



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2HX6  
Title : Solution structure analysis of the phage T4 endoribonuclease RegB  
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Deposited on : 2006-08-02

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

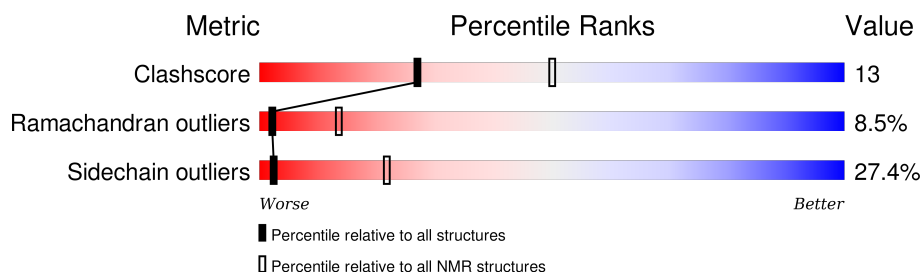
# 1 Overall quality at a glance

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	153	

## 2 Ensemble composition and analysis ⓘ

This entry contains 15 models. Model 8 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:4-A:81, A:102-A:141, A:150-A:153 (122)	0.82	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 2 clusters and 1 single-model cluster was found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2528 atoms, of which 1266 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ribonuclease.

Mol	Chain	Residues	Atoms						Trace
1	A	153	Total	C	H	N	O	S	0
			2528	798	1266	228	231	5	

There is a discrepancy between the modelled and reference sequences:

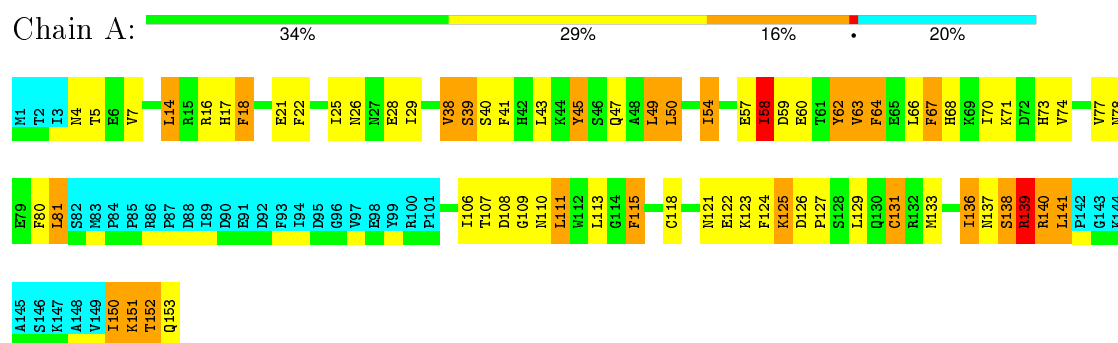
Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	HIS	ENGINEERED	UNP P13312

## 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: Ribonuclease

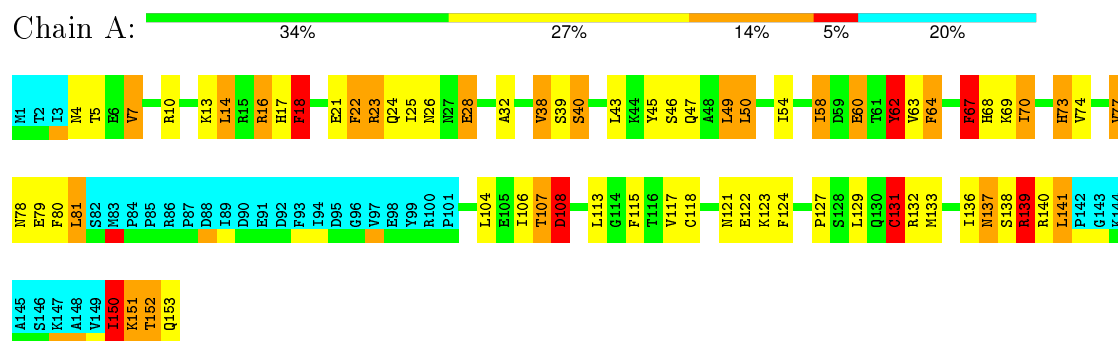


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

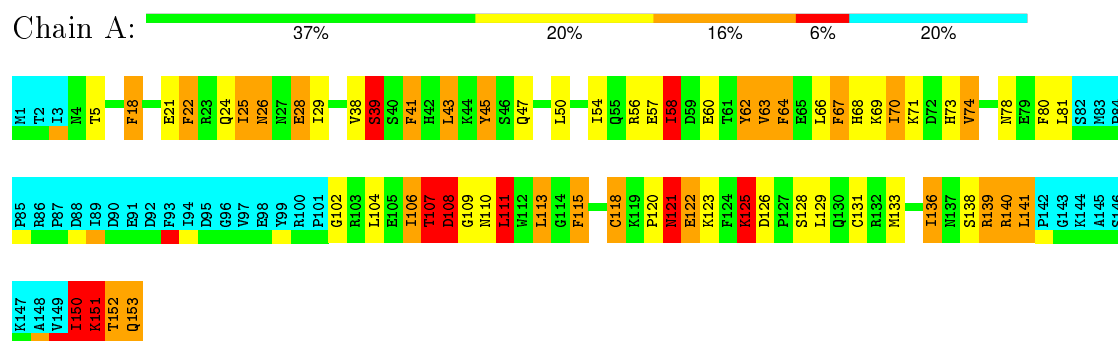
#### 4.2.1 Score per residue for model 1

- Molecule 1: Ribonuclease



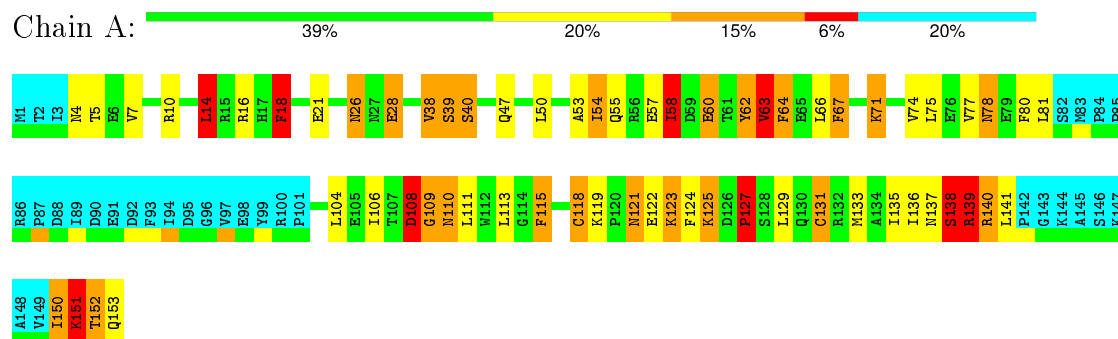
### 4.2.2 Score per residue for model 2

- Molecule 1: Ribonuclease



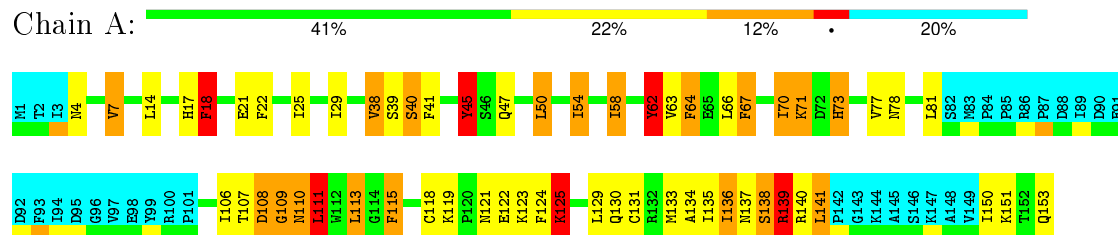
### 4.2.3 Score per residue for model 3

- Molecule 1: Ribonuclease



### 4.2.4 Score per residue for model 4

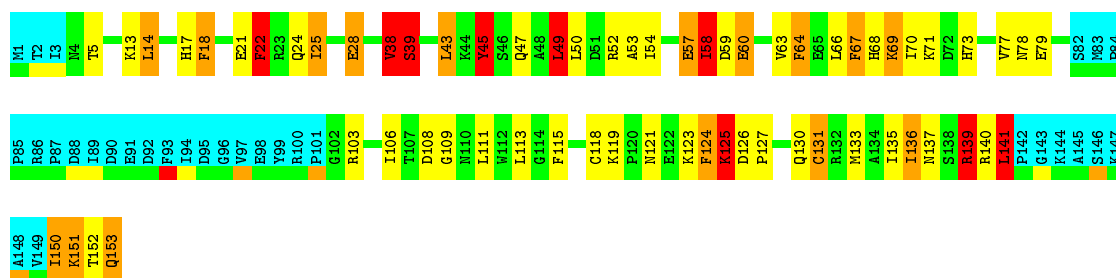
- Molecule 1: Ribonuclease



### 4.2.5 Score per residue for model 5

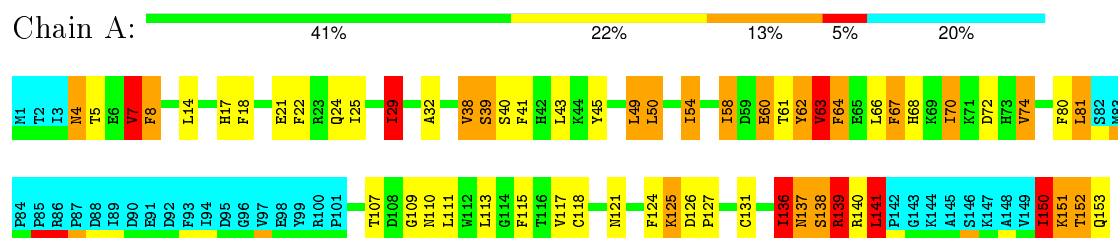
- Molecule 1: Ribonuclease





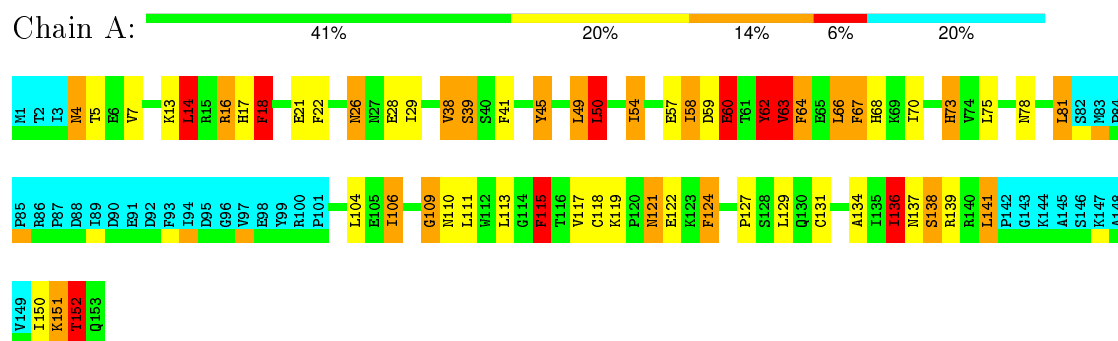
### 4.2.9 Score per residue for model 9

- Molecule 1: Ribonuclease



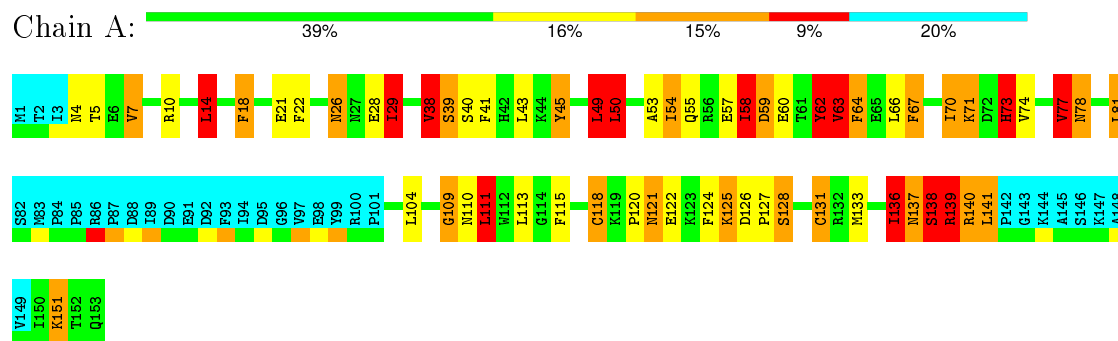
### 4.2.10 Score per residue for model 10

- Molecule 1: Ribonuclease



### 4.2.11 Score per residue for model 11

- Molecule 1: Ribonuclease

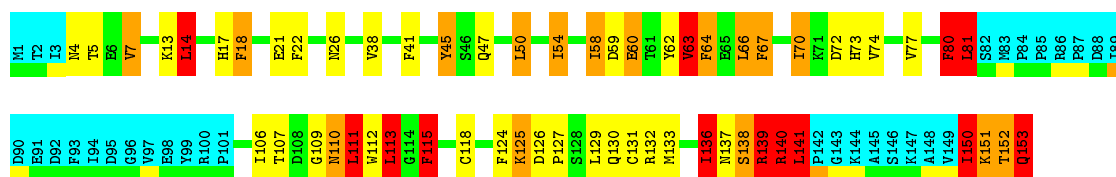


### 4.2.12 Score per residue for model 12

- Molecule 1: Ribonuclease

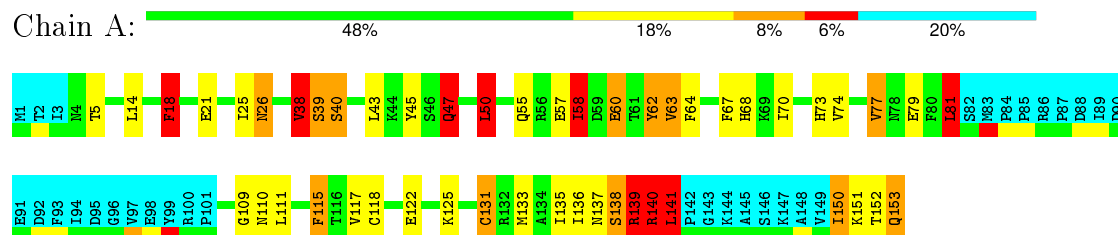






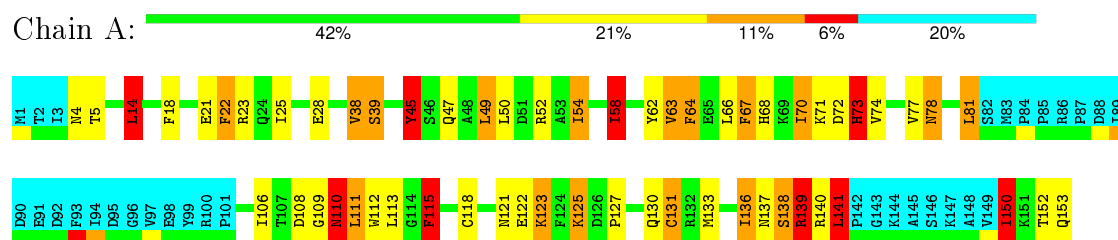
#### 4.2.13 Score per residue for model 13

- Molecule 1: Ribonuclease



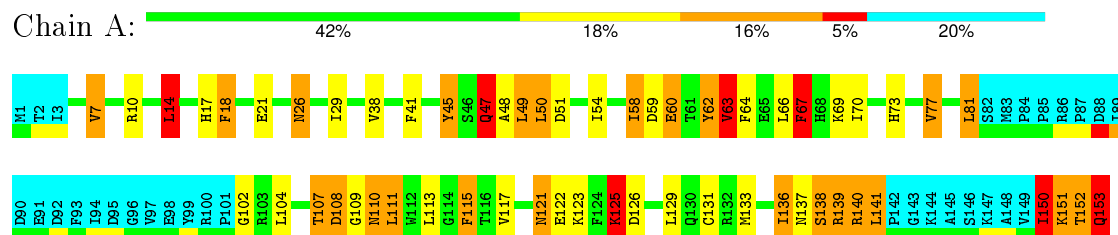
#### 4.2.14 Score per residue for model 14

- Molecule 1: Ribonuclease



#### 4.2.15 Score per residue for model 15

- Molecule 1: Ribonuclease



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *mix of manual and automatic NOE assignment procedure*.

Of the 30 calculated structures, 15 were deposited, based on the following criterion: *structures with acceptable covalent geometry, structures with favorable non-bond energy, structures with the least restraint violations*.

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

Software name	Classification	Version
INCA	structure solution	1.0
INCA	refinement	1.0

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 i

### 6.1 Standard geometry i

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	1.12±0.01	0±0/1041 (0.0±0.0%)	1.88±0.08	30±4/1395 (2.1±0.3%)
All	All	1.12	1/15615 (0.0%)	1.88	444/20925 (2.1%)

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	4.3±1.7
All	All	0	64

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	109	GLY	CA-C	-6.07	1.42	1.51	4	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	45	TYR	CB-CG-CD1	21.65	133.99	121.00	7	12
1	A	45	TYR	CB-CG-CD2	-20.64	108.61	121.00	7	11
1	A	62	TYR	CB-CG-CD1	15.79	130.47	121.00	4	10
1	A	62	TYR	CB-CG-CD2	-15.63	111.62	121.00	4	3
1	A	150	ILE	C-N-CA	12.56	153.11	121.70	1	7
1	A	138	SER	N-CA-CB	11.79	128.18	110.50	15	5
1	A	140	ARG	C-N-CA	11.53	150.52	121.70	13	3
1	A	115	PHE	CB-CG-CD1	11.40	128.78	120.80	13	6
1	A	152	THR	C-N-CA	10.66	148.36	121.70	5	7
1	A	125	LYS	CB-CA-C	9.78	129.95	110.40	5	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	PHE	CB-CG-CD1	9.77	127.64	120.80	7	1
1	A	80	PHE	CB-CG-CD1	9.45	127.41	120.80	9	6
1	A	152	THR	CA-C-N	-9.44	96.44	117.20	5	5
1	A	81	LEU	CB-CG-CD1	9.37	126.94	111.00	15	3
1	A	22	PHE	CB-CG-CD2	-9.26	114.31	120.80	7	1
1	A	139	ARG	C-N-CA	9.26	144.85	121.70	15	3
1	A	29	ILE	CA-CB-CG1	9.24	128.55	111.00	11	2
1	A	111	LEU	N-CA-CB	8.89	128.17	110.40	8	6
1	A	141	LEU	N-CA-CB	8.78	127.97	110.40	5	1
1	A	77	VAL	CB-CA-C	8.75	128.02	111.40	8	7
1	A	18	PHE	CB-CG-CD2	8.73	126.91	120.80	11	4
1	A	115	PHE	CB-CG-CD2	-8.68	114.72	120.80	7	6
1	A	152	THR	CA-CB-CG2	-8.56	100.41	112.40	3	4
1	A	14	LEU	CB-CG-CD2	8.46	125.39	111.00	14	7
1	A	26	ASN	CB-CA-C	8.44	127.27	110.40	2	4
1	A	107	THR	CA-CB-CG2	8.39	124.15	112.40	2	3
1	A	60	GLU	CB-CA-C	8.33	127.06	110.40	9	6
1	A	67	PHE	CB-CG-CD2	-8.06	115.16	120.80	7	1
1	A	151	LYS	CB-CA-C	-7.96	94.49	110.40	1	7
1	A	60	GLU	C-N-CA	7.88	141.40	121.70	1	1
1	A	28	GLU	N-CA-CB	7.80	124.64	110.60	3	3
1	A	50	LEU	CD1-CG-CD2	7.67	133.53	110.50	13	1
1	A	45	TYR	CA-CB-CG	7.60	127.84	113.40	7	2
1	A	73	HIS	CA-CB-CG	7.57	126.46	113.60	11	1
1	A	18	PHE	CB-CG-CD1	-7.54	115.52	120.80	11	6
1	A	139	ARG	N-CA-CB	7.48	124.07	110.60	12	3
1	A	59	ASP	CB-CA-C	7.46	125.32	110.40	10	1
1	A	125	LYS	C-N-CA	7.45	140.32	121.70	15	2
1	A	125	LYS	N-CA-CB	7.42	123.95	110.60	4	3
1	A	110	ASN	CA-CB-CG	7.40	129.69	113.40	14	1
1	A	80	PHE	CB-CG-CD2	-7.38	115.63	120.80	9	5
1	A	133	MET	CG-SD-CE	-7.31	88.51	100.20	2	7
1	A	151	LYS	CA-CB-CG	7.30	129.46	113.40	2	1
1	A	109	GLY	C-N-CA	7.28	139.90	121.70	9	9
1	A	8	PHE	CB-CG-CD1	7.24	125.87	120.80	9	1
1	A	124	PHE	C-N-CA	7.21	139.72	121.70	4	2
1	A	122	GLU	C-N-CA	7.18	139.65	121.70	4	8
1	A	69	LYS	N-CA-CB	7.09	123.37	110.60	5	3
1	A	72	ASP	C-N-CA	7.08	139.39	121.70	14	2
1	A	43	LEU	CB-CA-C	7.07	123.64	110.20	2	2
1	A	139	ARG	CB-CG-CD	7.05	129.93	111.60	5	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	67	PHE	N-CA-CB	7.05	123.28	110.60	9	11
1	A	64	PHE	CB-CG-CD2	-7.04	115.88	120.80	4	1
1	A	71	LYS	C-N-CA	6.95	139.08	121.70	4	2
1	A	128	SER	N-CA-CB	6.95	120.92	110.50	11	2
1	A	152	THR	N-CA-C	6.91	129.65	111.00	10	1
1	A	50	LEU	CB-CA-C	6.81	123.14	110.20	4	5
1	A	153	GLN	CB-CA-C	6.75	123.90	110.40	15	2
1	A	121	ASN	N-CA-C	6.75	129.22	111.00	2	2
1	A	141	LEU	CB-CG-CD1	-6.67	99.66	111.00	2	4
1	A	152	THR	N-CA-CB	-6.60	97.77	110.30	2	3
1	A	151	LYS	N-CA-CB	-6.57	98.77	110.60	7	4
1	A	110	ASN	C-N-CA	6.56	138.10	121.70	4	4
1	A	81	LEU	CB-CG-CD2	-6.54	99.88	111.00	14	6
1	A	21	GLU	CB-CA-C	6.54	123.47	110.40	7	1
1	A	131	CYS	N-CA-CB	6.52	122.34	110.60	11	6
1	A	136	ILE	C-N-CA	6.52	137.99	121.70	11	5
1	A	40	SER	N-CA-CB	6.51	120.27	110.50	4	5
1	A	38	VAL	C-N-CA	6.51	137.97	121.70	10	5
1	A	74	VAL	CA-CB-CG2	-6.50	101.15	110.90	3	2
1	A	129	LEU	CB-CG-CD1	6.48	122.02	111.00	4	3
1	A	63	VAL	CA-CB-CG1	6.46	120.58	110.90	15	12
1	A	22	PHE	CB-CG-CD1	6.44	125.31	120.80	7	3
1	A	63	VAL	CG1-CB-CG2	-6.44	100.59	110.90	9	4
1	A	118	CYS	C-N-CA	6.44	137.80	121.70	3	2
1	A	121	ASN	C-N-CA	6.44	137.80	121.70	6	1
1	A	8	PHE	CB-CG-CD2	-6.42	116.31	120.80	9	1
1	A	107	THR	N-CA-CB	6.38	122.42	110.30	1	1
1	A	78	ASN	CB-CA-C	6.33	123.06	110.40	3	1
1	A	49	LEU	CB-CA-C	-6.30	98.22	110.20	11	1
1	A	108	ASP	N-CA-CB	6.27	121.89	110.60	4	5
1	A	58	ILE	CB-CA-C	6.27	124.14	111.60	11	3
1	A	141	LEU	N-CA-C	6.27	127.92	111.00	12	2
1	A	78	ASN	CA-CB-CG	6.24	127.13	113.40	14	2
1	A	141	LEU	CB-CG-CD2	6.24	121.60	111.00	9	3
1	A	137	ASN	CB-CA-C	6.21	122.81	110.40	1	1
1	A	70	ILE	C-N-CA	6.20	137.19	121.70	14	2
1	A	139	ARG	CA-CB-CG	6.15	126.94	113.40	11	7
1	A	120	PRO	C-N-CA	6.14	137.05	121.70	2	1
1	A	54	ILE	CG1-CB-CG2	-6.12	97.93	111.40	8	5
1	A	50	LEU	CB-CG-CD2	-6.12	100.60	111.00	12	1
1	A	126	ASP	CA-C-N	6.02	133.96	117.10	2	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	64	PHE	CB-CG-CD1	-6.00	116.60	120.80	8	2
1	A	57	GLU	C-N-CA	5.99	136.68	121.70	2	3
1	A	38	VAL	CG1-CB-CG2	5.96	120.44	110.90	5	1
1	A	54	ILE	CA-CB-CG1	5.95	122.30	111.00	15	2
1	A	67	PHE	CB-CA-C	5.88	122.17	110.40	5	2
1	A	140	ARG	N-CA-CB	5.87	121.16	110.60	15	1
1	A	111	LEU	CB-CA-C	-5.84	99.10	110.20	4	1
1	A	113	LEU	CB-CA-C	-5.82	99.14	110.20	6	2
1	A	45	TYR	N-CA-CB	5.82	121.08	110.60	9	1
1	A	108	ASP	C-N-CA	5.81	134.49	122.30	3	1
1	A	127	PRO	CB-CA-C	5.80	126.50	112.00	3	2
1	A	18	PHE	CB-CA-C	-5.79	98.81	110.40	13	1
1	A	39	SER	CB-CA-C	5.79	121.11	110.10	2	1
1	A	151	LYS	N-CA-C	5.79	126.64	111.00	7	2
1	A	58	ILE	N-CA-C	5.79	126.62	111.00	2	3
1	A	138	SER	C-N-CA	5.77	136.12	121.70	3	1
1	A	122	GLU	N-CA-C	-5.73	95.53	111.00	13	1
1	A	118	CYS	N-CA-CB	5.73	120.91	110.60	1	2
1	A	45	TYR	CB-CA-C	-5.72	98.95	110.40	15	1
1	A	153	GLN	N-CA-C	5.70	126.39	111.00	12	1
1	A	58	ILE	CA-CB-CG1	5.69	121.81	111.00	11	1
1	A	73	HIS	C-N-CA	5.67	135.86	121.70	14	1
1	A	139	ARG	N-CA-C	-5.66	95.72	111.00	4	2
1	A	38	VAL	CA-CB-CG2	5.65	119.38	110.90	14	1
1	A	74	VAL	CB-CA-C	-5.60	100.75	111.40	2	1
1	A	138	SER	CB-CA-C	-5.60	99.45	110.10	11	1
1	A	47	GLN	CA-C-N	5.58	129.49	117.20	8	2
1	A	53	ALA	CB-CA-C	-5.58	101.73	110.10	3	1
1	A	7	VAL	CG1-CB-CG2	5.57	119.81	110.90	15	4
1	A	152	THR	CA-C-O	5.55	131.76	120.10	5	1
1	A	150	ILE	N-CA-C	5.55	125.99	111.00	9	1
1	A	136	ILE	CA-CB-CG1	5.55	121.54	111.00	12	1
1	A	4	ASN	C-N-CA	5.53	135.51	121.70	14	1
1	A	139	ARG	CA-C-N	5.52	129.35	117.20	13	1
1	A	150	ILE	CA-CB-CG1	5.52	121.49	111.00	8	1
1	A	77	VAL	CA-CB-CG2	5.52	119.17	110.90	8	3
1	A	49	LEU	CB-CG-CD2	5.50	120.35	111.00	5	1
1	A	134	ALA	N-CA-CB	-5.49	102.41	110.10	4	1
1	A	47	GLN	CB-CA-C	5.49	121.38	110.40	13	1
1	A	68	HIS	CB-CA-C	5.49	121.37	110.40	7	1
1	A	81	LEU	CA-CB-CG	5.47	127.89	115.30	13	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	70	ILE	CA-CB-CG1	-5.46	100.64	111.00	9	1
1	A	39	SER	N-CA-C	5.45	125.72	111.00	9	1
1	A	136	ILE	CB-CA-C	-5.44	100.72	111.60	10	1
1	A	72	ASP	CB-CA-C	-5.43	99.55	110.40	9	2
1	A	23	ARG	CA-CB-CG	5.42	125.33	113.40	1	1
1	A	23	ARG	N-CA-CB	5.42	120.35	110.60	1	1
1	A	124	PHE	CB-CG-CD1	5.39	124.57	120.80	5	1
1	A	55	GLN	CB-CA-C	-5.38	99.65	110.40	3	1
1	A	22	PHE	N-CA-CB	5.36	120.25	110.60	1	1
1	A	127	PRO	CA-N-CD	-5.33	104.03	111.50	3	2
1	A	151	LYS	O-C-N	-5.33	114.17	122.70	12	1
1	A	124	PHE	CB-CA-C	-5.32	99.75	110.40	12	2
1	A	113	LEU	N-CA-CB	5.31	121.02	110.40	15	2
1	A	41	PHE	N-CA-CB	5.29	120.13	110.60	11	1
1	A	112	TRP	CB-CG-CD2	-5.29	119.72	126.60	12	1
1	A	63	VAL	CB-CA-C	5.28	121.43	111.40	7	1
1	A	58	ILE	C-N-CA	5.24	134.80	121.70	7	1
1	A	49	LEU	CB-CG-CD1	5.23	119.89	111.00	6	1
1	A	123	LYS	CB-CA-C	5.21	120.81	110.40	2	1
1	A	74	VAL	CA-CB-CG1	5.20	118.70	110.90	3	1
1	A	53	ALA	C-N-CA	5.19	134.69	121.70	11	1
1	A	50	LEU	CB-CG-CD1	-5.19	102.18	111.00	13	1
1	A	63	VAL	C-N-CA	5.15	134.57	121.70	9	2
1	A	129	LEU	N-CA-C	-5.15	97.11	111.00	7	1
1	A	132	ARG	N-CA-C	-5.11	97.20	111.00	12	2
1	A	48	ALA	C-N-CA	5.09	134.41	121.70	15	1
1	A	129	LEU	CB-CG-CD2	-5.05	102.41	111.00	4	1
1	A	60	GLU	N-CA-CB	5.05	119.69	110.60	15	1
1	A	117	VAL	CA-CB-CG1	5.05	118.47	110.90	1	1
1	A	17	HIS	N-CA-CB	5.04	119.66	110.60	10	1
1	A	111	LEU	CB-CG-CD1	5.01	119.53	111.00	2	1
1	A	39	SER	N-CA-CB	5.00	118.00	110.50	7	2

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	64	PHE	Sidechain	12
1	A	62	TYR	Sidechain	12
1	A	45	TYR	Sidechain	8

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	151	LYS	Mainchain,Peptide	7
1	A	115	PHE	Sidechain	5
1	A	139	ARG	Sidechain,Peptide	4
1	A	41	PHE	Sidechain	3
1	A	73	HIS	Sidechain	2
1	A	150	ILE	Peptide	2
1	A	80	PHE	Sidechain	2
1	A	140	ARG	Peptide	1
1	A	138	SER	Peptide	1
1	A	109	GLY	Peptide	1
1	A	81	LEU	Peptide	1
1	A	18	PHE	Sidechain	1
1	A	56	ARG	Sidechain	1
1	A	126	ASP	Peptide	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	1023	1031	1031	27±6
All	All	15345	15465	15461	400

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD12	1:A:111:LEU:HD12	1.00	1.32	2	1
1:A:150:ILE:HD13	1:A:151:LYS:HB3	0.88	1.44	2	1
1:A:50:LEU:HD23	1:A:54:ILE:HD11	0.85	1.48	8	4
1:A:66:LEU:HD12	1:A:111:LEU:HD23	0.85	1.49	3	1
1:A:66:LEU:CD1	1:A:111:LEU:HD12	0.82	2.04	2	1
1:A:136:ILE:HD13	1:A:141:LEU:HD11	0.75	1.56	4	1
1:A:73:HIS:CD2	1:A:152:THR:HB	0.74	2.17	7	1
1:A:50:LEU:CD2	1:A:54:ILE:HD11	0.72	2.13	8	4
1:A:150:ILE:HD13	1:A:151:LYS:O	0.70	1.86	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:ILE:HD13	1:A:151:LYS:HG2	0.70	1.64	12	1
1:A:73:HIS:CD2	1:A:151:LYS:HG3	0.68	2.24	2	1
1:A:50:LEU:HD23	1:A:54:ILE:CD1	0.68	2.18	8	3
1:A:66:LEU:HD13	1:A:111:LEU:HD13	0.67	1.65	5	1
1:A:62:TYR:CE2	1:A:136:ILE:HG21	0.67	2.24	10	2
1:A:73:HIS:NE2	1:A:151:LYS:HG3	0.66	2.06	2	2
1:A:111:LEU:HA	1:A:136:ILE:HG23	0.66	1.67	10	2
1:A:66:LEU:HD11	1:A:151:LYS:HE3	0.65	1.67	3	1
1:A:49:LEU:HD22	1:A:50:LEU:H	0.65	1.51	9	3
1:A:45:TYR:CZ	1:A:50:LEU:HD12	0.65	2.27	14	2
1:A:45:TYR:CE1	1:A:50:LEU:HD12	0.65	2.27	8	1
1:A:106:ILE:HD13	1:A:153:GLN:HG2	0.65	1.68	12	1
1:A:73:HIS:CD2	1:A:152:THR:HA	0.64	2.28	1	1
1:A:73:HIS:CD2	1:A:153:GLN:HA	0.64	2.27	13	1
1:A:106:ILE:HG23	1:A:150:ILE:HD12	0.64	1.67	2	1
1:A:38:VAL:HG22	1:A:81:LEU:HD23	0.64	1.69	14	1
1:A:106:ILE:HD12	1:A:113:LEU:HD23	0.64	1.70	4	1
1:A:111:LEU:HD13	1:A:136:ILE:HD12	0.63	1.69	12	1
1:A:136:ILE:HD13	1:A:141:LEU:HD12	0.63	1.69	7	1
1:A:38:VAL:HG23	1:A:81:LEU:HD11	0.63	1.71	13	2
1:A:29:ILE:HD13	1:A:41:PHE:CE1	0.62	2.29	10	2
1:A:139:ARG:HD3	1:A:140:ARG:HG2	0.62	1.72	1	4
1:A:66:LEU:CD1	1:A:111:LEU:HD23	0.62	2.21	3	1
1:A:138:SER:CB	1:A:141:LEU:HD21	0.62	2.25	10	1
1:A:111:LEU:HB3	1:A:136:ILE:HG23	0.61	1.72	12	5
1:A:111:LEU:HG	1:A:136:ILE:HG23	0.61	1.71	9	1
1:A:39:SER:HB3	1:A:81:LEU:HD21	0.61	1.72	14	1
1:A:18:PHE:O	1:A:22:PHE:HB2	0.60	1.95	7	1
1:A:138:SER:HB3	1:A:141:LEU:HD21	0.60	1.73	10	1
1:A:49:LEU:H	1:A:49:LEU:HD13	0.60	1.56	9	1
1:A:49:LEU:HD22	1:A:50:LEU:N	0.60	2.11	9	1
1:A:49:LEU:HD13	1:A:50:LEU:H	0.60	1.55	14	1
1:A:14:LEU:HD12	1:A:54:ILE:HA	0.60	1.74	8	3
1:A:137:ASN:HA	1:A:141:LEU:HB2	0.60	1.73	11	1
1:A:45:TYR:CE2	1:A:50:LEU:HD12	0.60	2.32	14	1
1:A:60:GLU:O	1:A:63:VAL:HG12	0.60	1.97	3	6
1:A:150:ILE:HD13	1:A:152:THR:H	0.59	1.56	7	1
1:A:70:ILE:HD13	1:A:153:GLN:HB2	0.59	1.74	13	1
1:A:73:HIS:CE1	1:A:106:ILE:HD12	0.59	2.33	1	1
1:A:150:ILE:CD1	1:A:152:THR:H	0.58	2.11	3	2
1:A:70:ILE:HD13	1:A:153:GLN:N	0.58	2.14	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HG	1:A:111:LEU:HD21	0.58	1.75	14	2
1:A:136:ILE:HG22	1:A:137:ASN:H	0.58	1.59	11	5
1:A:139:ARG:CD	1:A:140:ARG:H	0.57	2.11	12	1
1:A:21:GLU:HB3	1:A:64:PHE:CD1	0.57	2.33	14	12
1:A:4:ASN:HA	1:A:7:VAL:HG13	0.57	1.77	12	4
1:A:57:GLU:OE1	1:A:136:ILE:HD12	0.57	1.99	10	1
1:A:18:PHE:CE2	1:A:50:LEU:HD11	0.57	2.33	11	1
1:A:107:THR:O	1:A:150:ILE:HG22	0.57	2.00	12	1
1:A:70:ILE:HD12	1:A:151:LYS:HE2	0.57	1.74	2	1
1:A:66:LEU:CD2	1:A:109:GLY:HA3	0.57	2.30	15	1
1:A:152:THR:O	1:A:152:THR:HG23	0.57	2.00	2	2
1:A:50:LEU:O	1:A:54:ILE:HG22	0.56	1.99	9	1
1:A:50:LEU:HD23	1:A:54:ILE:CG1	0.56	2.30	6	4
1:A:49:LEU:H	1:A:49:LEU:HD22	0.56	1.60	11	1
1:A:45:TYR:CD2	1:A:50:LEU:HD13	0.56	2.35	7	2
1:A:39:SER:HB2	1:A:81:LEU:HD11	0.56	1.77	7	1
1:A:49:LEU:HD11	1:A:133:MET:HA	0.56	1.78	1	1
1:A:106:ILE:HD11	1:A:115:PHE:CE1	0.56	2.36	12	2
1:A:111:LEU:CD2	1:A:136:ILE:HG23	0.55	2.31	4	1
1:A:70:ILE:HG23	1:A:73:HIS:CD2	0.55	2.36	11	1
1:A:70:ILE:HD12	1:A:73:HIS:CE1	0.55	2.35	5	1
1:A:49:LEU:HD13	1:A:50:LEU:N	0.55	2.17	7	3
1:A:108:ASP:HB2	1:A:150:ILE:HG22	0.55	1.79	14	1
1:A:18:PHE:CE1	1:A:50:LEU:HD11	0.55	2.37	3	5
1:A:139:ARG:CD	1:A:140:ARG:HG2	0.55	2.32	8	4
1:A:73:HIS:HE1	1:A:150:ILE:HD11	0.54	1.62	5	1
1:A:38:VAL:HG23	1:A:81:LEU:HD23	0.54	1.79	4	1
1:A:63:VAL:HG23	1:A:111:LEU:HD21	0.54	1.77	15	2
1:A:63:VAL:HG13	1:A:67:PHE:CE1	0.54	2.37	15	1
1:A:81:LEU:HD12	1:A:126:ASP:HA	0.54	1.80	7	1
1:A:66:LEU:HD12	1:A:111:LEU:CD1	0.54	2.21	2	1
1:A:14:LEU:HD23	1:A:54:ILE:HA	0.54	1.79	4	2
1:A:39:SER:CB	1:A:81:LEU:HD11	0.54	2.33	7	1
1:A:25:ILE:HG12	1:A:68:HIS:CE1	0.54	2.37	2	6
1:A:66:LEU:HG	1:A:109:GLY:HA3	0.54	1.80	8	5
1:A:57:GLU:HG2	1:A:136:ILE:HD11	0.53	1.80	7	1
1:A:14:LEU:HG	1:A:59:ASP:HA	0.53	1.80	15	1
1:A:139:ARG:CD	1:A:141:LEU:HD23	0.53	2.33	9	1
1:A:73:HIS:CG	1:A:153:GLN:HG2	0.53	2.38	13	1
1:A:108:ASP:HB3	1:A:151:LYS:H	0.53	1.64	3	1
1:A:57:GLU:CG	1:A:141:LEU:HD23	0.53	2.33	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:ASN:O	1:A:136:ILE:HG22	0.53	2.03	2	2
1:A:18:PHE:CZ	1:A:50:LEU:HG	0.52	2.39	13	3
1:A:106:ILE:CD1	1:A:113:LEU:HD23	0.52	2.33	4	1
1:A:57:GLU:HA	1:A:141:LEU:HD22	0.52	1.79	10	2
1:A:50:LEU:HD21	1:A:54:ILE:HD12	0.52	1.81	9	2
1:A:18:PHE:CE1	1:A:50:LEU:HD21	0.52	2.39	12	1
1:A:66:LEU:HD12	1:A:111:LEU:HD21	0.52	1.80	6	3
1:A:66:LEU:HD13	1:A:111:LEU:CD1	0.52	2.34	5	1
1:A:73:HIS:CG	1:A:153:GLN:HA	0.52	2.39	4	1
1:A:152:THR:HG23	1:A:152:THR:O	0.52	2.04	9	2
1:A:66:LEU:CG	1:A:111:LEU:HD21	0.52	2.34	14	2
1:A:22:PHE:CZ	1:A:45:TYR:CE2	0.52	2.98	14	2
1:A:140:ARG:HG3	1:A:141:LEU:HD13	0.51	1.82	12	1
1:A:66:LEU:HD11	1:A:151:LYS:HD3	0.51	1.80	7	1
1:A:150:ILE:HD11	1:A:153:GLN:H	0.51	1.65	8	1
1:A:66:LEU:HD23	1:A:109:GLY:HA3	0.51	1.82	15	1
1:A:66:LEU:HD21	1:A:151:LYS:HD3	0.50	1.84	7	1
1:A:69:LYS:O	1:A:152:THR:HG21	0.50	2.06	1	1
1:A:104:LEU:HD23	1:A:106:ILE:HD11	0.50	1.84	10	1
1:A:73:HIS:CE1	1:A:152:THR:N	0.50	2.79	10	1
1:A:32:ALA:CB	1:A:74:VAL:HG11	0.50	2.37	1	1
1:A:118:CYS:CB	1:A:121:ASN:HD21	0.50	2.20	10	2
1:A:139:ARG:O	1:A:141:LEU:N	0.50	2.45	13	1
1:A:106:ILE:HG23	1:A:150:ILE:CD1	0.50	2.36	2	1
1:A:66:LEU:HD22	1:A:153:GLN:C	0.50	2.26	2	1
1:A:18:PHE:CZ	1:A:50:LEU:HD21	0.49	2.42	12	1
1:A:62:TYR:CD2	1:A:141:LEU:HD13	0.49	2.42	4	1
1:A:111:LEU:HD23	1:A:111:LEU:H	0.49	1.67	11	2
1:A:38:VAL:HG23	1:A:81:LEU:HD22	0.49	1.83	7	1
1:A:62:TYR:CD2	1:A:136:ILE:HG21	0.49	2.41	10	1
1:A:136:ILE:HB	1:A:141:LEU:HD12	0.49	1.83	11	1
1:A:63:VAL:HG21	1:A:136:ILE:HD11	0.49	1.85	5	1
1:A:81:LEU:HD22	1:A:125:LYS:HB2	0.49	1.85	11	1
1:A:49:LEU:HD12	1:A:50:LEU:H	0.49	1.68	15	1
1:A:14:LEU:HD13	1:A:54:ILE:HG23	0.49	1.84	12	1
1:A:106:ILE:HG21	1:A:153:GLN:HG2	0.49	1.84	7	1
1:A:106:ILE:HD12	1:A:115:PHE:CE1	0.48	2.42	10	1
1:A:141:LEU:N	1:A:141:LEU:HD23	0.48	2.23	11	1
1:A:138:SER:HB2	1:A:141:LEU:HB2	0.48	1.84	1	1
1:A:14:LEU:HD13	1:A:54:ILE:HG13	0.48	1.85	3	1
1:A:70:ILE:HD11	1:A:106:ILE:HD12	0.48	1.84	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:141:LEU:CD2	1:A:141:LEU:N	0.48	2.76	7	1
1:A:38:VAL:HG21	1:A:78:ASN:ND2	0.48	2.24	8	2
1:A:49:LEU:HD23	1:A:134:ALA:H	0.48	1.68	10	1
1:A:66:LEU:CD1	1:A:111:LEU:HD21	0.48	2.39	14	3
1:A:38:VAL:HG22	1:A:39:SER:H	0.48	1.68	3	1
1:A:139:ARG:CG	1:A:140:ARG:H	0.48	2.21	6	2
1:A:150:ILE:CD1	1:A:151:LYS:HB3	0.48	2.28	2	1
1:A:70:ILE:HD13	1:A:153:GLN:HE21	0.47	1.68	2	1
1:A:18:PHE:CD1	1:A:50:LEU:HD11	0.47	2.44	8	5
1:A:21:GLU:HB3	1:A:64:PHE:CD2	0.47	2.44	10	2
1:A:66:LEU:HD11	1:A:113:LEU:HD13	0.47	1.87	12	1
1:A:67:PHE:HA	1:A:70:ILE:HB	0.47	1.87	1	1
1:A:151:LYS:H	1:A:151:LYS:CD	0.47	2.22	15	1
1:A:81:LEU:HD13	1:A:125:LYS:HB3	0.47	1.87	9	1
1:A:13:LYS:HA	1:A:16:ARG:HG3	0.47	1.87	8	4
1:A:50:LEU:CD2	1:A:54:ILE:HD12	0.47	2.39	14	2
1:A:78:ASN:O	1:A:81:LEU:HD23	0.47	2.09	10	1
1:A:38:VAL:CG2	1:A:81:LEU:HD23	0.47	2.39	14	1
1:A:4:ASN:HA	1:A:7:VAL:CG1	0.47	2.40	8	4
1:A:111:LEU:HD13	1:A:136:ILE:CG1	0.47	2.40	10	1
1:A:150:ILE:HD12	1:A:151:LYS:O	0.47	2.10	9	1
1:A:125:LYS:H	1:A:127:PRO:HD3	0.47	1.69	5	1
1:A:74:VAL:HA	1:A:77:VAL:CG1	0.47	2.39	13	1
1:A:138:SER:CB	1:A:139:ARG:HD2	0.46	2.40	3	1
1:A:24:GLN:HE21	1:A:68:HIS:CE1	0.46	2.28	9	2
1:A:106:ILE:HD12	1:A:115:PHE:CZ	0.46	2.45	10	1
1:A:25:ILE:HD13	1:A:68:HIS:CE1	0.46	2.45	5	1
1:A:138:SER:HB2	1:A:139:ARG:CD	0.46	2.40	11	1
1:A:66:LEU:HD12	1:A:111:LEU:CD2	0.46	2.32	3	1
1:A:45:TYR:CE1	1:A:50:LEU:HD13	0.46	2.46	1	2
1:A:138:SER:HB2	1:A:139:ARG:HD2	0.46	1.87	3	1
1:A:73:HIS:CE1	1:A:153:GLN:HE22	0.46	2.27	5	1
1:A:111:LEU:H	1:A:111:LEU:HD23	0.46	1.70	14	1
1:A:58:ILE:HD13	1:A:59:ASP:N	0.45	2.25	11	1
1:A:26:ASN:HA	1:A:29:ILE:HG13	0.45	1.87	10	2
1:A:32:ALA:HB3	1:A:74:VAL:HG21	0.45	1.87	9	1
1:A:64:PHE:HA	1:A:67:PHE:CD2	0.45	2.46	7	1
1:A:47:GLN:HA	1:A:50:LEU:CB	0.45	2.40	13	1
1:A:26:ASN:HA	1:A:29:ILE:CG1	0.45	2.41	10	1
1:A:49:LEU:HD22	1:A:49:LEU:C	0.45	2.32	14	1
1:A:66:LEU:HD11	1:A:113:LEU:CD1	0.45	2.42	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:ILE:CD1	1:A:67:PHE:CD1	0.45	3.00	4	2
1:A:18:PHE:CE1	1:A:50:LEU:CD1	0.45	3.00	7	2
1:A:106:ILE:HG23	1:A:150:ILE:O	0.45	2.12	1	1
1:A:14:LEU:HD12	1:A:58:ILE:HA	0.45	1.87	14	2
1:A:45:TYR:CE2	1:A:50:LEU:HD13	0.45	2.47	7	1
1:A:139:ARG:HD2	1:A:140:ARG:H	0.44	1.72	12	1
1:A:38:VAL:HG21	1:A:78:ASN:HB3	0.44	1.89	2	1
1:A:111:LEU:HD23	1:A:136:ILE:HG23	0.44	1.89	4	1
1:A:38:VAL:CG2	1:A:39:SER:N	0.44	2.80	5	1
1:A:73:HIS:CE1	1:A:152:THR:H	0.44	2.31	10	1
1:A:70:ILE:CG1	1:A:153:GLN:HA	0.44	2.42	9	1
1:A:64:PHE:O	1:A:68:HIS:CD2	0.44	2.70	7	4
1:A:151:LYS:HE3	1:A:153:GLN:N	0.44	2.28	2	1
1:A:139:ARG:HG2	1:A:140:ARG:HG2	0.44	1.89	13	1
1:A:67:PHE:CE1	1:A:113:LEU:HD11	0.44	2.48	7	1
1:A:111:LEU:HD13	1:A:113:LEU:HD23	0.44	1.88	2	1
1:A:24:GLN:CG	1:A:68:HIS:CE1	0.44	3.00	6	1
1:A:73:HIS:CB	1:A:152:THR:O	0.44	2.66	12	1
1:A:106:ILE:HD11	1:A:115:PHE:CZ	0.44	2.47	14	2
1:A:66:LEU:O	1:A:70:ILE:HG13	0.44	2.12	4	1
1:A:29:ILE:HD13	1:A:41:PHE:CE2	0.44	2.47	9	1
1:A:24:GLN:HB3	1:A:68:HIS:CE1	0.44	2.48	1	1
1:A:62:TYR:CZ	1:A:136:ILE:HG21	0.44	2.48	4	1
1:A:49:LEU:HD22	1:A:131:CYS:SG	0.44	2.53	1	1
1:A:73:HIS:HB2	1:A:153:GLN:HB3	0.44	1.88	13	1
1:A:50:LEU:O	1:A:50:LEU:HD13	0.44	2.13	13	1
1:A:139:ARG:HD3	1:A:140:ARG:HG3	0.44	1.90	11	1
1:A:62:TYR:CE2	1:A:141:LEU:HD13	0.43	2.47	4	1
1:A:81:LEU:HD13	1:A:125:LYS:HB2	0.43	1.90	14	1
1:A:13:LYS:O	1:A:16:ARG:HD2	0.43	2.12	7	1
1:A:106:ILE:HA	1:A:150:ILE:O	0.43	2.13	1	1
1:A:111:LEU:CA	1:A:136:ILE:HG23	0.43	2.43	8	2
1:A:49:LEU:HD21	1:A:132:ARG:O	0.43	2.14	1	1
1:A:71:LYS:O	1:A:74:VAL:HG23	0.43	2.13	2	1
1:A:63:VAL:CG2	1:A:111:LEU:HD21	0.43	2.43	15	1
1:A:136:ILE:HB	1:A:141:LEU:HD21	0.43	1.90	4	1
1:A:151:LYS:CE	1:A:153:GLN:HB3	0.43	2.44	2	1
1:A:138:SER:HB2	1:A:141:LEU:HG	0.43	1.91	6	1
1:A:17:HIS:CD2	1:A:61:THR:HG22	0.43	2.48	9	1
1:A:74:VAL:HA	1:A:77:VAL:HG13	0.43	1.90	11	2
1:A:108:ASP:HB2	1:A:151:LYS:HB2	0.43	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:LEU:HD13	1:A:49:LEU:H	0.43	1.72	8	1
1:A:73:HIS:HB2	1:A:152:THR:O	0.43	2.13	12	1
1:A:10:ARG:HE	1:A:58:ILE:HD11	0.43	1.72	1	1
1:A:66:LEU:CG	1:A:111:LEU:HD23	0.43	2.44	15	1
1:A:22:PHE:CZ	1:A:45:TYR:CZ	0.43	3.07	14	1
1:A:73:HIS:CD2	1:A:153:GLN:HE22	0.43	2.31	5	1
1:A:74:VAL:O	1:A:78:ASN:HB3	0.43	2.14	14	1
1:A:66:LEU:HD21	1:A:108:ASP:HB3	0.43	1.90	5	1
1:A:14:LEU:HD22	1:A:18:PHE:CD2	0.43	2.48	5	1
1:A:24:GLN:HG2	1:A:68:HIS:CE1	0.43	2.49	2	1
1:A:70:ILE:HD13	1:A:153:GLN:OXT	0.43	2.14	15	1
1:A:14:LEU:HD12	1:A:54:ILE:HG13	0.42	1.90	7	1
1:A:63:VAL:HA	1:A:111:LEU:HD11	0.42	1.90	4	1
1:A:49:LEU:O	1:A:52:ARG:HB2	0.42	2.13	14	1
1:A:81:LEU:O	1:A:81:LEU:HD23	0.42	2.13	1	1
1:A:62:TYR:CD2	1:A:141:LEU:HD21	0.42	2.49	14	1
1:A:150:ILE:HD11	1:A:152:THR:H	0.42	1.73	3	1
1:A:70:ILE:HG23	1:A:73:HIS:NE2	0.42	2.30	11	1
1:A:150:ILE:HD13	1:A:152:THR:N	0.42	2.29	7	1
1:A:28:GLU:CG	1:A:71:LYS:HG2	0.42	2.45	11	1
1:A:14:LEU:HD22	1:A:59:ASP:N	0.42	2.30	6	1
1:A:49:LEU:H	1:A:49:LEU:CD1	0.42	2.23	9	1
1:A:73:HIS:CD2	1:A:152:THR:CB	0.42	2.98	7	1
1:A:57:GLU:HA	1:A:140:ARG:HG3	0.42	1.92	5	1
1:A:47:GLN:O	1:A:51:ASP:N	0.42	2.53	15	2
1:A:62:TYR:HE2	1:A:136:ILE:HG21	0.42	1.74	8	2
1:A:138:SER:HB3	1:A:139:ARG:HG3	0.42	1.92	1	1
1:A:45:TYR:CD1	1:A:50:LEU:HD13	0.42	2.50	1	2
1:A:73:HIS:CE1	1:A:150:ILE:HD11	0.41	2.48	5	1
1:A:38:VAL:HG12	1:A:39:SER:H	0.41	1.75	2	1
1:A:38:VAL:HG23	1:A:81:LEU:HD21	0.41	1.92	12	1
1:A:63:VAL:HG13	1:A:67:PHE:CZ	0.41	2.51	8	1
1:A:110:ASN:HD21	1:A:141:LEU:HD11	0.41	1.75	14	1
1:A:60:GLU:OE1	1:A:136:ILE:HD11	0.41	2.16	12	1
1:A:28:GLU:CD	1:A:71:LYS:HB2	0.41	2.36	5	1
1:A:136:ILE:HG22	1:A:137:ASN:O	0.41	2.15	6	1
1:A:118:CYS:HB2	1:A:121:ASN:HD21	0.41	1.76	11	1
1:A:38:VAL:HG21	1:A:78:ASN:CB	0.41	2.45	5	1
1:A:111:LEU:CB	1:A:136:ILE:HG23	0.41	2.43	12	1
1:A:22:PHE:CE2	1:A:45:TYR:CD2	0.41	3.09	5	1
1:A:4:ASN:HA	1:A:7:VAL:HB	0.41	1.90	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:VAL:HG23	1:A:81:LEU:HD13	0.41	1.92	1	1
1:A:13:LYS:O	1:A:17:HIS:CG	0.41	2.73	12	2
1:A:28:GLU:HG2	1:A:71:LYS:HG2	0.41	1.93	11	1
1:A:73:HIS:CD2	1:A:152:THR:CA	0.41	3.03	1	1
1:A:81:LEU:HA	1:A:125:LYS:HB2	0.41	1.93	3	1
1:A:70:ILE:HD11	1:A:153:GLN:CB	0.41	2.46	9	1
1:A:53:ALA:HB1	1:A:60:GLU:CD	0.41	2.36	5	1
1:A:50:LEU:O	1:A:54:ILE:HG13	0.41	2.16	10	2
1:A:106:ILE:HG13	1:A:113:LEU:HD12	0.41	1.93	2	1
1:A:138:SER:HB3	1:A:139:ARG:HD2	0.41	1.93	6	1
1:A:77:VAL:HG23	1:A:80:PHE:CE1	0.40	2.51	12	1
1:A:106:ILE:HD13	1:A:153:GLN:OXT	0.40	2.16	4	1
1:A:49:LEU:CD2	1:A:50:LEU:H	0.40	2.30	8	1
1:A:38:VAL:HG11	1:A:78:ASN:CG	0.40	2.36	11	1
1:A:66:LEU:HD11	1:A:153:GLN:NE2	0.40	2.31	2	1
1:A:41:PHE:HA	1:A:127:PRO:O	0.40	2.16	12	1
1:A:45:TYR:CD2	1:A:50:LEU:CD1	0.40	3.04	11	1
1:A:66:LEU:HD13	1:A:66:LEU:C	0.40	2.37	3	1
1:A:73:HIS:CD2	1:A:153:GLN:CA	0.40	3.04	13	1
1:A:54:ILE:O	1:A:58:ILE:HG22	0.40	2.16	5	1
1:A:64:PHE:O	1:A:68:HIS:CG	0.40	2.75	2	1
1:A:73:HIS:CE1	1:A:151:LYS:HB2	0.40	2.50	15	1
1:A:66:LEU:HD12	1:A:113:LEU:HD21	0.40	1.93	9	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	121/153 (79%)	100±3 (82±2%)	11±3 (9±2%)	10±2 (8±2%)	2	13
All	All	1815/2295 (79%)	1496 (82%)	165 (9%)	154 (8%)	2	13

All 30 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	131	CYS	15
1	A	58	ILE	14
1	A	110	ASN	11
1	A	39	SER	9
1	A	138	SER	9
1	A	40	SER	8
1	A	118	CYS	8
1	A	127	PRO	8
1	A	121	ASN	6
1	A	140	ARG	5
1	A	126	ASP	5
1	A	71	LYS	5
1	A	139	ARG	5
1	A	4	ASN	5
1	A	123	LYS	4
1	A	119	LYS	4
1	A	47	GLN	4
1	A	124	PHE	4
1	A	59	ASP	4
1	A	125	LYS	4
1	A	109	GLY	3
1	A	122	GLU	3
1	A	60	GLU	2
1	A	102	GLY	2
1	A	74	VAL	2
1	A	120	PRO	1
1	A	57	GLU	1
1	A	141	LEU	1
1	A	73	HIS	1
1	A	108	ASP	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	112/139 (81%)	81±3 (73±3%)	31±3 (27±3%)	2	22
All	All	1680/2085 (81%)	1220 (73%)	460 (27%)	2	22

All 80 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	58	ILE	15
1	A	136	ILE	15
1	A	137	ASN	14
1	A	67	PHE	14
1	A	141	LEU	14
1	A	139	ARG	14
1	A	18	PHE	14
1	A	14	LEU	12
1	A	115	PHE	12
1	A	63	VAL	12
1	A	22	PHE	12
1	A	5	THR	12
1	A	38	VAL	11
1	A	150	ILE	11
1	A	125	LYS	10
1	A	49	LEU	10
1	A	121	ASN	10
1	A	111	LEU	9
1	A	26	ASN	9
1	A	153	GLN	9
1	A	47	GLN	9
1	A	7	VAL	8
1	A	113	LEU	8
1	A	43	LEU	7
1	A	28	GLU	7
1	A	70	ILE	7
1	A	73	HIS	7
1	A	151	LYS	7
1	A	39	SER	6
1	A	50	LEU	6
1	A	123	LYS	5
1	A	81	LEU	5
1	A	10	ARG	5
1	A	104	LEU	5
1	A	135	ILE	5
1	A	129	LEU	5
1	A	108	ASP	5
1	A	16	ARG	5
1	A	17	HIS	5
1	A	77	VAL	5
1	A	55	GLN	4
1	A	124	PHE	4

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Mol	Chain	Res	Type	Models (Total)
1	A	140	ARG	4
1	A	80	PHE	4
1	A	62	TYR	4
1	A	106	ILE	4
1	A	54	ILE	4
1	A	138	SER	4
1	A	60	GLU	4
1	A	133	MET	4
1	A	29	ILE	4
1	A	45	TYR	4
1	A	78	ASN	4
1	A	130	GLN	4
1	A	79	GLU	3
1	A	117	VAL	3
1	A	75	LEU	3
1	A	126	ASP	3
1	A	127	PRO	2
1	A	23	ARG	2
1	A	25	ILE	2
1	A	66	LEU	2
1	A	112	TRP	2
1	A	46	SER	2
1	A	152	THR	2
1	A	110	ASN	2
1	A	107	THR	2
1	A	56	ARG	1
1	A	52	ARG	1
1	A	118	CYS	1
1	A	8	PHE	1
1	A	57	GLU	1
1	A	61	THR	1
1	A	69	LYS	1
1	A	103	ARG	1
1	A	21	GLU	1
1	A	128	SER	1
1	A	131	CYS	1
1	A	71	LYS	1
1	A	4	ASN	1

### 6.3.3 RNA ⓘ

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](#)

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

No chemical shift data were provided