

# wwPDB NMR Structure Validation Summary Report (i)

#### May 29, 2020 – 12:58 am BST

PDB ID	:	2REL
$\operatorname{Title}$	:	SOLUTION STRUCTURE OF R-ELAFIN, A SPECIFIC INHIBITOR OF
		ELASTASE, NMR, 11 STRUCTURES
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Deposited on	:	1997-04-01

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

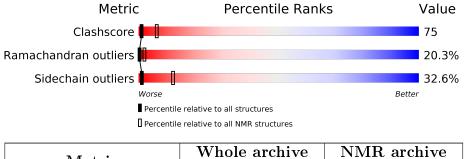
Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$	:	Kelley et al. (1996)
$\operatorname{MolProbity}$	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. $(2010)$
${ m ShiftChecker}$	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

# 1 Overall quality at a glance (i)

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	(#Entries)	(#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=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 <=5%

Mol	Chain	Length	Quality of chain			
1	А	57	5% 63%	16%	•	14%



# 2 Ensemble composition and analysis (i)

This entry contains 11 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:9-A:57 (49)	1.18	8		

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

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

The models can be grouped into 3 clusters. No single-model clusters were found.

Cluster number	Models
1	2, 4, 7, 8, 10
2	1, 5, 6
3	3, 9, 11



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 830 atoms, of which 419 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called R-ELAFIN.

Mol	Chain	Residues		Atoms			Trace		
1	Λ	57	Total	С	Η	Ν	0	S	0
	A	57	830	254	419	72	75	10	0



# 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: R-ELAFIN

Chain A: 5%		63%	16%	• 14%
A1 Q2 F2 F4 F6 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7 C7	T11 X12 X12 X12 V13 C14 C14 V17 V17 V12 V12 V12 V12 V12 V12 V12 V12 V12 V12	A24 A25 L26 L26 N27 P28 P28 R31 C32 C32 C32 C32 C32 C32 C32 C32 C38 C38 C38 C38 C38 C38 C38 C38 C38 C38	640 141 142 142 143 144 144 144 144 144 144 144 144 144	C 449 G 50 M 51 A 52 C 53 F 54 V 55 P 56 D 57

# 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

• Molecule 1: R-ELAFIN

Chain A:	28%	35%	19%	• 149	%
A1 G2 F3 V5 V5 G7 P8	V9 210 711 711 713 713 713 713 713 713 713 713	10000000000000000000000000000000000000	K43 C444 C445 C445 G44 C446 C49 S50 M51	F54 V55 P56 <b>Q</b> 57	



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *DISTANCE GEOMETRY*, *SIMULATED ANNEALING*.

Of the 200 calculated structures, 11 were deposited, based on the following criterion: *NOE AND DIHEDRAL ANGLE VIOLATIONS, ENERGY.* 

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

Software name	Classification	Version	
X-PLOR	refinement	3.1	
X-PLOR	structure solution	3.1	

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)

There are no covalent bond-length or bond-angle outliers.

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	А	$0.0{\pm}0.0$	$1.8 \pm 0.4$
All	All	0	20

There are no bond-length outliers.

There are no bond-angle outliers.

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	А	31	ARG	Sidechain	10
1	А	22	ARG	Sidechain	10

## 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)	$H(model) \mid H(added) \mid C$		
1	А	354	359	359	$53 \pm 10$	
All	All	3894	3949	3949	588	

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 75.

5 of 406 unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom 2	Atom-2 Clash(Å) Distance(		Moo	dels	
Atom-1	Atom-2	Clash(A)	Distance(Å)	Worst	Total	
1:A:32:CYS:C	1:A:33:LEU:HD13	0.95	1.80	10	1	
1:A:20:LEU:HD13	1:A:21:ILE:N	0.94	1.77	5	1	
1:A:19:ILE:HD13	1:A:46:GLU:O	0.91	1.64	5	2	
1:A:19:ILE:HG21	1:A:47:GLY:C	0.90	1.86	3	5	
1:A:20:LEU:HD12	1:A:21:ILE:N	0.88	1.84	10	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	А	48/57~(84%)	$24\pm3 (50\pm5\%)$	$14\pm3 (30\pm6\%)$	$10\pm3~(20\pm7\%)$	0 2		
All	All	528/627~(84%)	262~(50%)	159~(30%)	107~(20%)	0 2		

5 of 35 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	$\mathbf{Res}$	Type	Models (Total)
1	А	21	ILE	9
1	А	23	CYS	7
1	А	13	PRO	6
1	А	34	LYS	5
1	А	14	GLY	5

#### 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	Rotameric Outliers		Percentiles		
1	А	43/49~(88%)	$29 \pm 1 \ (67 \pm 3\%)$	$14\pm1~(33\pm3\%)$	-	L	12	
All	All	473/539 (88%)	319~(67%)	154 (33%)	]	L	12	



Mol	Chain	Res	Type	Models (Total)
1	А	33	LEU	9
1	А	34	LYS	8
1	А	10	SER	7
1	А	20	LEU	7
1	А	45	CYS	7

5 of 33 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

#### 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)

There are no ligands in this entry.

## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 7 Chemical shift validation (i)

No chemical shift data were provided

