



Full wwPDB NMR Structure Validation Report ⓘ

Mar 9, 2026 – 08:27 AM UTC

PDB ID : 3USN / pdb_00003usn
Title : STRUCTURE OF THE CATALYTIC DOMAIN OF HUMAN FIBROBLAST STROMELYSIN-1 INHIBITED WITH THE THIADIAZOLE INHIBITOR IPNU-107859, NMR, 1 STRUCTURE
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Deposited on : 1998-06-18

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<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

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)
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

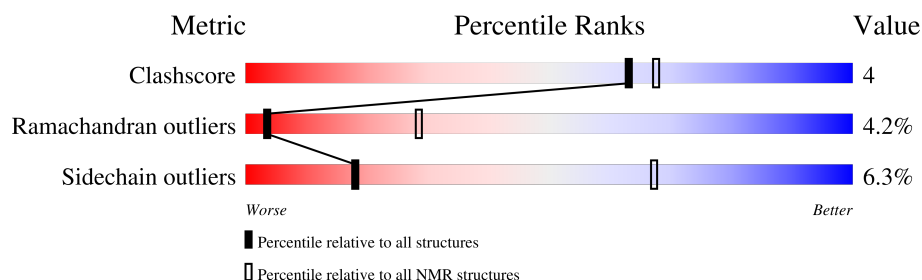
1 Overall quality at a glance

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	168	

2 Ensemble composition and analysis ⓘ

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2664 atoms, of which 1296 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STROMELYSIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	168	Total	C	H	N	O	S	0
			2617	861	1278	223	253	2	

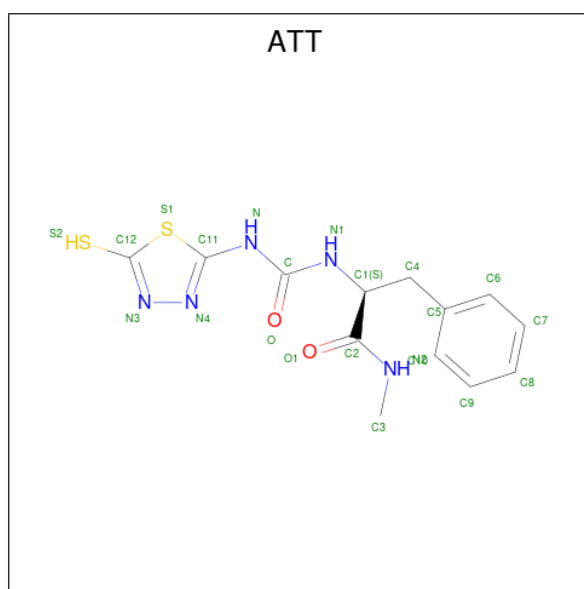
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	3	Total	Ca
			3	3

- Molecule 4 is 2-[3-(5-MERCAPTO-[1,3,4]THIADIAZOL-2-YL)-UREIDO]-N-METHYL-3-PHENYL-PROPIONAMIDE (CCD ID: ATT) (formula: C₁₃H₁₅N₅O₂S₂).



Mol	Chain	Residues	Atoms					
4	A	1	Total	C	H	N	O	S
			36	13	14	5	2	2

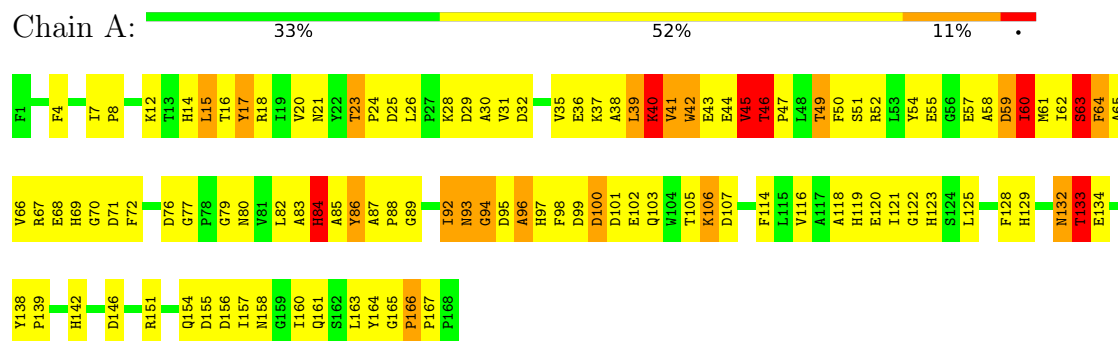
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		
5	A	2	Total	H	O
			6	4	2

4 Residue-property plots [i](#)

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



5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *RESTRAINED ENERGY MINIMIZATION AND RESTRAINED MOLECULAR DYNAMICS*.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version
Discover	refinement	
Discover	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: ZN, ATT, 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	2.53	98/1383 (7.1%)	2.70	120/1888 (6.4%)
All	All	2.53	98/1383 (7.1%)	2.70	120/1888 (6.4%)

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	7
All	All	0	7

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	167	PRO	CA-C	10.92	1.62	1.52
1	A	45	VAL	CA-CB	9.20	1.67	1.54
1	A	80	ASN	N-CA	8.31	1.56	1.46
1	A	97	HIS	CG-CD2	8.19	1.44	1.35
1	A	14	HIS	CG-CD2	8.01	1.44	1.35
1	A	142	HIS	ND1-CE1	7.91	1.40	1.32
1	A	57	GLU	CA-C	7.87	1.62	1.52
1	A	88	PRO	CA-C	7.72	1.62	1.52
1	A	92	ILE	CA-C	7.71	1.62	1.52
1	A	106	LYS	CA-C	7.70	1.62	1.52
1	A	121	ILE	CA-C	7.67	1.62	1.52
1	A	55	GLU	CA-C	7.67	1.62	1.52
1	A	40	LYS	C-N	7.51	1.43	1.33
1	A	164	TYR	CA-C	7.42	1.62	1.52
1	A	129	HIS	ND1-CE1	7.40	1.40	1.32
1	A	38	ALA	N-CA	7.35	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	PHE	CA-C	7.12	1.61	1.53
1	A	25	ASP	CG-OD2	7.08	1.38	1.25
1	A	85	ALA	CA-C	7.06	1.61	1.52
1	A	95	ASP	CG-OD2	7.05	1.38	1.25
1	A	26	LEU	CA-CB	6.95	1.63	1.54
1	A	119	HIS	CE1-NE2	6.92	1.39	1.32
1	A	20	VAL	N-CA	6.90	1.54	1.46
1	A	52	ARG	N-CA	6.90	1.54	1.46
1	A	66	VAL	CA-CB	6.88	1.63	1.54
1	A	84	HIS	CA-C	6.80	1.61	1.53
1	A	36	GLU	CD-OE2	6.80	1.38	1.25
1	A	84	HIS	C-O	6.65	1.31	1.23
1	A	41	VAL	CA-C	6.62	1.61	1.52
1	A	123	HIS	CG-CD2	6.57	1.43	1.35
1	A	39	LEU	N-CA	6.47	1.53	1.46
1	A	36	GLU	CA-C	6.46	1.61	1.52
1	A	107	ASP	CG-OD2	6.39	1.37	1.25
1	A	157	ILE	CA-CB	6.37	1.61	1.54
1	A	31	VAL	CA-C	6.36	1.60	1.52
1	A	14	HIS	CE1-NE2	6.36	1.39	1.32
1	A	122	GLY	CA-C	6.35	1.58	1.52
1	A	134	GLU	CD-OE2	6.35	1.37	1.25
1	A	12	LYS	CA-C	6.22	1.61	1.52
1	A	94	GLY	N-CA	6.20	1.54	1.45
1	A	67	ARG	CA-C	6.19	1.61	1.52
1	A	44	GLU	C-N	6.14	1.42	1.33
1	A	155	ASP	CG-OD2	6.05	1.36	1.25
1	A	100	ASP	CG-OD2	6.01	1.36	1.25
1	A	32	ASP	CG-OD2	5.99	1.36	1.25
1	A	63	SER	CA-C	5.98	1.60	1.52
1	A	8	PRO	CA-C	5.94	1.58	1.52
1	A	100	ASP	N-CA	5.91	1.54	1.46
1	A	41	VAL	N-CA	5.91	1.53	1.46
1	A	102	GLU	CD-OE2	5.87	1.36	1.25
1	A	57	GLU	CD-OE2	5.87	1.36	1.25
1	A	29	ASP	CG-OD2	5.85	1.36	1.25
1	A	107	ASP	CA-C	5.83	1.61	1.53
1	A	156	ASP	CG-OD2	5.82	1.36	1.25
1	A	14	HIS	CA-CB	5.81	1.61	1.53
1	A	35	VAL	CA-C	5.79	1.59	1.52
1	A	45	VAL	N-CA	5.75	1.53	1.46
1	A	71	ASP	CG-OD2	5.71	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	LYS	CA-C	5.71	1.60	1.52
1	A	161	GLN	CA-C	5.70	1.60	1.52
1	A	146	ASP	CG-OD2	5.68	1.36	1.25
1	A	64	PHE	CA-C	5.66	1.59	1.52
1	A	101	ASP	CG-OD2	5.65	1.36	1.25
1	A	16	THR	CA-C	5.64	1.59	1.52
1	A	76	ASP	CG-OD2	5.64	1.36	1.25
1	A	84	HIS	CD2-NE2	5.63	1.44	1.37
1	A	47	PRO	CA-C	5.60	1.60	1.53
1	A	93	ASN	CA-C	5.58	1.59	1.52
1	A	59	ASP	N-CA	5.54	1.53	1.46
1	A	118	ALA	CA-C	5.54	1.59	1.52
1	A	142	HIS	CE1-NE2	5.53	1.38	1.32
1	A	92	ILE	N-CA	5.53	1.53	1.46
1	A	51	SER	N-CA	5.50	1.52	1.46
1	A	62	ILE	CA-CB	5.45	1.60	1.53
1	A	119	HIS	CG-CD2	5.44	1.41	1.35
1	A	66	VAL	CA-C	5.43	1.59	1.52
1	A	59	ASP	CG-OD2	5.41	1.35	1.25
1	A	25	ASP	N-CA	5.40	1.53	1.46
1	A	133	THR	N-CA	5.40	1.53	1.46
1	A	30	ALA	CA-C	5.34	1.59	1.52
1	A	62	ILE	CA-C	5.23	1.59	1.53
1	A	160	ILE	N-CA	5.23	1.53	1.46
1	A	67	ARG	N-CA	5.22	1.52	1.46
1	A	84	HIS	ND1-CE1	5.19	1.37	1.32
1	A	68	GLU	CD-OE2	5.18	1.35	1.25
1	A	76	ASP	CA-C	5.18	1.59	1.52
1	A	54	TYR	CA-C	5.15	1.60	1.52
1	A	79	GLY	CA-C	5.15	1.59	1.51
1	A	7	ILE	CA-C	5.13	1.58	1.52
1	A	17	TYR	N-CA	5.13	1.52	1.45
1	A	119	HIS	ND1-CE1	5.12	1.37	1.32
1	A	151	ARG	CZ-NH2	-5.08	1.26	1.33
1	A	142	HIS	CG-CD2	5.06	1.41	1.35
1	A	38	ALA	CA-C	5.04	1.59	1.52
1	A	43	GLU	CA-C	5.02	1.59	1.52
1	A	101	ASP	CA-CB	5.01	1.61	1.53
1	A	120	GLU	CD-OE2	5.01	1.34	1.25
1	A	64	PHE	N-CA	5.00	1.52	1.45

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	HIS	ND1-CE1-NE2	15.10	123.50	108.40
1	A	97	HIS	ND1-CE1-NE2	15.06	123.46	108.40
1	A	99	ASP	CA-CB-CG	13.76	126.36	112.60
1	A	142	HIS	ND1-CE1-NE2	12.51	120.91	108.40
1	A	123	HIS	CE1-NE2-CD2	-12.41	96.59	109.00
1	A	97	HIS	CE1-NE2-CD2	-11.92	97.08	109.00
1	A	142	HIS	CE1-NE2-CD2	-11.85	97.15	109.00
1	A	119	HIS	ND1-CE1-NE2	11.84	120.24	108.40
1	A	14	HIS	ND1-CE1-NE2	11.81	120.21	108.40
1	A	69	HIS	ND1-CE1-NE2	11.41	119.81	108.40
1	A	69	HIS	CE1-NE2-CD2	-11.09	97.91	109.00
1	A	76	ASP	CA-CB-CG	10.70	123.30	112.60
1	A	84	HIS	CE1-NE2-CD2	-10.63	98.37	109.00
1	A	84	HIS	ND1-CE1-NE2	10.29	118.69	108.40
1	A	129	HIS	ND1-CE1-NE2	10.12	118.52	108.40
1	A	166	PRO	N-CA-C	10.02	122.93	110.70
1	A	47	PRO	CA-C-O	-9.93	113.73	121.38
1	A	63	SER	N-CA-C	9.76	131.58	110.80
1	A	119	HIS	CE1-NE2-CD2	-9.37	99.63	109.00
1	A	103	GLN	OE1-CD-NE2	-9.34	113.26	122.60
1	A	45	VAL	CA-CB-CG2	9.15	125.95	110.40
1	A	84	HIS	N-CA-C	-8.77	91.44	107.75
1	A	42	TRP	CB-CA-C	8.76	124.45	110.96
1	A	129	HIS	CE1-NE2-CD2	-8.56	100.44	109.00
1	A	100	ASP	N-CA-C	-8.45	93.82	108.52
1	A	64	PHE	N-CA-C	8.41	122.27	109.23
1	A	14	HIS	CE1-NE2-CD2	-8.41	100.59	109.00
1	A	84	HIS	CA-C-O	8.34	129.85	120.84
1	A	95	ASP	CA-CB-CG	8.30	120.90	112.60
1	A	80	ASN	CA-CB-CG	8.16	120.76	112.60
1	A	107	ASP	CA-CB-CG	7.92	120.53	112.60
1	A	35	VAL	N-CA-C	-7.69	103.04	110.42
1	A	87	ALA	N-CA-C	7.60	122.19	109.87
1	A	142	HIS	CA-CB-CG	7.60	121.40	113.80
1	A	84	HIS	N-CA-CB	7.38	122.57	110.39
1	A	36	GLU	CA-C-O	-7.38	112.73	120.55
1	A	156	ASP	CA-CB-CG	7.30	119.90	112.60
1	A	40	LYS	CA-C-O	-7.22	112.83	120.63
1	A	132	ASN	CA-CB-CG	7.19	119.79	112.60
1	A	65	ALA	CA-C-O	7.08	128.26	119.98
1	A	95	ASP	O-C-N	7.03	132.02	123.16
1	A	116	VAL	CA-C-O	-6.91	113.84	121.17
1	A	114	PHE	CA-CB-CG	6.84	120.64	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	LYS	N-CA-C	6.81	118.35	111.07
1	A	119	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	A	84	HIS	CB-CG-CD2	-6.79	122.38	131.20
1	A	154	GLN	OE1-CD-NE2	-6.78	115.83	122.60
1	A	4	PHE	CA-CB-CG	6.61	120.41	113.80
1	A	41	VAL	N-CA-CB	6.57	122.07	111.23
1	A	82	LEU	N-CA-C	-6.56	102.78	111.24
1	A	14	HIS	CA-C-O	-6.51	112.94	120.49
1	A	59	ASP	CA-C-O	6.46	129.75	120.51
1	A	72	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	158	ASN	OD1-CG-ND2	-6.35	116.25	122.60
1	A	85	ALA	N-CA-CB	6.30	119.74	110.35
1	A	47	PRO	N-CA-CB	-6.24	98.63	102.81
1	A	119	HIS	CG-ND1-CE1	-6.24	98.70	109.30
1	A	84	HIS	CA-CB-CG	6.21	120.01	113.80
1	A	92	ILE	N-CA-CB	6.21	118.23	110.47
1	A	52	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	119	HIS	N-CA-CB	-6.18	101.10	110.07
1	A	85	ALA	CA-C-O	-6.17	114.50	120.92
1	A	123	HIS	CG-ND1-CE1	-6.15	98.85	109.30
1	A	31	VAL	CA-CB-CG2	6.06	120.71	110.40
1	A	15	LEU	N-CA-C	6.05	119.74	110.36
1	A	142	HIS	CB-CG-CD2	-6.02	123.37	131.20
1	A	142	HIS	CG-ND1-CE1	-6.02	99.06	109.30
1	A	42	TRP	N-CA-CB	-5.99	101.17	109.91
1	A	14	HIS	CG-ND1-CE1	-5.92	99.24	109.30
1	A	29	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	163	LEU	O-C-N	-5.84	116.07	122.38
1	A	71	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	142	HIS	CB-CA-C	5.79	121.95	110.42
1	A	96	ALA	CA-C-N	5.74	129.82	121.26
1	A	96	ALA	C-N-CA	5.74	129.82	121.26
1	A	129	HIS	CG-ND1-CE1	-5.73	99.57	109.30
1	A	95	ASP	CB-CA-C	-5.72	98.90	109.37
1	A	100	ASP	N-CA-CB	5.68	118.77	110.58
1	A	97	HIS	CG-ND1-CE1	-5.67	99.66	109.30
1	A	142	HIS	CG-CD2-NE2	5.62	112.82	107.20
1	A	86	TYR	CA-C-N	5.61	130.66	121.57
1	A	86	TYR	C-N-CA	5.61	130.66	121.57
1	A	62	ILE	N-CA-CB	-5.58	105.49	111.46
1	A	46	THR	CB-CA-C	5.56	121.12	110.17
1	A	87	ALA	N-CA-CB	-5.55	102.66	110.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	LYS	N-CA-CB	-5.55	101.95	110.16
1	A	8	PRO	CB-CA-C	5.55	116.53	111.87
1	A	105	THR	CA-C-N	5.54	128.16	120.29
1	A	105	THR	C-N-CA	5.54	128.16	120.29
1	A	60	ILE	CB-CA-C	5.43	120.20	111.29
1	A	77	GLY	CA-C-O	-5.42	113.78	121.52
1	A	99	ASP	CB-CG-OD2	-5.39	106.01	118.40
1	A	84	HIS	CB-CA-C	5.38	120.34	111.31
1	A	165	GLY	CA-C-N	5.36	125.90	120.38
1	A	165	GLY	C-N-CA	5.36	125.90	120.38
1	A	23	THR	CA-CB-CG2	5.32	119.54	110.50
1	A	96	ALA	CB-CA-C	5.32	120.56	110.51
1	A	39	LEU	N-CA-C	-5.28	105.21	110.97
1	A	123	HIS	CA-CB-CG	5.28	119.08	113.80
1	A	21	ASN	OD1-CG-ND2	-5.28	117.32	122.60
1	A	24	PRO	N-CA-C	5.28	120.70	113.84
1	A	41	VAL	O-C-N	5.28	129.16	122.57
1	A	69	HIS	CG-ND1-CE1	-5.25	100.38	109.30
1	A	93	ASN	O-C-N	-5.23	116.02	122.82
1	A	89	GLY	O-C-N	-5.20	116.57	121.77
1	A	92	ILE	CA-CB-CG1	5.18	119.22	110.40
1	A	83	ALA	CA-C-N	-5.17	115.66	122.85
1	A	83	ALA	C-N-CA	-5.17	115.66	122.85
1	A	58	ALA	N-CA-C	-5.15	99.84	110.80
1	A	85	ALA	N-CA-C	-5.14	98.94	107.99
1	A	94	GLY	CA-C-N	5.13	131.13	122.87
1	A	94	GLY	C-N-CA	5.13	131.13	122.87
1	A	99	ASP	N-CA-CB	-5.08	102.72	110.49
1	A	59	ASP	N-CA-C	5.06	121.57	110.80
1	A	35	VAL	CB-CA-C	5.04	118.43	111.97
1	A	139	PRO	N-CA-C	5.04	121.11	113.81
1	A	128	PHE	CB-CA-C	5.03	120.43	110.42
1	A	138	TYR	CA-C-O	-5.03	115.97	120.19
1	A	163	LEU	N-CA-CB	5.02	118.12	110.39
1	A	23	THR	CA-C-O	-5.01	115.12	120.23

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	23	THR	Mainchain
1	A	63	SER	Mainchain

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Mol	Chain	Res	Type	Group
1	A	84	HIS	Sidechain
1	A	86	TYR	Sidechain
1	A	93	ASN	Mainchain
1	A	94	GLY	Mainchain
1	A	100	ASP	Mainchain

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	1339	1278	1268	11
All	All	1368	1296	1282	11

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:15:LEU:H	1:A:49:THR:C	0.58	2.07
1:A:18:ARG:HD3	1:A:61:MET:SD	0.53	2.43
1:A:40:LYS:CD	1:A:40:LYS:C	0.49	2.86
1:A:42:TRP:O	1:A:45:VAL:HG22	0.49	2.07
1:A:39:LEU:HD22	1:A:50:PHE:CG	0.47	2.44
1:A:45:VAL:CG2	1:A:46:THR:H	0.46	2.23
1:A:132:ASN:O	1:A:133:THR:OG1	0.45	2.35
1:A:63:SER:OG	1:A:96:ALA:O	0.43	2.37
1:A:41:VAL:O	1:A:45:VAL:HG13	0.43	2.13
1:A:64:PHE:HA	1:A:98:PHE:H	0.42	1.74
1:A:17:TYR:CZ	1:A:39:LEU:HD11	0.41	2.50

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	166/168 (99%)	130 (78%)	29 (17%)	7 (4%)	3	28
All	All	166/168 (99%)	130 (78%)	29 (17%)	7 (4%)	3	28

All 7 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	45	VAL
1	A	46	THR
1	A	59	ASP
1	A	60	ILE
1	A	70	GLY
1	A	133	THR
1	A	166	PRO

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	142/142 (100%)	133 (94%)	9 (6%)	18	67
All	All	142/142 (100%)	133 (94%)	9 (6%)	18	67

All 9 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	40	LYS
1	A	45	VAL
1	A	49	THR
1	A	60	ILE
1	A	63	SER
1	A	84	HIS
1	A	92	ILE
1	A	106	LYS
1	A	125	LEU

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 [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	ATT	A	174	2	22,23,23	1.89	7 (31%)

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	ATT	A	174	2	29,30,30	2.76	7 (24%)

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
4	ATT	A	174	2	-	2,18,18,18	0,2,2,2

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	174	ATT	C-N	3.70	1.31	1.39
4	A	174	ATT	C11-N4	3.44	1.26	1.31
4	A	174	ATT	C11-N	3.22	1.43	1.38
4	A	174	ATT	C12-S2	2.77	1.62	1.72
4	A	174	ATT	C3-N2	2.59	1.50	1.45
4	A	174	ATT	N4-N3	2.13	1.35	1.39
4	A	174	ATT	C1-C2	2.10	1.58	1.52

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	174	ATT	O1-C2-N2	9.23	107.74	123.13
4	A	174	ATT	C1-C2-N2	7.35	128.08	116.99
4	A	174	ATT	C11-N4-N3	4.61	117.89	112.02
4	A	174	ATT	C4-C1-C2	3.77	119.94	110.30
4	A	174	ATT	S1-C11-N4	3.55	110.56	114.52
4	A	174	ATT	S1-C11-N	2.85	127.54	123.72
4	A	174	ATT	S1-C12-N3	2.61	110.70	114.10

There are no chirality outliers.

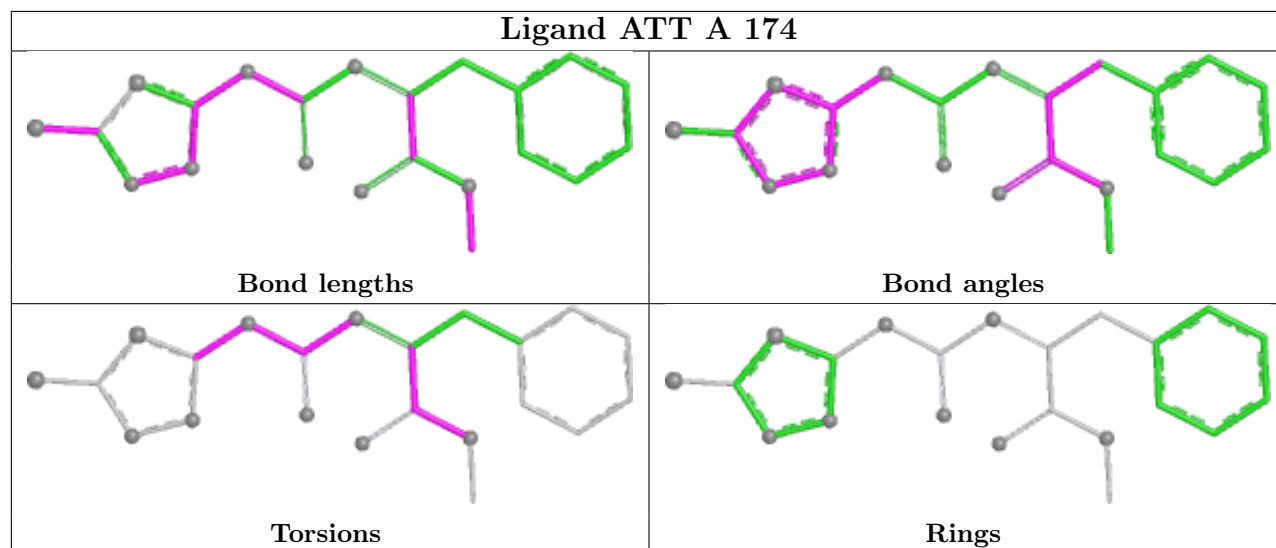
All torsion outliers are listed below.

Mol	Chain	Res	Type	Atoms
4	A	174	ATT	C1-C2-N2-C3
4	A	174	ATT	O1-C2-N2-C3

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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