.30	130.45	120.30	20	12
2	B	36	ARG	NE-CZ-NH1	20.05	130.32	120.30	7	13
2	B	50	ARG	NE-CZ-NH2	-16.07	112.27	120.30	7	7
2	B	56	ARG	NE-CZ-NH2	-14.55	113.03	120.30	3	14
2	B	36	ARG	NE-CZ-NH2	-14.29	113.15	120.30	11	8
2	B	59	ARG	NE-CZ-NH1	13.06	126.83	120.30	12	13
2	B	59	ARG	NE-CZ-NH2	-12.69	113.95	120.30	7	4
2	B	61	ARG	NE-CZ-NH2	-12.46	114.07	120.30	1	7
2	B	61	ARG	NE-CZ-NH1	12.21	126.40	120.30	18	10
2	B	87	PHE	CB-CG-CD2	11.88	129.12	120.80	4	5
2	B	63	ASP	CB-CG-OD1	11.62	128.75	118.30	13	2
2	B	56	ARG	NE-CZ-NH1	11.17	125.89	120.30	4	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	80	ASP	CB-CG-OD1	10.83	128.04	118.30	13	3
2	B	80	ASP	CB-CG-OD2	10.71	127.94	118.30	12	1
2	B	56	ARG	NH1-CZ-NH2	-10.25	108.13	119.40	15	2
2	B	85	ASP	CB-CG-OD1	-10.18	109.14	118.30	20	5
1	A	40	PHE	CB-CG-CD1	-10.08	113.75	120.80	13	6
2	B	26	ASP	CB-CG-OD1	9.64	126.97	118.30	12	5
2	B	60	PHE	CB-CG-CD2	9.38	127.37	120.80	16	4
2	B	47	TYR	CB-CG-CD1	-8.71	115.78	121.00	13	6
2	B	82	ASP	CB-CG-OD1	8.50	125.95	118.30	5	3
2	B	26	ASP	CB-CG-OD2	8.49	125.94	118.30	10	4
1	A	38	ASP	CB-CG-OD1	8.43	125.88	118.30	10	2
2	B	50	ARG	NH1-CZ-NH2	-8.37	110.20	119.40	20	2
1	A	40	PHE	CB-CG-CD2	-8.36	114.95	120.80	11	7
2	B	74	ALA	N-CA-CB	-8.35	98.41	110.10	11	1
2	B	47	TYR	CG-CD2-CE2	-8.33	114.63	121.30	3	3
2	B	62	PHE	CB-CG-CD2	-8.21	115.06	120.80	2	1
2	B	62	PHE	CB-CG-CD1	-8.19	115.07	120.80	5	3
2	B	50	ARG	CD-NE-CZ	8.14	135.00	123.60	13	3
2	B	47	TYR	CB-CG-CD2	-8.02	116.19	121.00	20	3
2	B	60	PHE	CB-CG-CD1	-7.71	115.40	120.80	13	6
2	B	85	ASP	CB-CG-OD2	7.69	125.22	118.30	7	2
2	B	63	ASP	CB-CG-OD2	7.58	125.12	118.30	6	5
1	A	42	VAL	CG1-CB-CG2	-7.52	98.87	110.90	10	4
1	A	38	ASP	CB-CG-OD2	7.50	125.05	118.30	11	4
2	B	66	PRO	N-CA-CB	7.40	112.18	103.30	8	2
2	B	49	GLU	OE1-CD-OE2	-7.33	114.51	123.30	19	1
1	A	45	ASP	CB-CG-OD1	7.31	124.88	118.30	17	2
2	B	30	VAL	CA-CB-CG2	7.20	121.70	110.90	4	4
2	B	87	PHE	CB-CG-CD1	-7.19	115.77	120.80	11	2
2	B	22	VAL	CA-CB-CG2	7.12	121.59	110.90	15	1
2	B	74	ALA	CB-CA-C	7.09	120.74	110.10	14	1
2	B	55	MET	CA-CB-CG	-6.96	101.47	113.30	4	2
2	B	59	ARG	NH1-CZ-NH2	-6.95	111.76	119.40	13	3
2	B	76	LEU	CB-CG-CD2	6.87	122.67	111.00	7	1
2	B	36	ARG	CD-NE-CZ	6.80	133.12	123.60	7	2
2	B	32	PHE	CB-CG-CD1	-6.75	116.08	120.80	2	3
2	B	36	ARG	NH1-CZ-NH2	-6.67	112.06	119.40	13	7
2	B	56	ARG	CB-CA-C	6.67	123.74	110.40	2	1
2	B	23	ALA	N-CA-CB	-6.66	100.77	110.10	7	2
2	B	39	PRO	N-CA-CB	6.59	111.21	103.30	7	1
2	B	77	GLU	CB-CA-C	6.49	123.39	110.40	11	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	42	VAL	CA-CB-CG2	6.49	120.63	110.90	8	3
2	B	38	THR	CA-CB-CG2	6.48	121.47	112.40	5	1
2	B	30	VAL	CA-CB-CG1	6.40	120.50	110.90	5	2
1	A	39	ALA	CB-CA-C	6.36	119.63	110.10	8	1
2	B	33	LYS	CB-CA-C	6.32	123.04	110.40	5	1
1	A	45	ASP	CB-CG-OD2	6.31	123.98	118.30	2	3
2	B	60	PHE	CG-CD1-CE1	-6.31	113.86	120.80	13	1
2	B	37	HIS	O-C-N	-6.30	112.62	122.70	3	1
2	B	73	PRO	N-CA-CB	6.25	110.80	103.30	20	4
2	B	71	ASP	CB-CG-OD2	6.21	123.89	118.30	11	2
2	B	60	PHE	CD1-CG-CD2	6.20	126.36	118.30	13	1
2	B	30	VAL	CG1-CB-CG2	-6.12	101.10	110.90	16	1
2	B	73	PRO	N-CD-CG	6.12	112.38	103.20	5	1
2	B	54	SER	N-CA-CB	-6.08	101.37	110.50	12	1
2	B	32	PHE	CB-CG-CD2	-6.06	116.56	120.80	8	6
1	A	41	ILE	CA-CB-CG1	6.05	122.50	111.00	9	3
2	B	71	ASP	CB-CG-OD1	6.05	123.74	118.30	18	4
2	B	76	LEU	CB-CA-C	5.98	121.57	110.20	8	2
2	B	23	ALA	CA-C-O	5.96	132.61	120.10	13	1
2	B	23	ALA	CB-CA-C	-5.94	101.19	110.10	13	1
2	B	30	VAL	C-N-CA	5.93	136.51	121.70	8	1
2	B	47	TYR	CG-CD1-CE1	-5.92	116.57	121.30	19	2
2	B	76	LEU	N-CA-CB	-5.91	98.59	110.40	3	1
2	B	82	ASP	CB-CG-OD2	5.89	123.60	118.30	17	4
2	B	77	GLU	OE1-CD-OE2	-5.84	116.29	123.30	18	2
1	A	40	PHE	CZ-CE2-CD2	-5.79	113.15	120.10	14	2
2	B	78	MET	CG-SD-CE	-5.78	90.96	100.20	17	1
2	B	61	ARG	NH1-CZ-NH2	-5.73	113.10	119.40	11	2
2	B	86	VAL	CG1-CB-CG2	-5.64	101.88	110.90	4	1
2	B	34	ILE	CA-CB-CG1	5.64	121.71	111.00	13	1
2	B	18	ILE	C-N-CA	5.62	135.75	121.70	16	1
2	B	34	ILE	CA-CB-CG2	5.61	122.13	110.90	7	1
2	B	58	ILE	CA-CB-CG1	5.61	121.66	111.00	14	1
2	B	62	PHE	CZ-CE2-CD2	-5.60	113.38	120.10	9	2
2	B	62	PHE	CG-CD1-CE1	-5.59	114.65	120.80	7	1
2	B	44	MET	CG-SD-CE	5.58	109.13	100.20	3	3
2	B	67	ILE	O-C-N	5.57	131.62	122.70	12	1
2	B	31	GLN	O-C-N	-5.56	113.80	122.70	10	1
2	B	29	VAL	CA-CB-CG2	5.51	119.16	110.90	1	1
2	B	52	GLY	O-C-N	-5.50	113.89	122.70	15	1
2	B	76	LEU	CB-CG-CD1	-5.46	101.71	111.00	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	40	LEU	CB-CG-CD2	5.44	120.25	111.00	15	1
1	A	45	ASP	N-CA-CB	-5.43	100.82	110.60	8	1
2	B	40	LEU	CB-CG-CD1	5.43	120.22	111.00	14	1
2	B	85	ASP	OD1-CG-OD2	5.42	133.60	123.30	20	1
2	B	47	TYR	CD1-CE1-CZ	-5.41	114.93	119.80	6	1
2	B	44	MET	CA-CB-CG	5.38	122.44	113.30	3	1
2	B	69	GLU	OE1-CD-OE2	-5.38	116.85	123.30	20	2
2	B	38	THR	CA-CB-OG1	5.36	120.26	109.00	6	1
2	B	83	THR	CA-CB-CG2	5.36	119.90	112.40	4	1
2	B	25	GLN	C-N-CA	5.35	135.09	121.70	5	1
2	B	47	TYR	CZ-CE2-CD2	5.34	124.61	119.80	17	1
2	B	32	PHE	CD1-CE1-CZ	-5.34	113.69	120.10	1	1
2	B	39	PRO	N-CD-CG	5.33	111.19	103.20	16	1
2	B	17	HIS	N-CA-CB	-5.32	101.02	110.60	10	1
1	A	43	ILE	CA-CB-CG1	5.32	121.11	111.00	12	1
2	B	27	GLY	C-N-CA	5.29	134.91	121.70	1	1
2	B	75	GLN	CB-CA-C	5.27	120.95	110.40	6	1
2	B	66	PRO	N-CD-CG	5.25	111.08	103.20	11	1
2	B	29	VAL	CG1-CB-CG2	-5.25	102.50	110.90	14	1
2	B	70	THR	CA-C-N	5.24	128.73	117.20	17	1
2	B	72	THR	CA-CB-CG2	-5.22	105.09	112.40	9	2
2	B	43	LEU	CD1-CG-CD2	-5.22	94.84	110.50	19	1
2	B	59	ARG	CD-NE-CZ	5.21	130.89	123.60	11	1
2	B	55	MET	CG-SD-CE	5.17	108.47	100.20	13	1
2	B	85	ASP	CB-CA-C	-5.13	100.13	110.40	2	1
2	B	18	ILE	CB-CA-C	5.13	121.86	111.60	13	1
2	B	20	LEU	CB-CG-CD2	5.13	119.72	111.00	16	1
2	B	48	CYS	N-CA-CB	-5.12	101.39	110.60	5	1
2	B	37	HIS	CA-CB-CG	5.11	122.28	113.60	9	1
2	B	79	GLU	OE1-CD-OE2	-5.07	117.21	123.30	12	1
2	B	20	LEU	CB-CG-CD1	-5.05	102.41	111.00	15	1
2	B	44	MET	O-C-N	-5.04	114.64	122.70	18	1
2	B	26	ASP	O-C-N	-5.04	114.64	123.20	7	1
2	B	60	PHE	CG-CD2-CE2	-5.03	115.27	120.80	13	1
2	B	20	LEU	CB-CA-C	5.03	119.75	110.20	2	1
2	B	25	GLN	O-C-N	-5.01	114.68	122.70	16	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)
2	B	36	ARG	Sidechain	4
2	B	53	LEU	Peptide	3
2	B	56	ARG	Sidechain	3
2	B	87	PHE	Sidechain	3
2	B	47	TYR	Sidechain	3
2	B	50	ARG	Sidechain	3
1	A	40	PHE	Sidechain	2
2	B	59	ARG	Sidechain	2
2	B	81	GLU	Peptide	2
2	B	25	GLN	Peptide	1
2	B	29	VAL	Peptide	1
1	A	43	ILE	Mainchain	1
2	B	24	GLY	Mainchain	1
2	B	60	PHE	Sidechain	1
2	B	17	HIS	Sidechain	1
2	B	39	PRO	Mainchain	1
2	B	43	LEU	Mainchain	1
2	B	37	HIS	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	55	53	53	0±0
2	B	593	588	588	1±1
All	All	12960	12820	12820	11

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:17:HIS:CG	2:B:33:LYS:HE2	0.55	2.36	14	2
2:B:17:HIS:ND1	2:B:33:LYS:HE2	0.46	2.25	10	1
1:A:41:ILE:HD12	2:B:30:VAL:HG11	0.46	1.88	2	1
2:B:43:LEU:HD12	2:B:43:LEU:N	0.45	2.26	12	2
2:B:60:PHE:CD2	2:B:86:VAL:HG22	0.45	2.47	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:40:LEU:O	2:B:44:MET:HG3	0.45	2.12	19	1
2:B:72:THR:H	2:B:75:GLN:HB3	0.43	1.73	1	1
2:B:41:SER:HB3	2:B:69:GLU:O	0.42	2.14	15	1
2:B:58:ILE:HD12	2:B:60:PHE:CZ	0.41	2.51	5	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	7/15 (47%)	5±1 (70±13%)	2±1 (28±13%)	0±0 (2±5%)	8	48
2	B	73/95 (77%)	71±1 (97±2%)	2±1 (3±2%)	0±0 (0±1%)	38	78
All	All	1600/2200 (73%)	1509 (94%)	84 (5%)	7 (0%)	32	76

All 4 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	39	ALA	3
2	B	69	GLU	2
2	B	81	GLU	1
2	B	34	ILE	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	6/9 (67%)	6±0 (94±8%)	0±0 (6±8%)	19	71
2	B	66/84 (79%)	65±1 (99±1%)	1±1 (1±1%)	66	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1440/1860 (77%)	1417 (98%)	23 (2%)	58 93

All 15 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	40	PHE	4
2	B	82	ASP	2
2	B	57	GLN	2
2	B	29	VAL	2
1	A	41	ILE	2
2	B	80	ASP	2
1	A	42	VAL	1
2	B	30	VAL	1
2	B	20	LEU	1
2	B	81	GLU	1
2	B	43	LEU	1
2	B	50	ARG	1
2	B	31	GLN	1
2	B	37	HIS	1
2	B	85	ASP	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	SEP	A	44	1	8,9,10	1.50±0.22	2±1 (21±11%)
1	SEP	A	46	1	8,9,10	1.62±0.31	2±1 (26±12%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	SEP	A	44	1	7,12,14	2.16±0.88	1±1 (17±11%)
1	SEP	A	46	1	7,12,14	1.98±0.86	2±1 (23±12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	A	46	1	-	0±0,6,8,10	-
1	SEP	A	44	1	-	0±0,6,8,10	-

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	46	SEP	CA-N	3.92	1.59	1.48	10	3
1	A	44	SEP	P-O2P	3.45	1.42	1.54	12	14
1	A	46	SEP	CB-CA	3.35	1.61	1.52	14	5
1	A	46	SEP	P-OG	3.32	1.49	1.60	5	2
1	A	46	SEP	P-O2P	3.17	1.43	1.54	19	12
1	A	46	SEP	P-O3P	3.11	1.43	1.54	20	14
1	A	44	SEP	P-O3P	3.06	1.43	1.54	12	13
1	A	44	SEP	CA-N	2.82	1.55	1.48	7	1
1	A	46	SEP	P-O1P	2.66	1.42	1.50	9	3
1	A	44	SEP	P-O1P	2.64	1.42	1.50	18	1
1	A	46	SEP	OG-CB	2.59	1.34	1.44	13	2
1	A	46	SEP	O-C	2.56	1.29	1.20	6	2
1	A	44	SEP	P-OG	2.49	1.52	1.60	13	3
1	A	44	SEP	CB-CA	2.33	1.58	1.52	7	1
1	A	44	SEP	O-C	2.20	1.28	1.20	3	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	44	SEP	OG-CB-CA	12.47	120.28	108.14	16	16
1	A	46	SEP	OG-CB-CA	9.97	117.85	108.14	10	14
1	A	46	SEP	OG-P-O1P	3.46	97.09	106.44	13	10
1	A	46	SEP	O3P-P-O2P	3.05	119.24	107.80	2	7
1	A	46	SEP	O3P-P-OG	2.91	99.09	106.67	20	1
1	A	44	SEP	O3P-P-OG	2.90	99.10	106.67	1	2
1	A	44	SEP	O3P-P-O2P	2.70	117.93	107.80	1	4
1	A	44	SEP	OG-P-O1P	2.38	100.00	106.44	13	2
1	A	44	SEP	O3P-P-O1P	2.14	119.17	110.83	9	1
1	A	46	SEP	O3P-P-O1P	2.12	119.09	110.83	11	1

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 29% for the well-defined parts and 27% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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	392
Number of shifts mapped to atoms	392
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	81	$-0.08 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	74	$-0.18 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	75	$0.05 \pm 0.07$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	81	$0.59 \pm 0.39$	None needed (imprecise)

#### 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 29%, i.e. 322 atoms were assigned a chemical shift out of a possible 1126. 0 out of 10 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	261/398 (66%)	67/161 (42%)	127/160 (79%)	67/77 (87%)
Sidechain	61/655 (9%)	0/421 (0%)	61/204 (30%)	0/30 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	0/73 (0%)	0/37 (0%)	0/34 (0%)	0/2 (0%)
Overall	322/1126 (29%)	67/619 (11%)	188/398 (47%)	67/109 (61%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 392 atoms were assigned a chemical shift out of a possible 1435. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	318/530 (60%)	81/216 (38%)	156/212 (74%)	81/102 (79%)
Sidechain	74/823 (9%)	0/525 (0%)	74/262 (28%)	0/36 (0%)
Aromatic	0/82 (0%)	0/41 (0%)	0/39 (0%)	0/2 (0%)
Overall	392/1435 (27%)	81/782 (10%)	230/513 (45%)	81/140 (58%)

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

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain B:

