



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 06:15 PM BST

PDB ID : 1X9L  
Title : Solution structure of CuI-DR1885 from Deinococcus Radiodurans  
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Deposited on : 2004-08-23

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

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

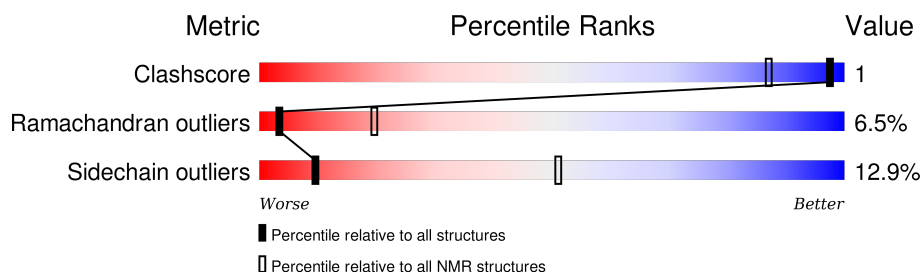
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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

Mol	Chain	Length	Quality of chain
1	A	149	

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *minimized average structure*.

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:28-A:144 (117)	0.52	9

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

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

The models can be grouped into 2 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2216 atoms, of which 1137 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CuI-DR1885.

Mol	Chain	Residues	Atoms						Trace
1	A	149	Total	C	H	N	O	S	0
			2215	673	1137	195	200	10	

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q9RT80
A	146	ILE	-	CLONING ARTIFACT	UNP Q9RT80
A	147	GLU	-	CLONING ARTIFACT	UNP Q9RT80
A	148	GLY	-	CLONING ARTIFACT	UNP Q9RT80
A	149	ARG	-	CLONING ARTIFACT	UNP Q9RT80

- Molecule 2 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

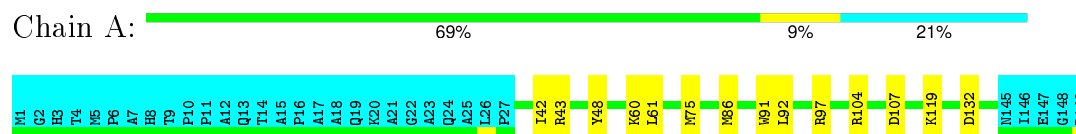
Mol	Chain	Residues	Atoms	
2	A	1	Total	Cu
			1	1

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

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

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: CuI-DR1885

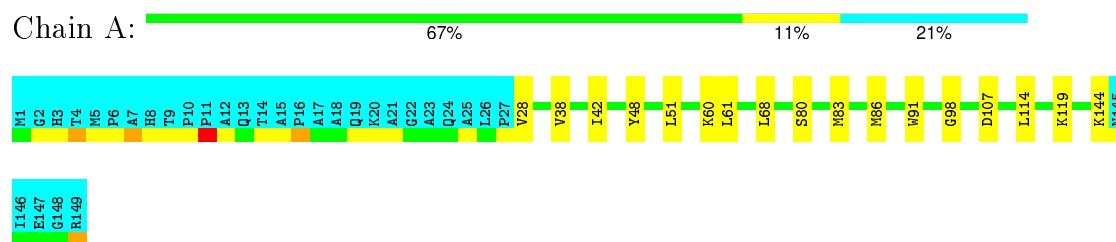


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

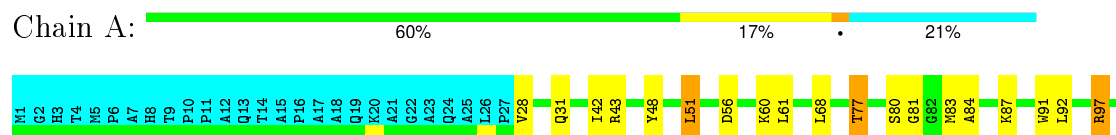
#### 4.2.1 Score per residue for model 1

- Molecule 1: CuI-DR1885



#### 4.2.2 Score per residue for model 2

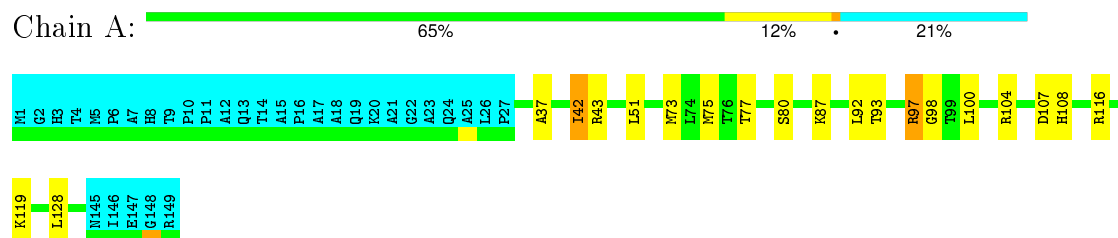
- Molecule 1: CuI-DR1885





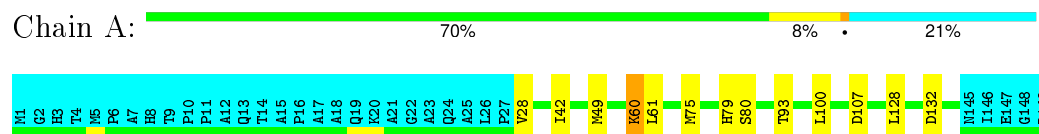
### 4.2.3 Score per residue for model 3

- Molecule 1: CuI-DR1885



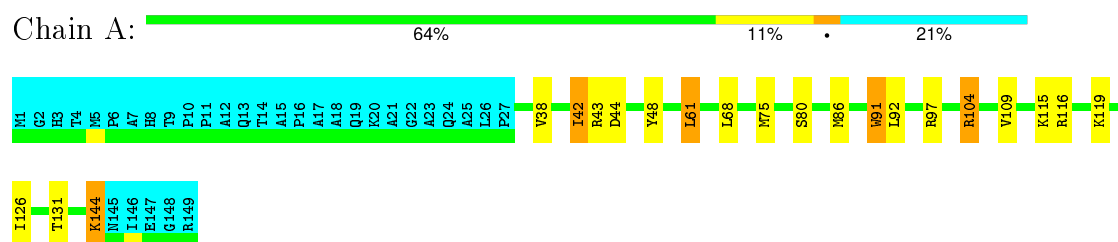
### 4.2.4 Score per residue for model 4

- Molecule 1: CuI-DR1885



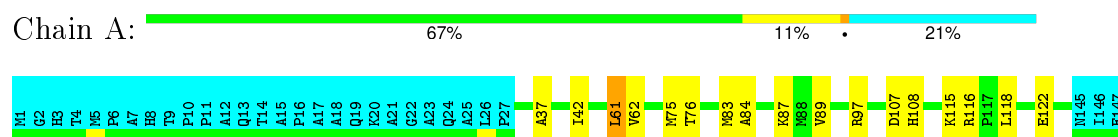
### 4.2.5 Score per residue for model 5

- Molecule 1: CuI-DR1885



### 4.2.6 Score per residue for model 6

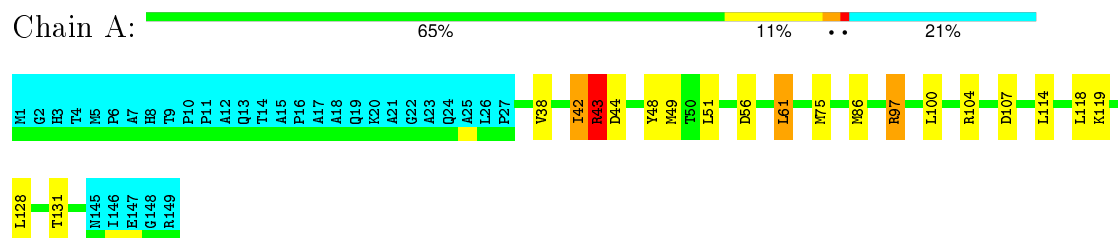
- Molecule 1: CuI-DR1885





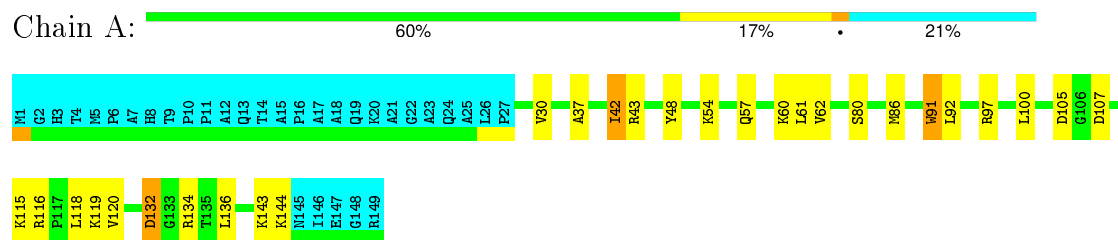
#### 4.2.7 Score per residue for model 7

- Molecule 1: CuI-DR1885



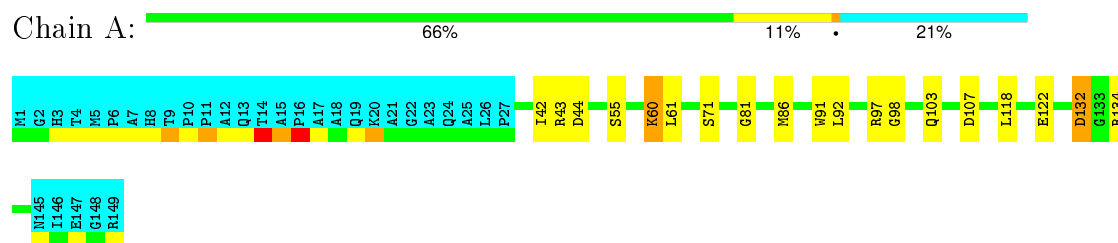
#### 4.2.8 Score per residue for model 8

- Molecule 1: CuI-DR1885



#### 4.2.9 Score per residue for model 9 (medoid)

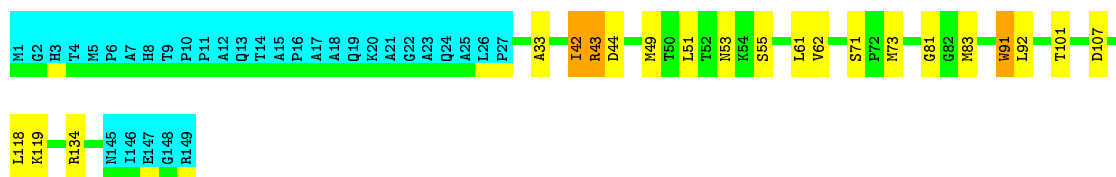
- Molecule 1: CuI-DR1885



#### 4.2.10 Score per residue for model 10

- Molecule 1: CuI-DR1885

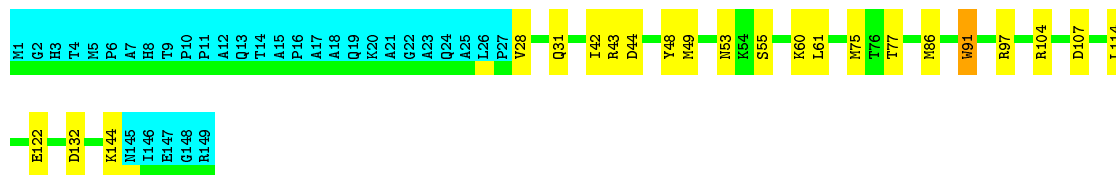




#### 4.2.11 Score per residue for model 11

- Molecule 1: CuI-DR1885

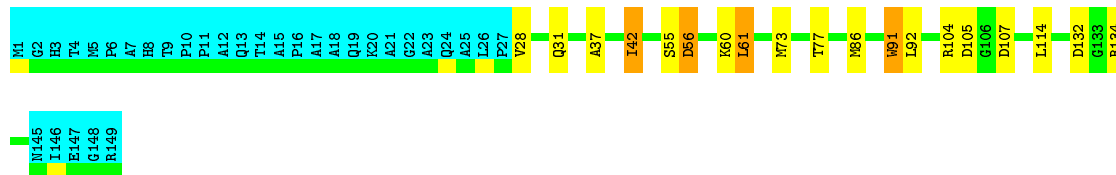
Chain A: 64%



#### 4.2.12 Score per residue for model 12

- Molecule 1: CuI-DR1885

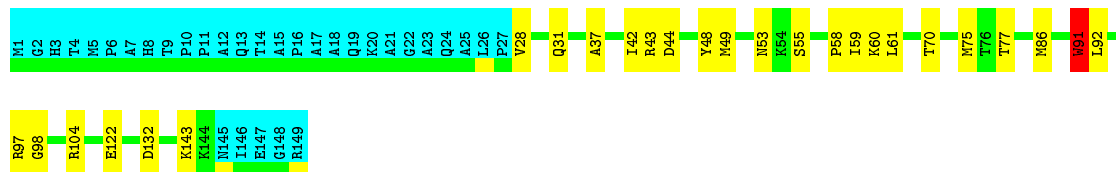
Chain A: 66%



#### 4.2.13 Score per residue for model 13

- Molecule 1: CuI-DR1885

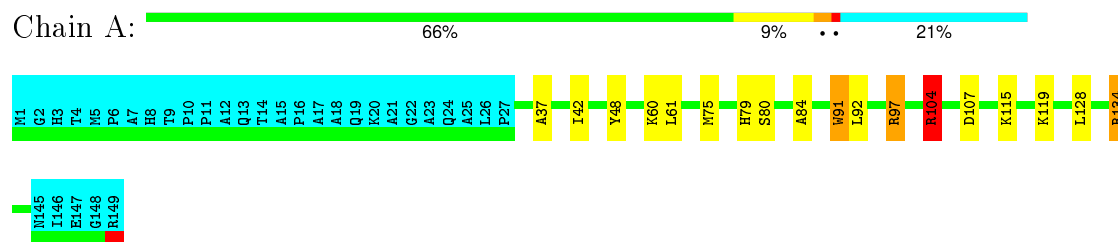
Chain A: 61%



#### 4.2.14 Score per residue for model 14

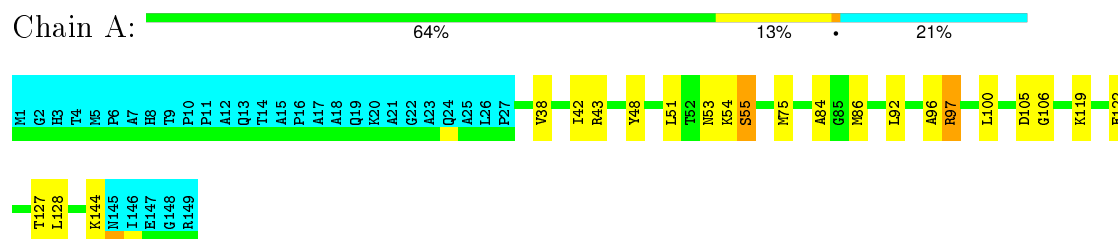
- Molecule 1: CuI-DR1885





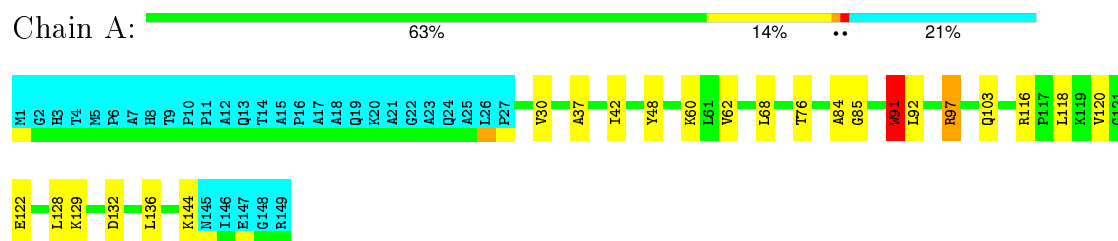
#### 4.2.15 Score per residue for model 15

- Molecule 1: CuI-DR1885



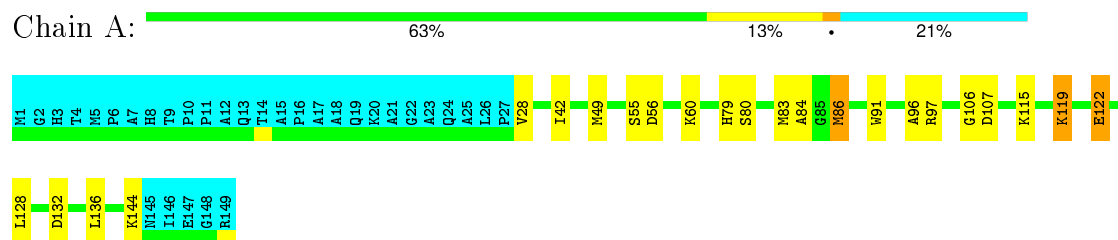
#### 4.2.16 Score per residue for model 16

- Molecule 1: CuI-DR1885



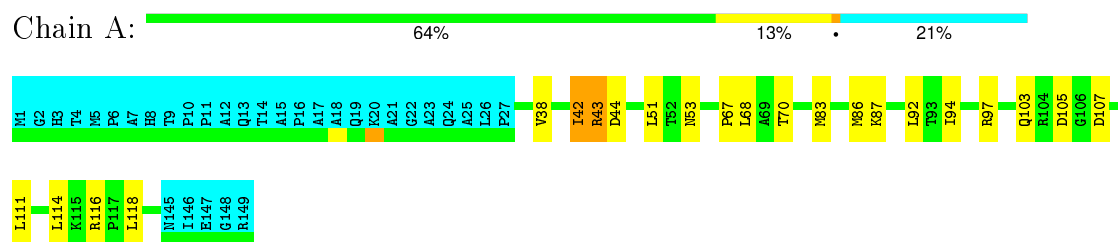
#### 4.2.17 Score per residue for model 17

- Molecule 1: CuI-DR1885



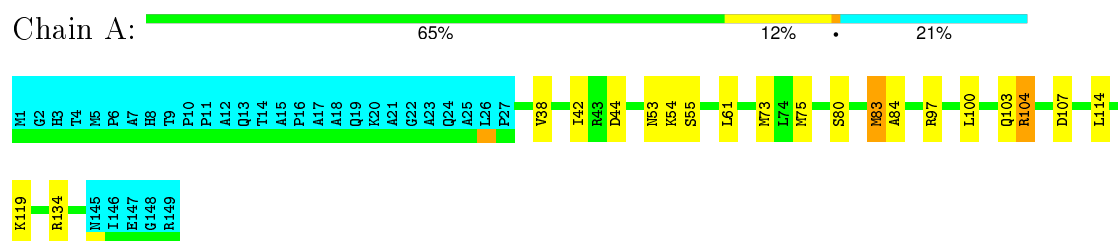
### 4.2.18 Score per residue for model 18

- Molecule 1: CuI-DR1885



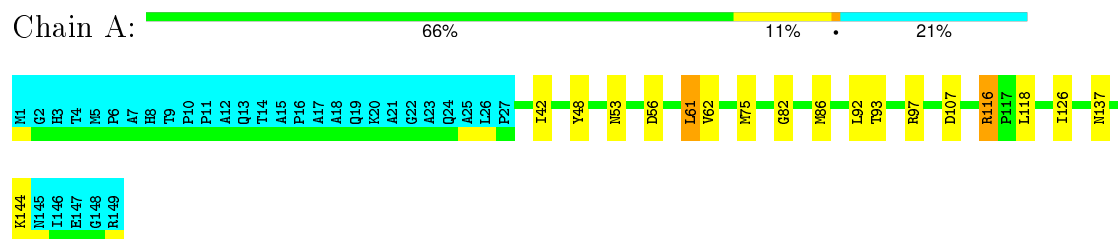
### 4.2.19 Score per residue for model 19

- Molecule 1: CuI-DR1885



### 4.2.20 Score per residue for model 20

- Molecule 1: CuI-DR1885



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 20 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
DYANA	refinement	1.5

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality

### 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU1

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	0.47±0.00	0±0/866 (0.0±0.0%)	0.96±0.03	0±1/1180 (0.0±0.1%)
All	All	0.47	0/17320 (0.0%)	0.97	6/23600 (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	1.2±0.9
All	All	0	24

There are no bond-length outliers.

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	104	ARG	NE-CZ-NH2	-5.95	117.32	120.30	14	1
1	A	97	ARG	NE-CZ-NH2	-5.93	117.33	120.30	15	1
1	A	91	TRP	CB-CG-CD2	5.24	133.41	126.60	16	1
1	A	77	THR	CA-CB-CG2	5.18	119.65	112.40	2	1
1	A	134	ARG	NE-CZ-NH1	5.14	122.87	120.30	2	1
1	A	134	ARG	NE-CZ-NH2	-5.12	117.74	120.30	14	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	48	TYR	Sidechain	11
1	A	97	ARG	Sidechain	3
1	A	104	ARG	Sidechain	3
1	A	37	ALA	Peptide	2
1	A	134	ARG	Sidechain	2
1	A	83	MET	Peptide	1
1	A	108	HIS	Sidechain	1
1	A	55	SER	Peptide	1

## 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	853	914	914	1±1
All	All	17080	18280	18280	27

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:53:ASN:HD21	1:A:94:ILE:HD12	0.58	1.57	18	1
1:A:42:ILE:HG22	1:A:43:ARG:H	0.46	1.69	8	5
1:A:62:VAL:HB	1:A:91:TRP:CD1	0.45	2.46	16	1
1:A:61:LEU:HD13	1:A:61:LEU:C	0.45	2.32	6	3
1:A:61:LEU:C	1:A:61:LEU:HD13	0.44	2.33	12	3
1:A:42:ILE:HG22	1:A:43:ARG:N	0.43	2.28	3	2
1:A:60:LYS:NZ	1:A:132:ASP:OD1	0.43	2.51	4	1
1:A:28:VAL:HG22	1:A:51:LEU:HG	0.43	1.91	2	1
1:A:51:LEU:HD23	1:A:94:ILE:HD13	0.42	1.92	18	1
1:A:91:TRP:C	1:A:92:LEU:HD22	0.42	2.35	13	1
1:A:58:PRO:C	1:A:59:ILE:HD12	0.42	2.36	13	1
1:A:81:GLY:HA3	1:A:100:LEU:HD13	0.41	1.91	2	1
1:A:60:LYS:NZ	1:A:132:ASP:OD2	0.41	2.53	17	2
1:A:79:HIS:CD2	1:A:84:ALA:CB	0.41	3.04	17	1
1:A:119:LYS:NZ	1:A:122:GLU:OE2	0.40	2.54	17	1
1:A:28:VAL:O	1:A:28:VAL:HG13	0.40	2.16	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:ASP:OD2	1:A:97:ARG:NH1	0.40	2.55	20	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	117/149 (79%)	81±4 (69±3%)	28±3 (24±3%)	8±1 (6±1%)	<b>3</b>	<b>19</b>
All	All	2340/2980 (79%)	1626 (69%)	563 (24%)	151 (6%)	<b>3</b>	<b>19</b>

All 35 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	42	ILE	20
1	A	107	ASP	15
1	A	91	TRP	11
1	A	80	SER	9
1	A	55	SER	8
1	A	116	ARG	7
1	A	97	ARG	7
1	A	38	VAL	6
1	A	84	ALA	6
1	A	28	VAL	6
1	A	37	ALA	5
1	A	98	GLY	4
1	A	62	VAL	4
1	A	86	MET	4
1	A	43	ARG	3
1	A	105	ASP	3
1	A	132	ASP	3
1	A	144	LYS	3
1	A	120	VAL	2
1	A	79	HIS	2
1	A	106	GLY	2

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ASP	2
1	A	131	THR	2
1	A	83	MET	2
1	A	114	LEU	2
1	A	81	GLY	2
1	A	96	ALA	2
1	A	30	VAL	2
1	A	118	LEU	1
1	A	68	LEU	1
1	A	67	PRO	1
1	A	108	HIS	1
1	A	82	GLY	1
1	A	85	GLY	1
1	A	33	ALA	1

### 6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	94/115 (82%)	82±2 (87±3%)	12±2 (13±3%)	9	51
All	All	1880/2300 (82%)	1638 (87%)	242 (13%)	9	51

All 51 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	61	LEU	14
1	A	92	LEU	12
1	A	75	MET	11
1	A	119	LYS	10
1	A	97	ARG	10
1	A	60	LYS	10
1	A	91	TRP	9
1	A	86	MET	9
1	A	118	LEU	8
1	A	44	ASP	8
1	A	122	GLU	8

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Mol	Chain	Res	Type	Models (Total)
1	A	104	ARG	8
1	A	128	LEU	7
1	A	53	ASN	6
1	A	43	ARG	6
1	A	49	MET	6
1	A	100	LEU	6
1	A	51	LEU	6
1	A	83	MET	5
1	A	77	THR	5
1	A	132	ASP	5
1	A	115	LYS	5
1	A	144	LYS	5
1	A	73	MET	4
1	A	134	ARG	4
1	A	136	LEU	4
1	A	68	LEU	4
1	A	103	GLN	4
1	A	114	LEU	4
1	A	87	LYS	4
1	A	31	GLN	4
1	A	56	ASP	3
1	A	93	THR	3
1	A	126	ILE	2
1	A	71	SER	2
1	A	105	ASP	2
1	A	54	LYS	2
1	A	70	THR	2
1	A	76	THR	2
1	A	143	LYS	2
1	A	107	ASP	1
1	A	101	THR	1
1	A	57	GLN	1
1	A	116	ARG	1
1	A	127	THR	1
1	A	109	VAL	1
1	A	129	LYS	1
1	A	111	LEU	1
1	A	137	ASN	1
1	A	42	ILE	1
1	A	89	VAL	1



### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

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

### 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

No chemical shift data were provided