



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1BM6 / pdb_00001bm6
Title : SOLUTION STRUCTURE OF THE CATALYTIC DOMAIN OF HUMAN STROMELYSIN-1 COMPLEXED TO A POTENT NON-PEPTIDIC INHIBITOR, NMR, 20 STRUCTURES
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with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

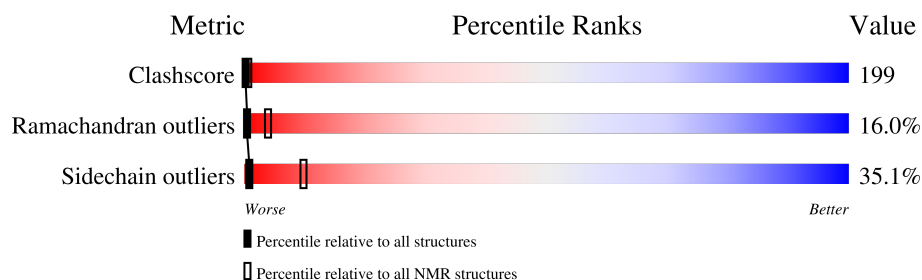
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	173	

2 Ensemble composition and analysis

This entry contains 20 models. Model 15 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:91-A:149, A:156-A:246 (150)	0.56	15

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

3 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2728 atoms, of which 1321 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STROMELYSIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	173	Total	C	H	N	O	S	0
			2674	882	1298	228	264	2	

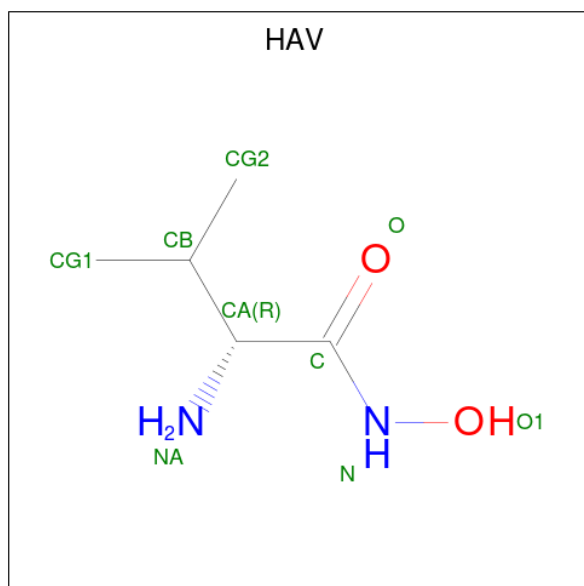
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

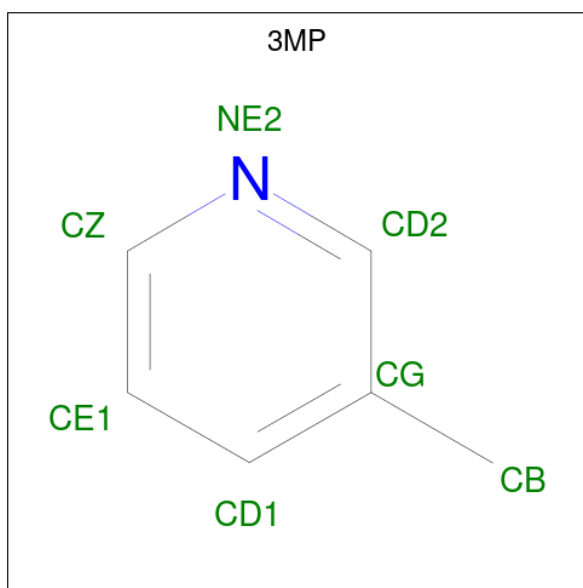
Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

- Molecule 4 is HYDROXYAMINOVALINE (CCD ID: HAV) (formula: C₅H₁₂N₂O₂).



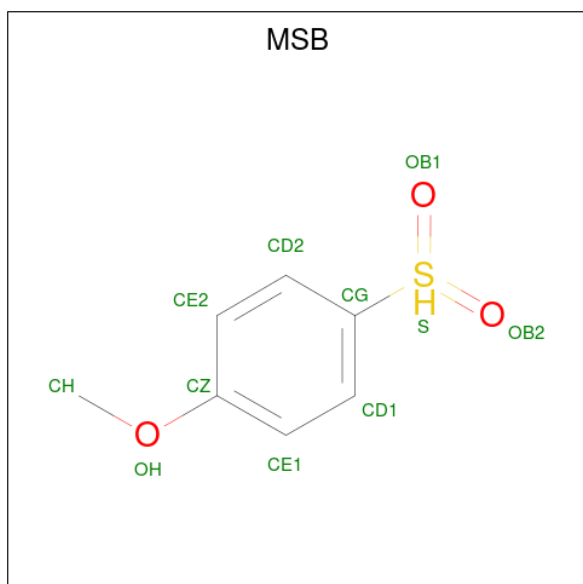
Mol	Chain	Residues	Atoms				
4	A	1	Total	C	H	N	O
			19	5	10	2	2

- Molecule 5 is 3-METHYLPYRIDINE (CCD ID: 3MP) (formula: C_6H_7N).



Mol	Chain	Residues	Atoms			
			Total	C	H	N
5	A	1	13	6	6	1

- Molecule 6 is 1-METHYLOXY-4-SULFONE-BENZENE (CCD ID: MSB) (formula: $C_7H_8O_3S$).



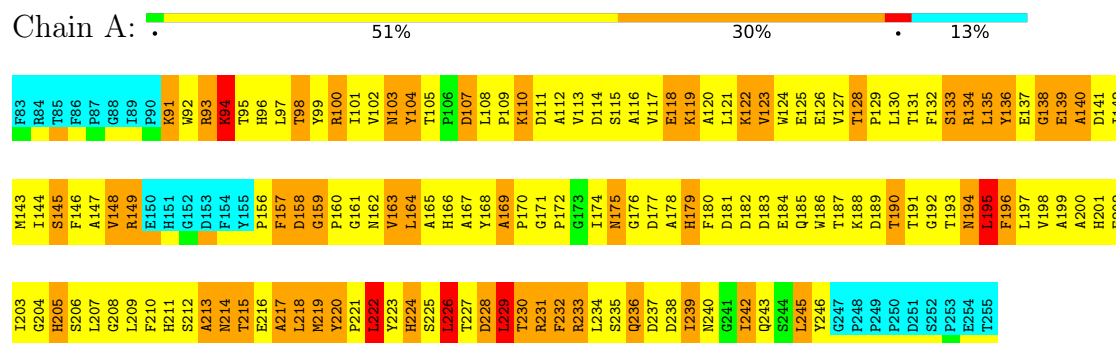
Mol	Chain	Residues	Atoms				
			Total	C	H	O	S
6	A	1	18	7	7	3	1

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

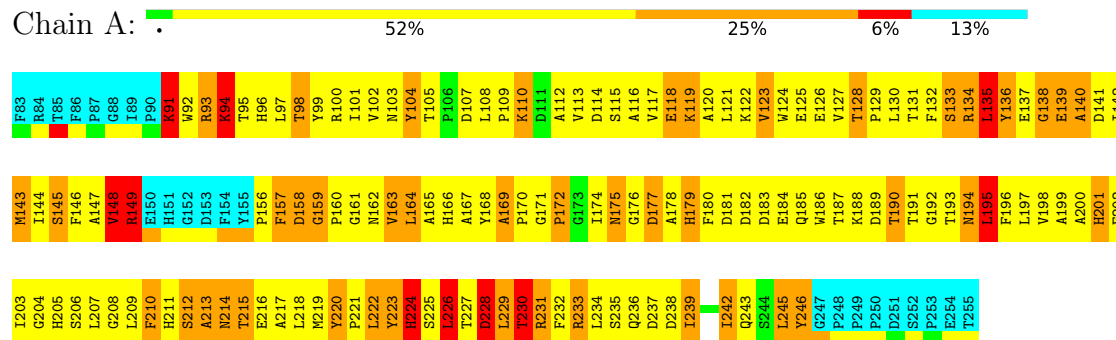
- Molecule 1: STROMELYSIN-1



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

The representative model is number 15. Colouring as in section 4.1 above.

- Molecule 1: STROMELYSIN-1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LEAST RESTRAINT VIOLATION, ENERGY MINIMIZATION*.

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

Software name	Classification	Version
X-PLOR	refinement	3.1
BRUKER XWINNMR	structure solution	XWINNMR
MSI NMRCOMPASS	structure solution	NMRCOMPASS
Felix	structure solution	
NMRPipe	structure solution	

No chemical shift data was provided.

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: MSB, HAV, ZN, 3MP, CA

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	1.44±0.01	0±0/1228 (0.0± 0.0%)	1.32±0.01	2±1/1676 (0.1± 0.0%)
All	All	1.44	4/24560 (0.0%)	1.32	41/33520 (0.1%)

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
1	A	192	GLY	N-CA	5.65	1.49	1.45	18	1
1	A	164	LEU	CA-C	5.42	1.55	1.52	10	1
1	A	246	TYR	N-CA	5.19	1.49	1.46	11	1
1	A	159	GLY	N-CA	5.01	1.51	1.44	1	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	215	THR	N-CA-C	-6.16	103.87	111.75	14	20
1	A	201	HIS	CA-CB-CG	-5.60	108.20	113.80	3	8
1	A	200	ALA	N-CA-C	-5.55	106.35	113.01	1	5
1	A	216	GLU	N-CA-C	-5.27	107.50	114.04	20	6
1	A	157	PHE	CA-CB-CG	-5.26	108.53	113.80	12	2

There are no chirality outliers.

There are no planarity outliers.

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	1193	1139	1139	472±17
4	A	9	10	10	6±4
5	A	7	6	5	2±1
6	A	11	7	7	16±2
All	All	24480	23240	23207	9499

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 199.

5 of 2150 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:LEU:HD13	1:A:195:LEU:HD22	1.11	1.20	3	4
1:A:97:LEU:HD13	1:A:132:PHE:CZ	1.09	1.82	13	3
1:A:135:LEU:HD21	1:A:140:ALA:HB2	1.08	1.20	8	10
1:A:164:LEU:HD21	1:A:193:THR:HG21	1.05	1.28	4	4
1:A:147:ALA:HB3	1:A:179:HIS:CE1	1.05	1.85	3	16

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	150/173 (87%)	92±3 (61±2%)	34±4 (23±3%)	24±3 (16±2%)	0	4
All	All	3000/3460 (87%)	1831 (61%)	689 (23%)	480 (16%)	0	4

5 of 45 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	94	LYS	20
1	A	148	VAL	20
1	A	195	LEU	20
1	A	220	TYR	20
1	A	226	LEU	20

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	127/147 (86%)	82±4 (65±3%)	45±4 (35±3%)	1	10
All	All	2540/2940 (86%)	1649 (65%)	891 (35%)	1	10

5 of 101 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	91	LYS	20
1	A	94	LYS	20
1	A	135	LEU	20
1	A	145	SER	20
1	A	179	HIS	20

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 oligosaccharides in this entry.

6.6 Ligand geometry

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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
4	HAV	A	1	6,2,5	6,8,8	0.53±0.06	0±0 (0±0%)
5	3MP	A	2	4	7,7,7	0.45±0.01	0±0 (0±0%)
6	MSB	A	3	4	9,11,11	1.06±0.02	1±0 (10±2%)

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
4	HAV	A	1	6,2,5	5,10,10	0.86±0.10	0±0 (6±9%)
5	3MP	A	2	4	8,8,8	0.48±0.01	0±0 (0±0%)
6	MSB	A	3	4	13,14,14	0.86±0.02	1±0 (7±0%)

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
6	MSB	A	3	4	-	0±0,6,6,6	0±0,1,1,1
4	HAV	A	1	6,2,5	-	0±0,10,10,10	-
5	3MP	A	2	4	-	-	0±0,1,1,1

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
6	A	3	MSB	CG-S	2.47	1.75	1.80	9	19

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
6	A	3	MSB	OB1-S-CG	2.54	110.26	104.55	15	20
4	A	1	HAV	O-C-CA	2.38	122.55	120.66	15	6

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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