



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 03:07 AM BST

PDB ID : 2LVZ  
Title : Solution structure of a Eosinophil Cationic Protein-trisaccharide heparin mimetic complex  
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Deposited on : 2012-07-17

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 : 1.7.1 (RC1), CSD as537be (2016)  
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

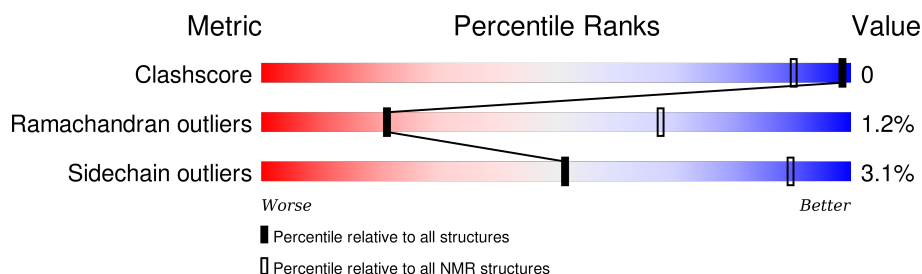
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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	133	<div> <div style="width: 76%; background-color: green;"></div> <div style="width: 23%; background-color: yellow;"></div> <div style="width: 1%; background-color: cyan;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>76% 23% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	SGN	203	2	-

## 2 Ensemble composition and analysis

This entry contains 20 models. Model 13 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:133 (132)	0.43	13

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 4 clusters and 6 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2259 atoms, of which 1107 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Eosinophil cationic protein.

Mol	Chain	Residues	Atoms						Trace
1	A	133	Total	C	H	N	O	S	0
			2169	677	1075	224	184	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	ARG	THR	CONFLICT	UNP P12724

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

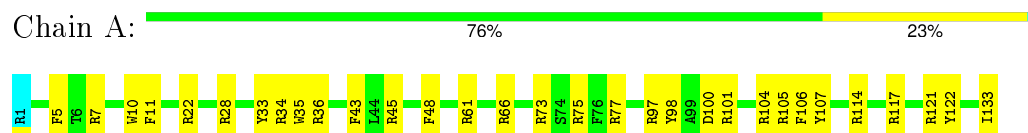
Mol	Chain	Residues	Atoms					
2	A	3	Total	C	H	N	O	S
			90	21	32	2	30	5

## 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: Eosinophil cationic protein

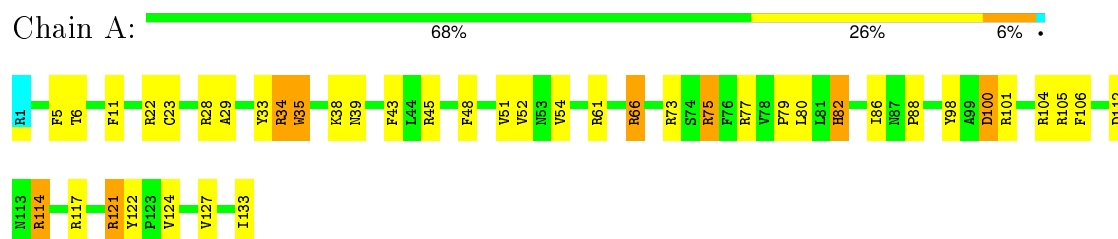


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

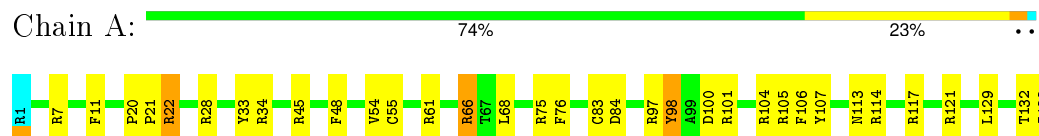
#### 4.2.1 Score per residue for model 1

- Molecule 1: Eosinophil cationic protein



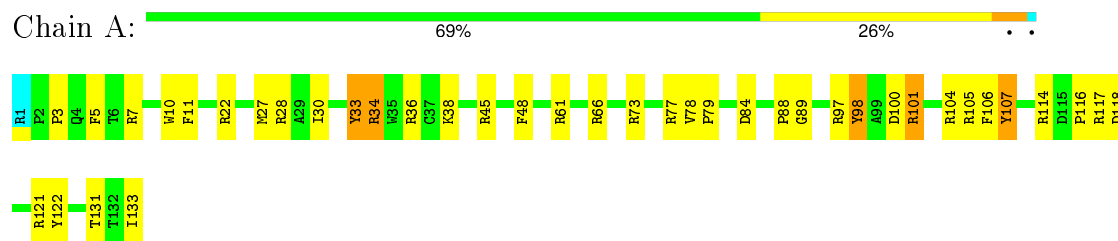
#### 4.2.2 Score per residue for model 2

- Molecule 1: Eosinophil cationic protein



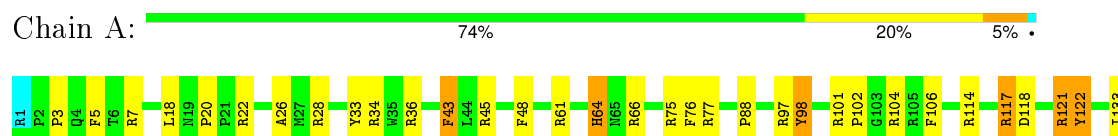
### 4.2.3 Score per residue for model 3

- Molecule 1: Eosinophil cationic protein



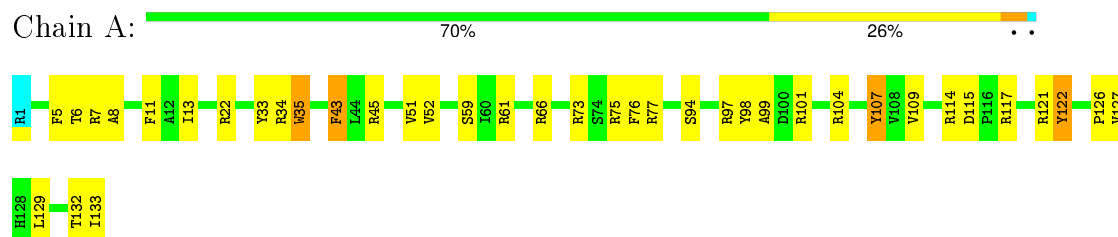
### 4.2.4 Score per residue for model 4

- Molecule 1: Eosinophil cationic protein



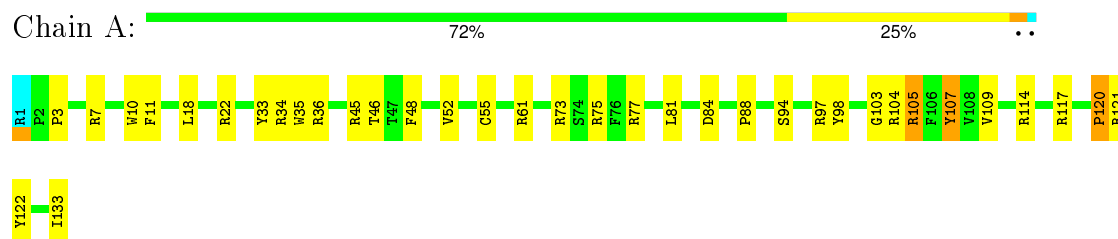
### 4.2.5 Score per residue for model 5

- Molecule 1: Eosinophil cationic protein



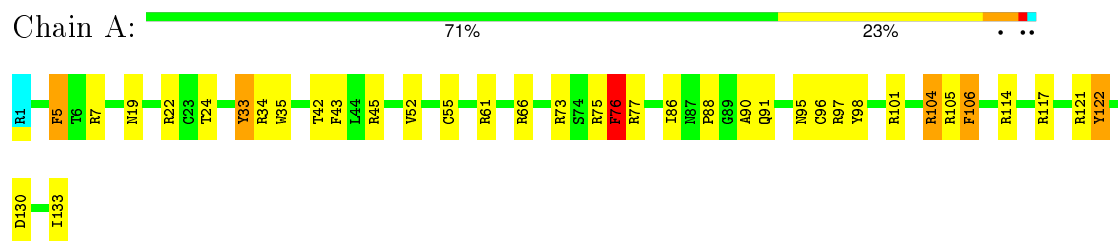
### 4.2.6 Score per residue for model 6

- Molecule 1: Eosinophil cationic protein



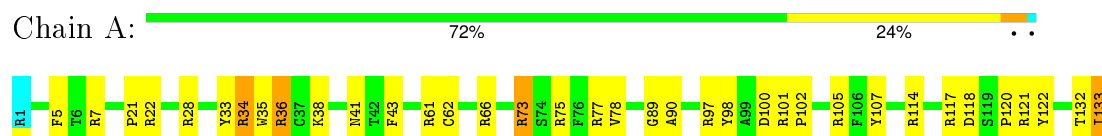
### 4.2.7 Score per residue for model 7

- Molecule 1: Eosinophil cationic protein



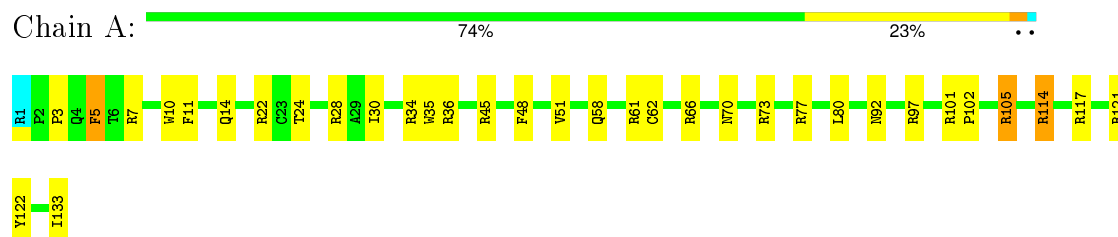
### 4.2.8 Score per residue for model 8

- Molecule 1: Eosinophil cationic protein



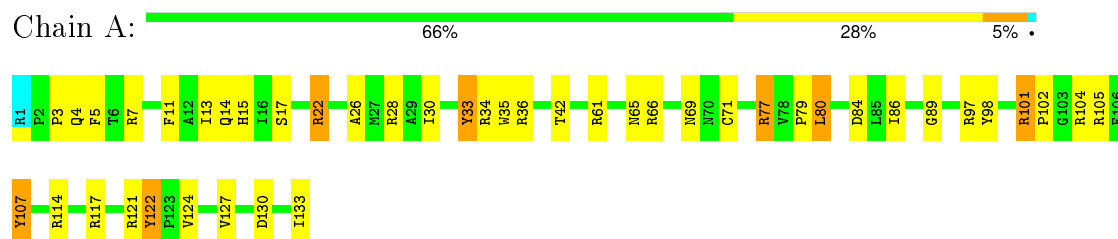
### 4.2.9 Score per residue for model 9

- Molecule 1: Eosinophil cationic protein



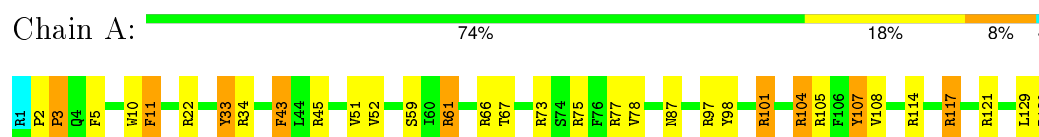
### 4.2.10 Score per residue for model 10

- Molecule 1: Eosinophil cationic protein



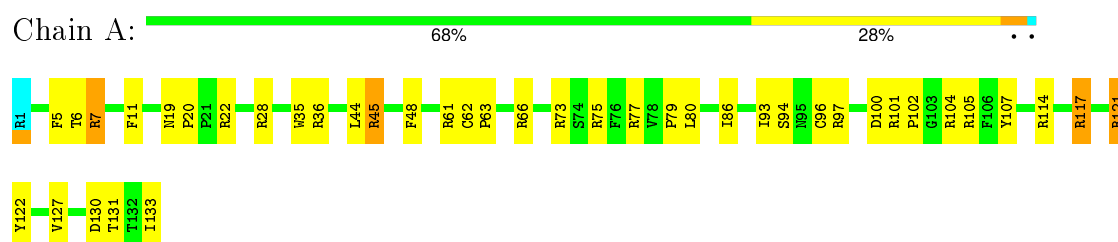
### 4.2.11 Score per residue for model 11

- Molecule 1: Eosinophil cationic protein



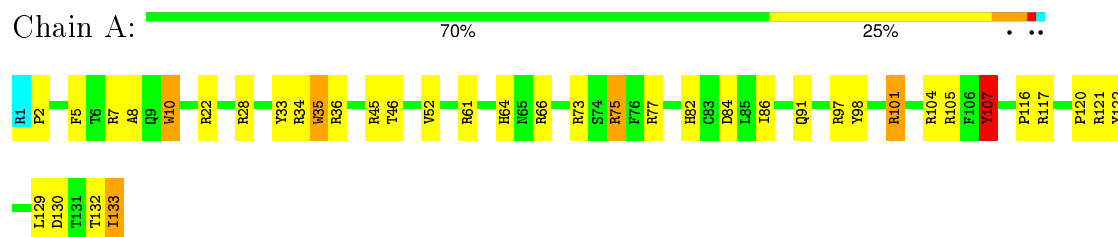
### 4.2.12 Score per residue for model 12

- Molecule 1: Eosinophil cationic protein



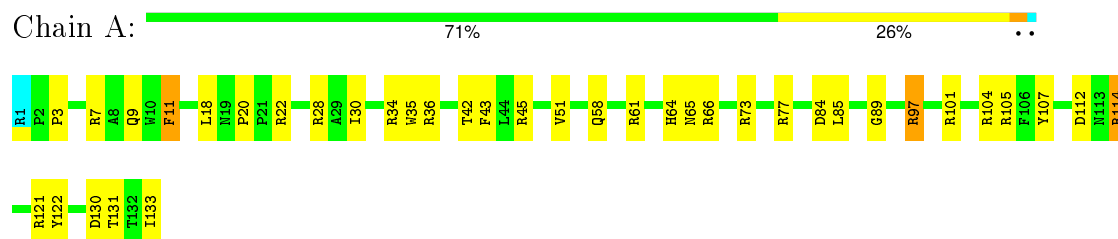
### 4.2.13 Score per residue for model 13 (medoid)

- Molecule 1: Eosinophil cationic protein



### 4.2.14 Score per residue for model 14

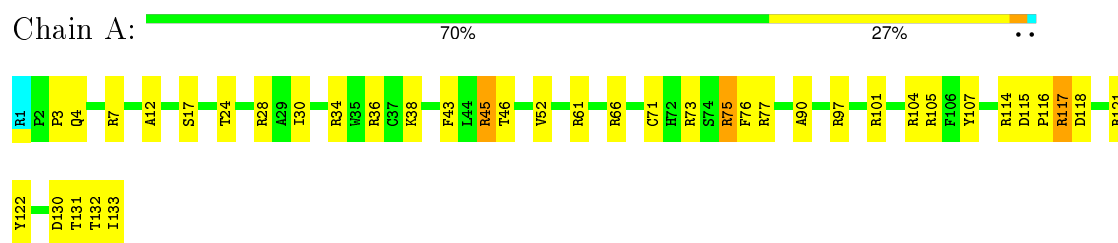
- Molecule 1: Eosinophil cationic protein





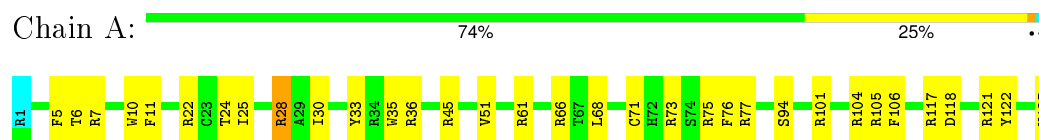
## 4.2.15 Score per residue for model 15

- Molecule 1: Eosinophil cationic protein



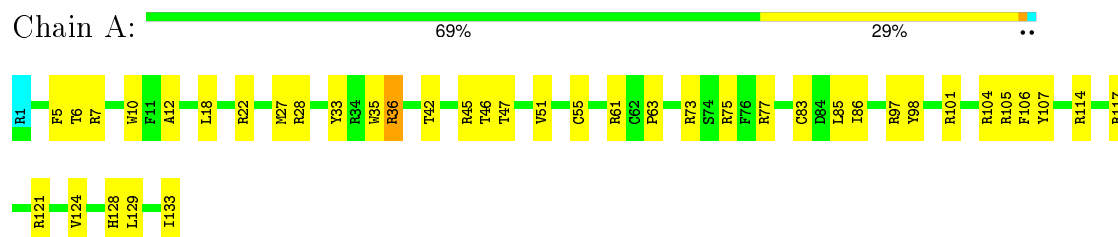
## 4.2.16 Score per residue for model 16

- Molecule 1: Eosinophil cationic protein



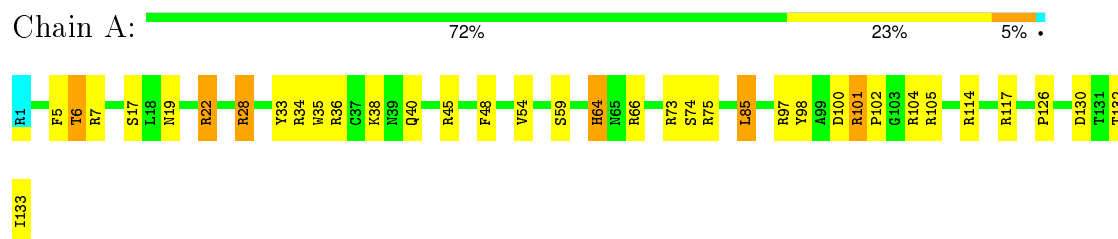
## 4.2.17 Score per residue for model 17

- Molecule 1: Eosinophil cationic protein



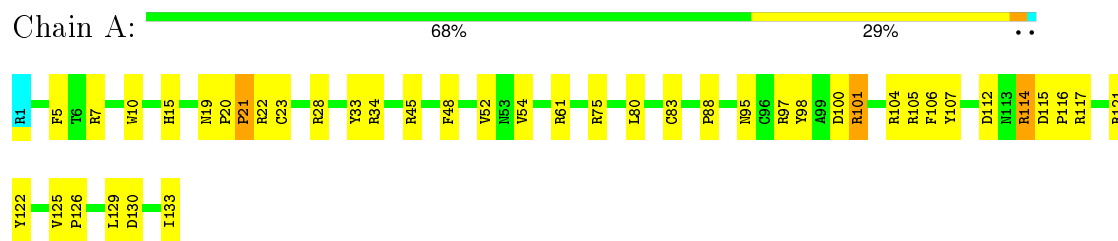
## 4.2.18 Score per residue for model 18

- Molecule 1: Eosinophil cationic protein



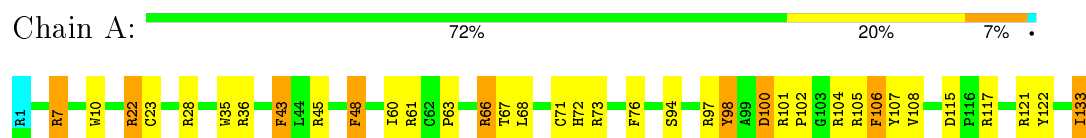
### 4.2.19 Score per residue for model 19

- Molecule 1: Eosinophil cationic protein



### 4.2.20 Score per residue for model 20

- Molecule 1: Eosinophil cationic protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
AMBER	structure solution	
CYANA	structure solution	
AMBER	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2lvz_cs.str
Number of chemical shift lists	1
Total number of shifts	1481
Number of shifts mapped to atoms	1481
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: LVZ, IDS, SGN

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	1.56±0.03	5±2/1113 (0.5±0.2%)	2.17±0.09	42±5/1515 (2.7±0.3%)
2	A	0.00±0.00	-	0.00±0.00	-
All	All	1.56	107/22260 (0.5%)	2.17	830/30300 (2.7%)

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	5.8±2.1
2	A	0.1±0.3	0.0±0.0
All	All	2	115

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	23	CYS	CB-SG	-7.98	1.68	1.82	19	1
1	A	63	PRO	N-CD	-7.97	1.36	1.47	12	2
1	A	61	ARG	CZ-NH1	-7.52	1.23	1.33	6	4
1	A	33	TYR	CG-CD1	7.24	1.48	1.39	17	1
1	A	22	ARG	CZ-NH1	-7.21	1.23	1.33	14	1
1	A	97	ARG	CZ-NH2	-7.06	1.23	1.33	7	3
1	A	75	ARG	CZ-NH1	-6.90	1.24	1.33	12	2
1	A	94	SER	CA-CB	6.62	1.62	1.52	12	2
1	A	122	TYR	CD1-CE1	6.55	1.49	1.39	4	1
1	A	62	CYS	CB-SG	-6.49	1.71	1.82	12	1
1	A	33	TYR	CE2-CZ	6.48	1.47	1.38	2	2
1	A	89	GLY	CA-C	6.45	1.62	1.51	8	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	75	ARG	NE-CZ	-6.41	1.24	1.33	19	1
1	A	7	ARG	CZ-NH2	-6.40	1.24	1.33	13	2
1	A	120	PRO	N-CA	6.32	1.57	1.47	8	1
1	A	59	SER	CB-OG	6.30	1.50	1.42	18	3
1	A	33	TYR	CE1-CZ	6.29	1.46	1.38	17	1
1	A	98	TYR	CG-CD2	6.25	1.47	1.39	5	2
1	A	97	ARG	CD-NE	6.25	1.57	1.46	11	1
1	A	28	ARG	CZ-NH1	-6.13	1.25	1.33	16	3
1	A	116	PRO	N-CD	-6.12	1.39	1.47	3	1
1	A	117	ARG	CZ-NH1	-6.06	1.25	1.33	18	2
1	A	122	TYR	CE1-CZ	6.01	1.46	1.38	6	1
1	A	114	ARG	CZ-NH2	-5.99	1.25	1.33	5	1
1	A	103	GLY	CA-C	5.97	1.61	1.51	6	1
1	A	117	ARG	CZ-NH2	-5.93	1.25	1.33	8	3
1	A	126	PRO	N-CA	-5.91	1.37	1.47	19	1
1	A	48	PHE	CE2-CZ	5.90	1.48	1.37	20	1
1	A	33	TYR	CB-CG	5.89	1.60	1.51	8	1
1	A	66	ARG	CZ-NH1	-5.89	1.25	1.33	20	1
1	A	10	TRP	CD2-CE2	5.85	1.48	1.41	20	1
1	A	33	TYR	CG-CD2	5.84	1.46	1.39	10	1
1	A	55	CYS	CB-SG	-5.83	1.72	1.81	2	1
1	A	34	ARG	CZ-NH1	-5.80	1.25	1.33	10	1
1	A	121	ARG	CZ-NH1	-5.79	1.25	1.33	19	1
1	A	94	SER	CB-OG	5.71	1.49	1.42	5	1
1	A	121	ARG	CZ-NH2	-5.70	1.25	1.33	2	3
1	A	126	PRO	N-CD	-5.70	1.39	1.47	18	2
1	A	122	TYR	CD2-CE2	5.70	1.47	1.39	5	1
1	A	28	ARG	NE-CZ	-5.69	1.25	1.33	3	1
1	A	7	ARG	CZ-NH1	-5.69	1.25	1.33	9	1
1	A	76	PHE	CG-CD2	5.68	1.47	1.38	4	1
1	A	10	TRP	CZ3-CH2	5.67	1.49	1.40	3	1
1	A	61	ARG	CD-NE	5.66	1.56	1.46	12	1
1	A	71	CYS	CB-SG	-5.66	1.72	1.81	15	1
1	A	17	SER	CB-OG	5.63	1.49	1.42	10	2
1	A	34	ARG	CZ-NH2	-5.62	1.25	1.33	8	1
1	A	122	TYR	CG-CD2	5.61	1.46	1.39	10	1
1	A	6	THR	N-CA	5.60	1.57	1.46	17	1
1	A	66	ARG	CZ-NH2	-5.53	1.25	1.33	3	1
1	A	48	PHE	CG-CD1	5.50	1.47	1.38	20	1
1	A	35	TRP	CD2-CE2	5.48	1.48	1.41	13	2
1	A	105	ARG	CZ-NH1	-5.47	1.25	1.33	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	78	VAL	CA-CB	5.46	1.66	1.54	3	1
1	A	17	SER	CA-CB	5.45	1.61	1.52	15	1
1	A	77	ARG	CZ-NH2	-5.43	1.25	1.33	5	1
1	A	102	PRO	N-CD	-5.42	1.40	1.47	8	2
1	A	75	ARG	CZ-NH2	-5.42	1.26	1.33	4	1
1	A	104	ARG	CZ-NH1	-5.34	1.26	1.33	7	1
1	A	22	ARG	CZ-NH2	-5.34	1.26	1.33	9	2
1	A	104	ARG	CZ-NH2	-5.32	1.26	1.33	18	2
1	A	129	LEU	CA-CB	5.32	1.66	1.53	2	1
1	A	36	ARG	CZ-NH2	-5.30	1.26	1.33	6	1
1	A	101	ARG	CZ-NH2	-5.30	1.26	1.33	20	1
1	A	107	TYR	CE2-CZ	5.22	1.45	1.38	20	1
1	A	48	PHE	CE1-CZ	5.21	1.47	1.37	9	1
1	A	98	TYR	CE2-CZ	5.21	1.45	1.38	10	1
1	A	20	PRO	C-N	5.20	1.44	1.34	4	1
1	A	43	PHE	CG-CD2	5.18	1.46	1.38	11	1
1	A	38	LYS	N-CA	5.17	1.56	1.46	15	1
1	A	3	PRO	N-CA	-5.17	1.38	1.47	6	1
1	A	107	TYR	CE1-CZ	5.15	1.45	1.38	11	1
1	A	105	ARG	CZ-NH2	-5.13	1.26	1.33	2	1
1	A	77	ARG	NE-CZ	5.12	1.39	1.33	7	1
1	A	94	SER	N-CA	5.12	1.56	1.46	6	1
1	A	69	ASN	N-CA	5.12	1.56	1.46	10	1
1	A	107	TYR	CB-CG	5.08	1.59	1.51	10	1
1	A	10	TRP	CG-CD2	5.07	1.52	1.43	9	1
1	A	34	ARG	N-CA	5.06	1.56	1.46	6	1
1	A	3	PRO	N-CD	-5.04	1.40	1.47	15	1
1	A	101	ARG	NE-CZ	-5.00	1.26	1.33	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	77	ARG	NE-CZ-NH1	24.71	132.65	120.30	5	10
1	A	34	ARG	NE-CZ-NH1	24.68	132.64	120.30	13	10
1	A	105	ARG	NE-CZ-NH1	22.62	131.61	120.30	17	14
1	A	97	ARG	NE-CZ-NH1	21.13	130.86	120.30	2	12
1	A	117	ARG	NE-CZ-NH1	20.34	130.47	120.30	7	13
1	A	28	ARG	NE-CZ-NH1	18.86	129.73	120.30	8	12
1	A	61	ARG	NE-CZ-NH1	18.74	129.67	120.30	3	12
1	A	7	ARG	NE-CZ-NH1	18.40	129.50	120.30	20	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	75	ARG	NE-CZ-NH1	18.22	129.41	120.30	16	10
1	A	101	ARG	NE-CZ-NH1	17.58	129.09	120.30	4	14
1	A	45	ARG	NE-CZ-NH1	17.26	128.93	120.30	6	12
1	A	22	ARG	NE-CZ-NH1	17.09	128.85	120.30	1	11
1	A	7	ARG	NE-CZ-NH2	-16.80	111.90	120.30	20	9
1	A	101	ARG	NE-CZ-NH2	-16.59	112.01	120.30	5	13
1	A	104	ARG	NE-CZ-NH1	16.26	128.43	120.30	2	9
1	A	114	ARG	NE-CZ-NH2	-15.69	112.45	120.30	4	8
1	A	105	ARG	NE-CZ-NH2	-14.83	112.89	120.30	7	9
1	A	77	ARG	NE-CZ-NH2	14.77	127.69	120.30	9	12
1	A	34	ARG	NE-CZ-NH2	-14.69	112.95	120.30	13	9
1	A	75	ARG	NE-CZ-NH2	-14.54	113.03	120.30	16	7
1	A	107	TYR	CB-CG-CD1	14.42	129.65	121.00	12	6
1	A	117	ARG	NE-CZ-NH2	-14.10	113.25	120.30	1	15
1	A	66	ARG	NE-CZ-NH1	14.10	127.35	120.30	2	11
1	A	45	ARG	NE-CZ-NH2	-13.98	113.31	120.30	13	8
1	A	121	ARG	NE-CZ-NH1	13.82	127.21	120.30	7	12
1	A	114	ARG	NE-CZ-NH1	12.95	126.78	120.30	4	13
1	A	121	ARG	NE-CZ-NH2	12.91	126.75	120.30	13	10
1	A	36	ARG	NE-CZ-NH1	12.84	126.72	120.30	4	8
1	A	107	TYR	CG-CD1-CE1	-12.32	111.44	121.30	19	2
1	A	117	ARG	NH1-CZ-NH2	-12.04	106.16	119.40	7	3
1	A	73	ARG	NE-CZ-NH2	-12.00	114.30	120.30	16	8
1	A	107	TYR	CB-CG-CD2	-11.71	113.97	121.00	12	5
1	A	66	ARG	NE-CZ-NH2	11.61	126.10	120.30	16	8
1	A	73	ARG	NE-CZ-NH1	11.51	126.05	120.30	8	13
1	A	61	ARG	NE-CZ-NH2	-11.36	114.62	120.30	9	11
1	A	77	ARG	NH1-CZ-NH2	-11.20	107.08	119.40	1	4
1	A	98	TYR	CB-CG-CD1	-11.09	114.35	121.00	19	5
1	A	130	ASP	CB-CG-OD1	11.05	128.25	118.30	18	4
1	A	5	PHE	CB-CG-CD2	-10.96	113.13	120.80	11	5
1	A	33	TYR	CB-CG-CD2	-10.95	114.43	121.00	13	5
1	A	11	PHE	CB-CG-CD1	-10.49	113.46	120.80	11	8
1	A	98	TYR	CB-CG-CD2	10.43	127.26	121.00	1	6
1	A	22	ARG	NE-CZ-NH2	10.27	125.44	120.30	11	9
1	A	36	ARG	NE-CZ-NH2	-10.22	115.19	120.30	10	10
1	A	97	ARG	NE-CZ-NH2	-10.10	115.25	120.30	5	9
1	A	5	PHE	CB-CG-CD1	-10.00	113.80	120.80	19	6
1	A	43	PHE	CB-CG-CD2	-9.80	113.94	120.80	4	4
1	A	61	ARG	NH1-CZ-NH2	-9.79	108.63	119.40	6	1
1	A	28	ARG	NE-CZ-NH2	-9.67	115.46	120.30	3	6

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	ARG	NH1-CZ-NH2	-9.60	108.84	119.40	2	2
1	A	43	PHE	CB-CG-CD1	-9.26	114.31	120.80	15	4
1	A	33	TYR	CB-CG-CD1	-9.22	115.47	121.00	16	5
1	A	5	PHE	CG-CD1-CE1	-9.13	110.76	120.80	19	1
1	A	97	ARG	NH1-CZ-NH2	-9.06	109.44	119.40	2	6
1	A	84	ASP	CB-CG-OD1	9.05	126.44	118.30	10	3
1	A	101	ARG	NH1-CZ-NH2	-8.90	109.61	119.40	11	2
1	A	105	ARG	NH1-CZ-NH2	-8.74	109.78	119.40	19	4
1	A	104	ARG	NE-CZ-NH2	-8.54	116.03	120.30	6	8
1	A	115	ASP	CB-CG-OD2	-8.41	110.73	118.30	5	2
1	A	35	TRP	CE2-CD2-CG	8.38	114.00	107.30	20	2
1	A	48	PHE	CB-CG-CD1	-8.36	114.95	120.80	12	5
1	A	106	PHE	CB-CG-CD1	-8.33	114.97	120.80	19	2
1	A	35	TRP	NE1-CE2-CD2	-8.12	99.18	107.30	20	2
1	A	73	ARG	NH1-CZ-NH2	-8.05	110.54	119.40	1	5
1	A	90	ALA	N-CA-CB	-8.04	98.84	110.10	8	1
1	A	101	ARG	CD-NE-CZ	8.03	134.84	123.60	9	3
1	A	122	TYR	CB-CG-CD2	-8.00	116.20	121.00	14	7
1	A	130	ASP	CB-CG-OD2	8.00	125.50	118.30	12	5
1	A	76	PHE	CB-CG-CD2	-7.98	115.21	120.80	16	2
1	A	115	ASP	CB-CG-OD1	-7.98	111.12	118.30	15	2
1	A	107	TYR	CD1-CG-CD2	7.95	126.64	117.90	19	2
1	A	75	ARG	NH1-CZ-NH2	-7.94	110.66	119.40	15	2
1	A	48	PHE	CB-CG-CD2	-7.93	115.25	120.80	18	4
1	A	66	ARG	NH1-CZ-NH2	-7.83	110.78	119.40	15	5
1	A	75	ARG	CD-NE-CZ	7.83	134.56	123.60	2	3
1	A	10	TRP	NE1-CE2-CD2	-7.80	99.50	107.30	3	2
1	A	22	ARG	CD-NE-CZ	7.75	134.45	123.60	7	4
1	A	11	PHE	CB-CG-CD2	-7.74	115.39	120.80	14	6
1	A	45	ARG	NH1-CZ-NH2	-7.66	110.97	119.40	5	7
1	A	11	PHE	CG-CD1-CE1	-7.63	112.41	120.80	12	1
1	A	46	THR	CA-CB-OG1	7.61	124.98	109.00	6	2
1	A	105	ARG	CD-NE-CZ	7.55	134.18	123.60	2	2
1	A	116	PRO	N-CA-CB	7.53	112.34	103.30	19	1
1	A	28	ARG	NH1-CZ-NH2	-7.47	111.18	119.40	8	2
1	A	76	PHE	CB-CG-CD1	-7.44	115.59	120.80	2	4
1	A	100	ASP	CB-CG-OD2	-7.42	111.62	118.30	8	3
1	A	100	ASP	CB-CG-OD1	-7.41	111.63	118.30	19	4
1	A	97	ARG	CD-NE-CZ	7.36	133.91	123.60	9	2
1	A	46	THR	CA-CB-CG2	7.34	122.68	112.40	17	2
1	A	10	TRP	CB-CG-CD2	7.26	136.04	126.60	16	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	3	PRO	N-CA-CB	7.25	112.00	103.30	3	2
1	A	117	ARG	CD-NE-CZ	7.13	133.58	123.60	5	4
1	A	35	TRP	CD1-NE1-CE2	7.09	115.38	109.00	20	3
1	A	10	TRP	CD1-NE1-CE2	7.08	115.37	109.00	3	4
1	A	11	PHE	CD1-CG-CD2	7.07	127.49	118.30	12	1
1	A	93	ILE	CA-CB-CG1	7.04	124.37	111.00	12	1
1	A	125	VAL	CG1-CB-CG2	-6.96	99.76	110.90	16	1
1	A	129	LEU	CB-CG-CD2	-6.94	99.20	111.00	19	1
1	A	107	TYR	CD1-CE1-CZ	-6.94	113.56	119.80	3	2
1	A	132	THR	CA-CB-CG2	6.93	122.10	112.40	8	4
1	A	68	LEU	CB-CG-CD2	6.92	122.77	111.00	20	1
1	A	2	PRO	N-CA-CB	6.90	111.58	103.30	13	1
1	A	54	VAL	CG1-CB-CG2	-6.87	99.91	110.90	1	2
1	A	121	ARG	NH1-CZ-NH2	-6.85	111.86	119.40	13	2
1	A	52	VAL	CA-CB-CG1	6.78	121.07	110.90	1	3
1	A	6	THR	CA-CB-CG2	6.75	121.84	112.40	16	3
1	A	45	ARG	CD-NE-CZ	6.73	133.02	123.60	14	2
1	A	61	ARG	CD-NE-CZ	6.71	132.99	123.60	12	2
1	A	51	VAL	CA-CB-CG2	6.71	120.96	110.90	1	4
1	A	127	VAL	CA-CB-CG2	6.70	120.94	110.90	10	3
1	A	63	PRO	N-CA-CB	6.69	111.33	103.30	17	1
1	A	54	VAL	CA-CB-CG1	6.66	120.88	110.90	19	2
1	A	112	ASP	CB-CG-OD1	6.65	124.29	118.30	19	2
1	A	132	THR	OG1-CB-CG2	-6.60	94.81	110.00	18	1
1	A	104	ARG	NH1-CZ-NH2	-6.60	112.14	119.40	11	3
1	A	22	ARG	NH1-CZ-NH2	-6.58	112.16	119.40	1	9
1	A	114	ARG	CD-NE-CZ	6.57	132.79	123.60	17	2
1	A	10	TRP	CG-CD2-CE3	6.55	139.79	133.90	20	2
1	A	79	PRO	O-C-N	-6.53	112.25	122.70	1	2
1	A	84	ASP	CB-CG-OD2	-6.52	112.43	118.30	14	1
1	A	115	ASP	N-CA-CB	-6.52	98.87	110.60	19	1
1	A	118	ASP	CB-CG-OD1	6.45	124.10	118.30	3	3
1	A	122	TYR	CG-CD2-CE2	-6.42	116.16	121.30	12	1
1	A	131	THR	CA-CB-CG2	6.42	121.38	112.40	14	3
1	A	36	ARG	CD-NE-CZ	6.38	132.53	123.60	16	3
1	A	98	TYR	CG-CD2-CE2	-6.37	116.21	121.30	20	3
1	A	106	PHE	CB-CG-CD2	-6.36	116.35	120.80	16	3
1	A	66	ARG	CD-NE-CZ	6.35	132.49	123.60	8	3
1	A	90	ALA	CB-CA-C	6.33	119.60	110.10	7	2
1	A	51	VAL	CG1-CB-CG2	-6.33	100.77	110.90	17	4
1	A	55	CYS	CA-CB-SG	6.30	125.34	114.00	6	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	84	ASP	N-CA-CB	-6.28	99.30	110.60	13	2
1	A	118	ASP	N-CA-CB	-6.28	99.31	110.60	8	1
1	A	73	ARG	CD-NE-CZ	6.26	132.36	123.60	3	2
1	A	80	LEU	CB-CA-C	6.26	122.09	110.20	12	1
1	A	20	PRO	N-CA-CB	6.22	110.76	103.30	19	2
1	A	88	PRO	N-CA-CB	6.21	110.75	103.30	3	2
1	A	107	TYR	CG-CD2-CE2	-6.17	116.36	121.30	17	3
1	A	33	TYR	CG-CD2-CE2	-6.14	116.39	121.30	10	1
1	A	122	TYR	CG-CD1-CE1	-6.12	116.41	121.30	4	1
1	A	86	ILE	CA-CB-CG1	6.08	122.54	111.00	13	1
1	A	80	LEU	CB-CG-CD1	6.07	121.33	111.00	10	1
1	A	3	PRO	N-CD-CG	6.07	112.30	103.20	11	1
1	A	33	TYR	CG-CD1-CE1	-6.07	116.45	121.30	2	3
1	A	122	TYR	CZ-CE2-CD2	6.04	125.24	119.80	6	4
1	A	133	ILE	CA-CB-CG1	6.04	122.47	111.00	8	4
1	A	33	TYR	N-CA-CB	-5.95	99.90	110.60	17	1
1	A	112	ASP	CB-CG-OD2	5.94	123.64	118.30	1	1
1	A	34	ARG	CD-NE-CZ	5.92	131.89	123.60	11	2
1	A	33	TYR	CZ-CE2-CD2	5.91	125.12	119.80	1	1
1	A	118	ASP	CB-CG-OD2	5.88	123.59	118.30	16	2
1	A	106	PHE	N-CA-CB	-5.84	100.08	110.60	3	1
1	A	39	ASN	N-CA-CB	-5.82	100.12	110.60	1	1
1	A	10	TRP	CB-CG-CD1	-5.81	119.44	127.00	11	2
1	A	8	ALA	CB-CA-C	5.80	118.81	110.10	5	1
1	A	77	ARG	CD-NE-CZ	5.79	131.70	123.60	16	1
1	A	98	TYR	CA-CB-CG	5.79	124.39	113.40	8	1
1	A	91	GLN	O-C-N	-5.78	113.45	122.70	13	1
1	A	124	VAL	CA-CB-CG2	5.76	119.54	110.90	17	1
1	A	125	VAL	CA-CB-CG1	5.75	119.53	110.90	16	1
1	A	44	LEU	CB-CG-CD2	-5.74	101.23	111.00	12	1
1	A	91	GLN	OE1-CD-NE2	-5.72	108.75	121.90	13	1
1	A	85	LEU	CB-CG-CD1	5.72	120.72	111.00	18	2
1	A	35	TRP	CG-CD2-CE3	-5.71	128.76	133.90	12	2
1	A	54	VAL	O-C-N	-5.70	113.58	122.70	18	1
1	A	98	TYR	CG-CD1-CE1	-5.69	116.75	121.30	3	3
1	A	120	PRO	N-CA-C	5.68	126.86	112.10	6	1
1	A	3	PRO	CA-N-CD	-5.67	103.57	111.50	11	1
1	A	25	ILE	CA-CB-CG1	5.66	121.76	111.00	16	1
1	A	120	PRO	C-N-CA	5.64	135.80	121.70	13	1
1	A	122	TYR	CB-CG-CD1	-5.63	117.62	121.00	7	3
1	A	64	HIS	CA-CB-CG	5.62	123.15	113.60	14	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	26	ALA	N-CA-CB	-5.61	102.25	110.10	10	1
1	A	24	THR	CA-CB-CG2	-5.60	104.55	112.40	7	1
1	A	81	LEU	CB-CA-C	5.59	120.83	110.20	6	1
1	A	5	PHE	CD1-CE1-CZ	-5.59	113.39	120.10	16	2
1	A	46	THR	OG1-CB-CG2	-5.56	97.20	110.00	15	1
1	A	94	SER	CB-CA-C	-5.56	99.54	110.10	16	1
1	A	42	THR	CA-CB-CG2	5.56	120.18	112.40	14	4
1	A	102	PRO	N-CA-CB	5.55	109.97	103.30	20	2
1	A	6	THR	CA-CB-OG1	5.54	120.64	109.00	1	1
1	A	7	ARG	CA-CB-CG	5.54	125.58	113.40	14	2
1	A	47	THR	CA-CB-OG1	5.54	120.63	109.00	17	1
1	A	78	VAL	CG1-CB-CG2	-5.52	102.06	110.90	8	1
1	A	62	CYS	CA-CB-SG	5.52	123.93	114.00	8	2
1	A	58	GLN	O-C-N	-5.51	113.88	122.70	9	1
1	A	106	PHE	CA-CB-CG	5.50	127.10	113.90	2	1
1	A	18	LEU	CB-CG-CD1	5.50	120.34	111.00	6	1
1	A	27	MET	O-C-N	-5.49	113.92	122.70	17	1
1	A	109	VAL	CG1-CB-CG2	-5.48	102.13	110.90	6	2
1	A	36	ARG	NH1-CZ-NH2	-5.48	113.38	119.40	15	1
1	A	52	VAL	CG1-CB-CG2	-5.47	102.14	110.90	7	3
1	A	45	ARG	N-CA-CB	5.47	120.44	110.60	1	1
1	A	5	PHE	CG-CD2-CE2	-5.46	114.80	120.80	1	1
1	A	15	HIS	N-CA-C	5.46	125.73	111.00	19	1
1	A	28	ARG	CD-NE-CZ	5.45	131.23	123.60	17	2
1	A	7	ARG	NH1-CZ-NH2	-5.45	113.41	119.40	12	2
1	A	104	ARG	O-C-N	5.44	131.41	122.70	10	1
1	A	43	PHE	CZ-CE2-CD2	-5.44	113.58	120.10	5	1
1	A	77	ARG	CB-CA-C	-5.43	99.53	110.40	14	1
1	A	122	TYR	CD1-CG-CD2	5.42	123.86	117.90	19	1
1	A	43	PHE	N-CA-CB	-5.42	100.85	110.60	20	1
1	A	21	PRO	N-CD-CG	5.41	111.31	103.20	19	2
1	A	17	SER	O-C-N	5.41	131.35	122.70	18	1
1	A	10	TRP	CE2-CD2-CG	5.40	111.62	107.30	3	2
1	A	104	ARG	CD-NE-CZ	5.39	131.15	123.60	6	1
1	A	113	ASN	N-CA-CB	-5.37	100.93	110.60	2	1
1	A	10	TRP	CB-CA-C	5.37	121.15	110.40	6	1
1	A	65	ASN	N-CA-CB	-5.36	100.95	110.60	14	2
1	A	79	PRO	N-CD-CG	5.33	111.19	103.20	12	1
1	A	8	ALA	N-CA-CB	-5.30	102.69	110.10	13	1
1	A	10	TRP	CE2-CD2-CE3	-5.30	112.34	118.70	20	1
1	A	71	CYS	CB-CA-C	5.27	120.93	110.40	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	7	ARG	CD-NE-CZ	5.26	130.97	123.60	7	1
1	A	64	HIS	O-C-N	-5.24	114.32	122.70	4	1
1	A	98	TYR	CD1-CG-CD2	5.24	123.66	117.90	20	1
1	A	98	TYR	CD1-CE1-CZ	5.23	124.51	119.80	3	1
1	A	40	GLN	CA-CB-CG	5.23	124.91	113.40	18	1
1	A	74	SER	CA-CB-OG	5.23	125.31	111.20	18	1
1	A	4	GLN	CB-CA-C	5.19	120.78	110.40	15	1
1	A	35	TRP	CE2-CD2-CE3	-5.18	112.48	118.70	20	1
1	A	52	VAL	CA-CB-CG2	-5.18	103.13	110.90	15	1
1	A	82	HIS	CB-CA-C	5.18	120.75	110.40	1	2
1	A	12	ALA	CB-CA-C	5.18	117.86	110.10	17	1
1	A	48	PHE	CG-CD1-CE1	-5.17	115.11	120.80	6	1
1	A	71	CYS	CA-C-N	-5.17	105.82	117.20	10	1
1	A	18	LEU	CB-CG-CD2	-5.17	102.21	111.00	17	1
1	A	89	GLY	CA-C-O	-5.16	111.31	120.60	10	1
1	A	114	ARG	NH1-CZ-NH2	-5.16	113.73	119.40	8	2
1	A	122	TYR	CD1-CE1-CZ	-5.14	115.17	119.80	19	1
1	A	92	ASN	N-CA-CB	-5.13	101.36	110.60	9	1
1	A	9	GLN	CB-CA-C	-5.11	100.19	110.40	14	1
1	A	61	ARG	C-N-CA	5.10	134.46	121.70	13	1
1	A	35	TRP	CG-CD1-NE1	5.09	115.19	110.10	16	1
1	A	33	TYR	CD1-CG-CD2	5.08	123.49	117.90	19	1
1	A	52	VAL	O-C-N	-5.08	114.57	122.70	13	1
1	A	80	LEU	CB-CG-CD2	-5.08	102.37	111.00	10	1
1	A	116	PRO	CA-N-CD	-5.08	104.39	111.50	19	1
1	A	22	ARG	CB-CG-CD	5.07	124.79	111.60	5	1
1	A	42	THR	OG1-CB-CG2	-5.07	98.34	110.00	14	1
1	A	83	CYS	N-CA-CB	-5.07	101.48	110.60	2	1
1	A	80	LEU	C-N-CA	5.06	134.34	121.70	12	1
1	A	117	ARG	N-CA-CB	-5.05	101.51	110.60	20	1
1	A	20	PRO	N-CD-CG	5.05	110.77	103.20	12	1
1	A	19	ASN	CA-CB-CG	5.03	124.47	113.40	7	1
1	A	95	ASN	N-CA-CB	-5.03	101.55	110.60	19	1
1	A	106	PHE	O-C-N	-5.02	114.67	122.70	4	1
1	A	116	PRO	CA-C-N	5.02	128.24	117.20	15	1
1	A	71	CYS	C-N-CA	5.02	134.25	121.70	16	1
1	A	96	CYS	CB-CA-C	5.01	120.43	110.40	12	1
1	A	131	THR	OG1-CB-CG2	-5.01	98.48	110.00	3	1
1	A	13	ILE	CA-CB-CG2	5.00	120.91	110.90	5	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	203	SGN	C1	2

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	107	TYR	Sidechain	9
1	A	5	PHE	Peptide,Sidechain	8
1	A	22	ARG	Sidechain	5
1	A	33	TYR	Sidechain	4
1	A	34	ARG	Sidechain,Mainchain	4
1	A	104	ARG	Sidechain	4
1	A	122	TYR	Sidechain,Mainchain	4
1	A	66	ARG	Sidechain	4
1	A	11	PHE	Sidechain	4
1	A	45	ARG	Sidechain	4
1	A	114	ARG	Sidechain,Peptide	4
1	A	106	PHE	Sidechain	4
1	A	117	ARG	Sidechain	4
1	A	75	ARG	Sidechain	4
1	A	121	ARG	Sidechain	4
1	A	36	ARG	Sidechain,Mainchain	3
1	A	43	PHE	Mainchain,Sidechain	3
1	A	28	ARG	Sidechain	3
1	A	105	ARG	Sidechain	3
1	A	14	GLN	Mainchain,Peptide	2
1	A	7	ARG	Sidechain	2
1	A	18	LEU	Mainchain,Peptide	2
1	A	83	CYS	Peptide	2
1	A	98	TYR	Sidechain	2
1	A	64	HIS	Peptide	2
1	A	97	ARG	Sidechain	2
1	A	48	PHE	Sidechain	1
1	A	99	ALA	Peptide	1
1	A	129	LEU	Peptide	1
1	A	82	HIS	Sidechain	1
1	A	73	ARG	Sidechain	1
1	A	6	THR	Peptide	1
1	A	77	ARG	Sidechain	1
1	A	2	PRO	Peptide	1
1	A	29	ALA	Mainchain	1
1	A	101	ARG	Sidechain	1
1	A	87	ASN	Sidechain	1
1	A	91	GLN	Mainchain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	21	PRO	Peptide	1
1	A	76	PHE	Sidechain	1
1	A	61	ARG	Sidechain	1
1	A	78	VAL	Peptide	1
1	A	13	ILE	Mainchain	1
1	A	70	ASN	Sidechain	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	1083	1060	1055	1±1
2	A	58	32	30	0±0
All	All	22820	21840	21707	15

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
1:A:38:LYS:HE2	2:A:203:SGN:HN	0.63	1.52	1	2
1:A:107:TYR:HB3	1:A:132:THR:HG22	0.53	1.79	13	1
1:A:80:LEU:HD12	1:A:80:LEU:C	0.51	2.25	19	1
1:A:128:HIS:CD2	1:A:129:LEU:H	0.47	2.28	17	1
1:A:60:ILE:HG13	1:A:71:CYS:SG	0.46	2.49	20	1
1:A:38:LYS:HG3	2:A:203:SGN:HN	0.46	1.69	8	1
1:A:23:CYS:SG	1:A:100:ASP:HA	0.44	2.52	1	2
1:A:108:VAL:O	1:A:129:LEU:HD12	0.42	2.14	11	1
1:A:26:ALA:HB1	1:A:43:PHE:CZ	0.42	2.49	4	1
1:A:38:LYS:HE2	2:A:203:SGN:H3	0.42	1.91	3	1
1:A:41:ASN:ND2	1:A:43:PHE:CE1	0.41	2.89	8	1
1:A:27:MET:HG3	1:A:98:TYR:CD1	0.41	2.51	3	1
1:A:72:HIS:O	1:A:108:VAL:HG13	0.40	2.16	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	131/133 (98%)	113±4 (87±3%)	16±3 (12±3%)	2±1 (1±1%)	21	68
All	All	2620/2660 (98%)	2267 (87%)	322 (12%)	31 (1%)	21	68

All 21 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	86	ILE	3
1	A	24	THR	3
1	A	102	PRO	3
1	A	88	PRO	2
1	A	89	GLY	2
1	A	85	LEU	2
1	A	3	PRO	2
1	A	12	ALA	1
1	A	58	GLN	1
1	A	68	LEU	1
1	A	55	CYS	1
1	A	96	CYS	1
1	A	127	VAL	1
1	A	15	HIS	1
1	A	66	ARG	1
1	A	79	PRO	1
1	A	121	ARG	1
1	A	120	PRO	1
1	A	4	GLN	1
1	A	20	PRO	1
1	A	95	ASN	1

### 6.3.2 Protein sidechains [i](#)

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

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	121/122 (99%)	117±2 (97±1%)	4±2 (3±1%)	51 90
All	All	2420/2440 (99%)	2344 (97%)	76 (3%)	51 90

All 28 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	133	ILE	20
1	A	35	TRP	9
1	A	30	ILE	6
1	A	101	ARG	5
1	A	19	ASN	3
1	A	122	TYR	3
1	A	80	LEU	3
1	A	3	PRO	2
1	A	86	ILE	2
1	A	124	VAL	2
1	A	67	THR	2
1	A	100	ASP	2
1	A	88	PRO	2
1	A	130	ASP	1
1	A	21	PRO	1
1	A	68	LEU	1
1	A	10	TRP	1
1	A	6	THR	1
1	A	43	PHE	1
1	A	129	LEU	1
1	A	116	PRO	1
1	A	125	VAL	1
1	A	114	ARG	1
1	A	76	PHE	1
1	A	98	TYR	1
1	A	64	HIS	1
1	A	61	ARG	1
1	A	121	ARG	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates ⓘ

3 carbohydrates 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
2	LVZ	A	201	2	22,23,23	1.93±0.33	0±1 (1±2%)
2	IDS	A	202	2	13,16,17	2.28±0.56	1±0 (4±3%)
2	SGN	A	203	2	18,19,20	1.93±0.50	0±1 (2±3%)

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
2	LVZ	A	201	2	28,35,35	1.80±0.32	1±1 (2±2%)
2	IDS	A	202	2	16,24,26	1.75±0.28	0±0 (1±2%)
2	SGN	A	203	2	24,29,31	2.06±0.26	1±1 (2±2%)

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
2	LVZ	A	201	2	-	0±0,15,35,35	0±0,1,1,1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IDS	A	202	2	-	0±0,5,26,29	0±0,1,1,1
2	SGN	A	203	2	-	0±0,11,28,31	0±0,1,1,1

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	A	202	IDS	O5-C5	10.26	1.54	1.43	15	9
2	A	203	SGN	S1-N	8.80	1.70	1.60	1	6
2	A	201	LVZ	S19-N9	8.58	1.69	1.60	3	4
2	A	203	SGN	O1S-S1	7.35	1.50	1.42	4	2
2	A	202	IDS	O5-C1	6.95	1.55	1.43	8	2
2	A	202	IDS	C1-C2	6.21	1.62	1.51	10	1
2	A	201	LVZ	O59-C59	5.93	1.59	1.44	20	1
2	A	201	LVZ	O3S-S19	5.88	1.48	1.42	6	2
2	A	203	SGN	O2S-S1	5.31	1.48	1.42	17	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	A	201	LVZ	O3S-S19-N9	9.27	95.75	108.63	4	8
2	A	203	SGN	C1-O5-C5	8.22	124.22	112.14	10	5
2	A	202	IDS	C1-C2-C3	7.29	120.38	109.48	11	3
2	A	202	IDS	C4-C3-C2	6.63	122.06	110.23	10	1
2	A	203	SGN	C2-N-S1	6.25	109.11	121.38	18	3
2	A	201	LVZ	O2S-S19-N9	6.16	117.18	108.63	8	1
2	A	203	SGN	C3-C4-C5	6.11	121.13	110.23	20	1
2	A	203	SGN	C3-C2-N	5.74	118.06	110.36	15	2
2	A	203	SGN	O1S-S1-N	5.40	101.12	108.63	17	1
2	A	202	IDS	O5-C5-C4	5.28	99.89	108.51	19	1
2	A	201	LVZ	C49-C39-C29	5.27	118.37	110.37	15	1
2	A	201	LVZ	O3S-S19-O2S	5.22	106.01	120.14	6	1
2	A	201	LVZ	O69-C69-C59	5.05	117.75	107.96	17	1

All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	203	SGN	C1	2

There are no torsion outliers.

There are no ring outliers.

## 6.6 Ligand geometry

There are no ligands in this entry.

## 6.7 Other polymers

There are no such molecules in this entry.

## 6.8 Polymer linkage issues

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 77% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2lvz\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

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

Total number of shifts	1481
Number of shifts mapped to atoms	1481
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	129	$-0.01 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	129	$-0.08 \pm 0.12$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	120	$1.12 \pm 0.39$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1355 atoms were assigned a chemical shift out of a possible 1755. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	500/636 (79%)	252/252 (100%)	128/264 (48%)	120/120 (100%)
Sidechain	775/969 (80%)	493/577 (85%)	256/316 (81%)	26/76 (34%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	80/150 (53%)	62/78 (79%)	16/60 (27%)	2/12 (17%)
Overall	1355/1755 (77%)	807/907 (89%)	400/640 (62%)	148/208 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 77%, i.e. 1366 atoms were assigned a chemical shift out of a possible 1778. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	502/641 (78%)	253/254 (100%)	129/266 (48%)	120/121 (99%)
Sidechain	784/987 (79%)	499/588 (85%)	259/320 (81%)	26/79 (33%)
Aromatic	80/150 (53%)	62/78 (79%)	16/60 (27%)	2/12 (17%)
Overall	1366/1778 (77%)	814/920 (88%)	404/646 (63%)	148/212 (70%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	117	ARG	H	0.30	11.29 – 5.19	-13.0
1	A	12	ALA	CB	38.40	28.03 – 9.93	10.7
1	A	14	GLN	HG3	0.58	3.75 – 0.85	-5.9
1	A	14	GLN	HB2	0.68	3.30 – 0.80	-5.5
1	A	126	PRO	HB3	0.07	3.81 – 0.21	-5.4
1	A	27	MET	HB3	0.28	3.70 – 0.30	-5.1
1	A	74	SER	HB3	2.44	5.25 – 2.45	-5.0

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

