



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 08:33 PM UTC

PDB ID : 1UMT / pdb_00001umt
Title : Stromelysin-1 catalytic domain with hydrophobic inhibitor bound, ph 7.0, 32oc, 20 mm cac12, 15% acetonitrile; nmr average of 20 structures minimized with restraints
Authors : Van Doren, S.R.; Kurochkin, A.V.; Hu, W.; Zuiderweg, E.R.P.
Deposited on : 1995-10-31

This is a Full wwPDB NMR Structure Validation 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 ⓘ 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

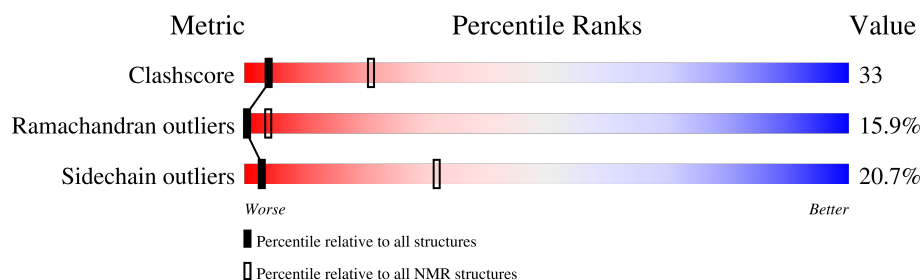
1 Overall quality at a glance

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	174	

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 4 unique types of molecules in this entry. The entry contains 2643 atoms, of which 1284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called STROMELYSIN-1.

Mol	Chain	Residues	Atoms						Trace
1	A	166	Total	C	H	N	O	S	0
			2572	851	1248	221	250	2	

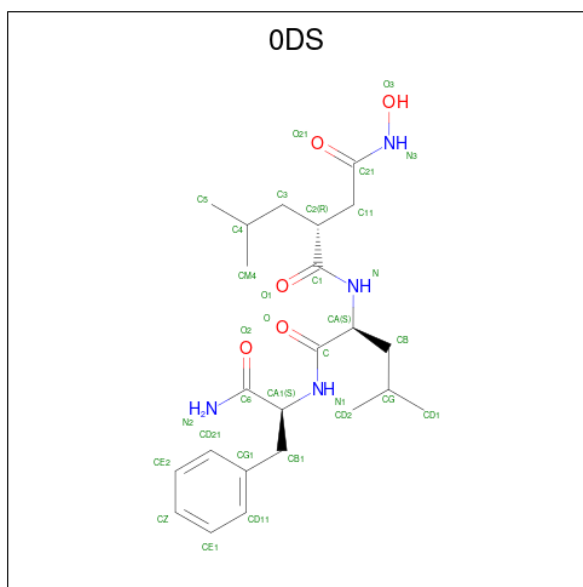
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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	1	Total	Ca
			1	1

- Molecule 4 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-L-leucyl-L-phenylalaninamide (CCD ID: 0DS) (formula: C₂₃H₃₆N₄O₅).

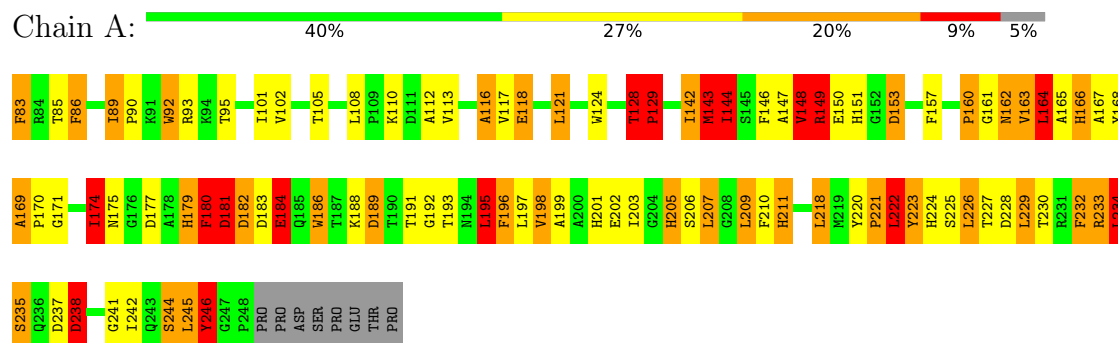


Mol	Chain	Residues	Atoms				
4	A	1	Total	C	H	N	O
			68	23	36	4	5

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: ?.

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
DGII	geometry optimization	
Discover	refinement	

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, ODS, 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	0.93	0/1366 (0.0%)	2.36	90/1864 (4.8%)
All	All	0.93	0/1366 (0.0%)	2.36	90/1864 (4.8%)

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

There are no bond-length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	CA-CB-CG	17.71	130.31	112.60
1	A	160	PRO	N-CA-CB	15.01	116.67	103.31
1	A	166	HIS	ND1-CE1-NE2	10.87	119.27	108.40
1	A	205	HIS	ND1-CE1-NE2	10.02	118.42	108.40
1	A	192	GLY	N-CA-C	-9.96	89.57	113.18
1	A	211	HIS	ND1-CE1-NE2	9.77	118.17	108.40
1	A	201	HIS	ND1-CE1-NE2	9.75	118.15	108.40
1	A	166	HIS	CE1-NE2-CD2	-9.74	99.26	109.00
1	A	174	ILE	N-CA-C	-9.68	93.62	107.37
1	A	151	HIS	ND1-CE1-NE2	9.47	117.87	108.40
1	A	218	LEU	N-CA-C	-9.37	101.27	112.89
1	A	128	THR	CA-C-N	9.35	131.53	119.84
1	A	128	THR	C-N-CA	9.35	131.53	119.84
1	A	166	HIS	CA-CB-CG	8.09	121.89	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TRP	CB-CA-C	7.78	121.90	109.61
1	A	166	HIS	CB-CA-C	7.59	124.12	111.51
1	A	182	ASP	CA-CB-CG	7.58	120.18	112.60
1	A	195	LEU	CA-C-N	7.51	133.13	121.19
1	A	195	LEU	C-N-CA	7.51	133.13	121.19
1	A	224	HIS	N-CA-C	-7.28	99.57	109.54
1	A	163	VAL	N-CA-CB	7.21	123.13	111.23
1	A	203	ILE	CA-C-N	7.13	127.71	119.94
1	A	203	ILE	C-N-CA	7.13	127.71	119.94
1	A	203	ILE	CA-CB-CG1	7.09	122.46	110.40
1	A	221	PRO	CB-CA-C	-7.00	100.88	111.44
1	A	83	PHE	CA-CB-CG	6.98	120.78	113.80
1	A	149	ARG	CA-C-N	6.93	134.77	121.54
1	A	149	ARG	C-N-CA	6.93	134.77	121.54
1	A	221	PRO	N-CA-C	6.57	122.11	114.03
1	A	108	LEU	N-CA-C	-6.54	100.53	110.07
1	A	205	HIS	CE1-NE2-CD2	-6.52	102.48	109.00
1	A	209	LEU	CA-C-N	6.52	134.00	121.54
1	A	209	LEU	C-N-CA	6.52	134.00	121.54
1	A	189	ASP	N-CA-C	-6.46	103.46	112.25
1	A	211	HIS	CE1-NE2-CD2	-6.46	102.54	109.00
1	A	143	MET	CB-CA-C	6.44	121.68	109.37
1	A	151	HIS	CE1-NE2-CD2	-6.44	102.56	109.00
1	A	237	ASP	N-CA-C	-6.41	104.50	112.90
1	A	167	ALA	N-CA-C	6.40	119.17	109.95
1	A	148	VAL	CG1-CB-CG2	6.39	124.86	110.80
1	A	171	GLY	CA-C-N	6.36	127.79	119.84
1	A	171	GLY	C-N-CA	6.36	127.79	119.84
1	A	116	ALA	CB-CA-C	6.35	120.73	110.96
1	A	201	HIS	CE1-NE2-CD2	-6.33	102.67	109.00
1	A	180	PHE	CA-C-O	-6.20	113.53	120.54
1	A	164	LEU	N-CA-CB	-6.18	100.04	110.49
1	A	148	VAL	N-CA-CB	6.12	121.32	111.23
1	A	222	LEU	CA-C-N	6.08	133.31	122.31
1	A	222	LEU	C-N-CA	6.08	133.31	122.31
1	A	246	TYR	CA-CB-CG	6.05	124.79	113.90
1	A	163	VAL	CB-CA-C	6.04	121.19	111.29
1	A	144	ILE	N-CA-C	6.01	116.52	108.11
1	A	151	HIS	ND1-CG-CD2	5.92	112.02	106.10
1	A	153	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	244	SER	CA-C-N	5.91	129.01	120.79
1	A	244	SER	C-N-CA	5.91	129.01	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	SER	CA-C-N	5.91	132.82	121.54
1	A	225	SER	C-N-CA	5.91	132.82	121.54
1	A	164	LEU	N-CA-C	5.90	123.37	110.80
1	A	201	HIS	ND1-CG-CD2	5.84	111.94	106.10
1	A	195	LEU	N-CA-CB	-5.70	101.13	110.14
1	A	210	PHE	CA-CB-CG	5.70	119.50	113.80
1	A	110	LYS	CA-C-N	5.68	128.47	120.28
1	A	110	LYS	C-N-CA	5.68	128.47	120.28
1	A	143	MET	CA-CB-CG	5.68	125.47	114.10
1	A	232	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	246	TYR	CA-C-N	5.67	125.27	121.13
1	A	246	TYR	C-N-CA	5.67	125.27	121.13
1	A	211	HIS	ND1-CG-CD2	5.63	111.73	106.10
1	A	177	ASP	CB-CA-C	-5.60	100.51	109.75
1	A	205	HIS	ND1-CG-CD2	5.54	111.64	106.10
1	A	151	HIS	CG-ND1-CE1	-5.49	99.97	109.30
1	A	89	ILE	CA-C-N	5.44	126.64	119.84
1	A	89	ILE	C-N-CA	5.44	126.64	119.84
1	A	238	ASP	N-CA-C	-5.44	105.35	111.28
1	A	245	LEU	N-CA-C	-5.42	104.41	111.02
1	A	177	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	201	HIS	CG-ND1-CE1	-5.41	100.11	109.30
1	A	129	PRO	CA-N-CD	-5.38	104.47	112.00
1	A	165	ALA	N-CA-C	-5.37	101.90	109.96
1	A	205	HIS	CG-ND1-CE1	-5.37	100.17	109.30
1	A	174	ILE	N-CA-CB	5.35	117.68	111.90
1	A	211	HIS	CG-ND1-CE1	-5.27	100.33	109.30
1	A	230	THR	CA-C-N	5.26	131.59	121.54
1	A	230	THR	C-N-CA	5.26	131.59	121.54
1	A	203	ILE	CB-CG1-CD1	5.22	124.76	113.80
1	A	166	HIS	N-CA-C	-5.21	96.24	107.49
1	A	199	ALA	N-CA-C	-5.18	105.33	110.97
1	A	112	ALA	CA-C-N	5.11	128.73	120.55
1	A	112	ALA	C-N-CA	5.11	128.73	120.55

There are no chirality outliers.

All planar outliers are listed below.

Mol	Chain	Res	Type	Group
1	A	128	THR	Peptide
1	A	146	PHE	Sidechain
1	A	168	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	180	PHE	Sidechain
1	A	196	PHE	Sidechain
1	A	223	TYR	Sidechain
1	A	246	TYR	Sidechain

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	1324	1248	1252	80
4	A	32	36	35	17
All	All	1359	1284	1287	88

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 33.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
4:A:261:0DS:HD1	4:A:261:0DS:CD11	1.09	0.97
4:A:261:0DS:CD21	4:A:261:0DS:HD2	1.08	0.97
4:A:261:0DS:CE1	4:A:261:0DS:CG1	0.95	2.43
4:A:261:0DS:CG1	4:A:261:0DS:CE2	0.94	2.43
4:A:261:0DS:HD2	4:A:261:0DS:CE2	0.80	2.06
4:A:261:0DS:HD1	4:A:261:0DS:CG1	0.79	2.07
4:A:261:0DS:HD1	4:A:261:0DS:CE1	0.79	2.07
1:A:116:ALA:HB1	1:A:196:PHE:N	0.79	1.93
4:A:261:0DS:HD2	4:A:261:0DS:CG1	0.78	2.07
1:A:164:LEU:HD23	1:A:198:VAL:HG21	0.70	1.63
1:A:113:VAL:HG13	1:A:195:LEU:HG	0.68	1.63
1:A:163:VAL:C	1:A:164:LEU:HD13	0.68	2.13
1:A:164:LEU:HD22	1:A:164:LEU:N	0.65	2.06
1:A:227:THR:HG23	1:A:232:PHE:CD1	0.65	2.26
1:A:148:VAL:CG1	1:A:181:ASP:HA	0.65	2.21
1:A:222:LEU:HD21	4:A:261:0DS:HB31	0.64	1.69
1:A:163:VAL:CG2	4:A:261:0DS:HA	0.64	2.23
1:A:164:LEU:HD22	1:A:198:VAL:HG11	0.62	1.70
1:A:164:LEU:CD2	1:A:198:VAL:HG21	0.62	2.23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:222:LEU:HD22	1:A:223:TYR:H	0.62	1.53
1:A:163:VAL:CA	1:A:164:LEU:HD13	0.61	2.26
1:A:164:LEU:N	1:A:164:LEU:CD2	0.60	2.65
1:A:160:PRO:HA	1:A:184:GLU:CD	0.60	2.21
1:A:222:LEU:HD13	1:A:223:TYR:N	0.59	2.12
1:A:113:VAL:HG13	1:A:195:LEU:CG	0.59	2.28
1:A:105:THR:CG2	1:A:186:TRP:CD1	0.59	2.85
1:A:116:ALA:HB1	1:A:196:PHE:CA	0.59	2.28
1:A:143:MET:HE3	1:A:174:ILE:CD1	0.58	2.28
1:A:169:ALA:HB1	1:A:170:PRO:CD	0.56	2.31
1:A:207:LEU:HD22	1:A:245:LEU:HD11	0.56	1.78
1:A:162:ASN:HA	4:A:261:ODS:CB1	0.55	2.32
1:A:143:MET:HE3	1:A:174:ILE:HD12	0.54	1.80
1:A:162:ASN:HA	4:A:261:ODS:HB21	0.53	1.81
1:A:148:VAL:CG2	1:A:181:ASP:HA	0.52	2.34
1:A:222:LEU:CD2	1:A:223:TYR:H	0.52	2.17
1:A:142:ILE:CG2	1:A:206:SER:HB2	0.52	2.35
1:A:164:LEU:CD2	1:A:198:VAL:HG11	0.52	2.34
1:A:143:MET:HE2	1:A:143:MET:N	0.51	2.21
1:A:105:THR:HG21	1:A:186:TRP:CD1	0.51	2.40
1:A:124:TRP:CZ3	1:A:234:LEU:CD2	0.51	2.94
1:A:169:ALA:HB1	1:A:170:PRO:HD3	0.50	1.83
1:A:148:VAL:HG23	1:A:149:ARG:N	0.50	2.21
1:A:222:LEU:HD22	1:A:223:TYR:N	0.50	2.22
1:A:142:ILE:CG2	1:A:206:SER:CB	0.49	2.90
1:A:153:ASP:HB2	1:A:166:HIS:CE1	0.49	2.43
1:A:113:VAL:HG22	1:A:195:LEU:HG	0.48	1.85
1:A:189:ASP:C	1:A:191:THR:H	0.48	2.16
1:A:89:ILE:CG1	1:A:245:LEU:O	0.48	2.62
1:A:163:VAL:C	1:A:164:LEU:CD1	0.48	2.85
1:A:163:VAL:HG22	4:A:261:ODS:H1	0.48	1.69
1:A:222:LEU:HD13	1:A:223:TYR:H	0.47	1.69
1:A:153:ASP:HB2	1:A:166:HIS:ND1	0.47	2.24
1:A:124:TRP:CZ3	1:A:234:LEU:HD23	0.46	2.45
1:A:197:LEU:CD1	1:A:223:TYR:HA	0.46	2.40
1:A:180:PHE:O	1:A:182:ASP:N	0.46	2.49
1:A:186:TRP:CE3	1:A:195:LEU:N	0.46	2.83
1:A:209:LEU:CD1	1:A:238:ASP:HB2	0.46	2.41
1:A:232:PHE:O	1:A:233:ARG:C	0.46	2.58
1:A:147:ALA:O	1:A:148:VAL:HG13	0.46	2.11
1:A:184:GLU:CG	1:A:193:THR:HG21	0.45	2.41
1:A:148:VAL:CG2	1:A:183:ASP:HB2	0.45	2.41

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:164:LEU:HD22	1:A:164:LEU:H	0.45	1.71
1:A:180:PHE:N	1:A:180:PHE:CD1	0.45	2.85
1:A:148:VAL:HG23	1:A:183:ASP:HB2	0.45	1.88
1:A:164:LEU:HD12	1:A:184:GLU:OE2	0.45	2.12
1:A:118:GLU:HA	1:A:121:LEU:HD23	0.44	1.88
1:A:86:PHE:CB	1:A:244:SER:CB	0.44	2.96
1:A:163:VAL:C	1:A:164:LEU:CG	0.44	2.86
1:A:218:LEU:HD11	1:A:232:PHE:CD2	0.43	2.48
1:A:179:HIS:CD2	1:A:179:HIS:N	0.43	2.86
1:A:169:ALA:CB	1:A:170:PRO:CD	0.43	2.97
1:A:148:VAL:HG21	1:A:181:ASP:OD1	0.43	2.13
1:A:162:ASN:CA	4:A:261:0DS:HB21	0.43	2.44
1:A:220:TYR:CD1	1:A:221:PRO:HD2	0.42	2.49
1:A:222:LEU:CG	1:A:223:TYR:H	0.42	2.28
1:A:163:VAL:HG22	4:A:261:0DS:N1	0.42	2.30
1:A:86:PHE:CB	1:A:244:SER:HB3	0.42	2.44
1:A:105:THR:HG21	1:A:186:TRP:NE1	0.42	2.29
1:A:144:ILE:HG23	1:A:180:PHE:CE1	0.42	2.50
1:A:113:VAL:HG13	1:A:195:LEU:CD1	0.42	2.45
1:A:222:LEU:CD2	4:A:261:0DS:HB31	0.41	2.42
1:A:153:ASP:CB	1:A:166:HIS:ND1	0.41	2.83
1:A:222:LEU:HD21	4:A:261:0DS:CB1	0.41	2.42
1:A:222:LEU:CD1	1:A:223:TYR:H	0.41	2.28
1:A:229:LEU:CD2	1:A:232:PHE:CD2	0.41	3.04
1:A:161:GLY:O	1:A:162:ASN:CB	0.41	2.69
1:A:235:SER:N	1:A:238:ASP:HB3	0.41	2.31
1:A:163:VAL:HG13	1:A:222:LEU:CD2	0.40	2.47

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	164/174 (94%)	88 (54%)	50 (30%)	26 (16%)	0	4
All	All	164/174 (94%)	88 (54%)	50 (30%)	26 (16%)	0	4

All 26 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	86	PHE
1	A	90	PRO
1	A	92	TRP
1	A	102	VAL
1	A	117	VAL
1	A	118	GLU
1	A	129	PRO
1	A	148	VAL
1	A	149	ARG
1	A	150	GLU
1	A	157	PHE
1	A	162	ASN
1	A	164	LEU
1	A	169	ALA
1	A	175	ASN
1	A	181	ASP
1	A	184	GLU
1	A	188	LYS
1	A	211	HIS
1	A	226	LEU
1	A	228	ASP
1	A	233	ARG
1	A	234	LEU
1	A	235	SER
1	A	241	GLY
1	A	246	TYR

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	140/148 (95%)	111 (79%)	29 (21%)	3	32
All	All	140/148 (95%)	111 (79%)	29 (21%)	3	32

All 29 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	83	PHE
1	A	85	THR
1	A	92	TRP
1	A	93	ARG
1	A	95	THR
1	A	101	ILE
1	A	121	LEU
1	A	128	THR
1	A	129	PRO
1	A	142	ILE
1	A	143	MET
1	A	144	ILE
1	A	148	VAL
1	A	164	LEU
1	A	174	ILE
1	A	179	HIS
1	A	184	GLU
1	A	195	LEU
1	A	198	VAL
1	A	202	GLU
1	A	205	HIS
1	A	207	LEU
1	A	222	LEU
1	A	226	LEU
1	A	229	LEU
1	A	234	LEU
1	A	238	ASP
1	A	242	ILE
1	A	246	TYR

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 ⓘ

There are no oligosaccharides in this entry.

6.6 Ligand geometry

Of 4 ligands modelled in this entry, 3 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	0DS	A	261	2	32,32,32	1.34	1 (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
4	0DS	A	261	2	40,42,42	1.04	3 (7%)

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	0DS	A	261	2	-	0,38,38,38	0,1,1,1

All bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	261	0DS	O3-N3	6.41	1.24	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	261	0DS	C11-C2-C1	3.12	114.15	109.71

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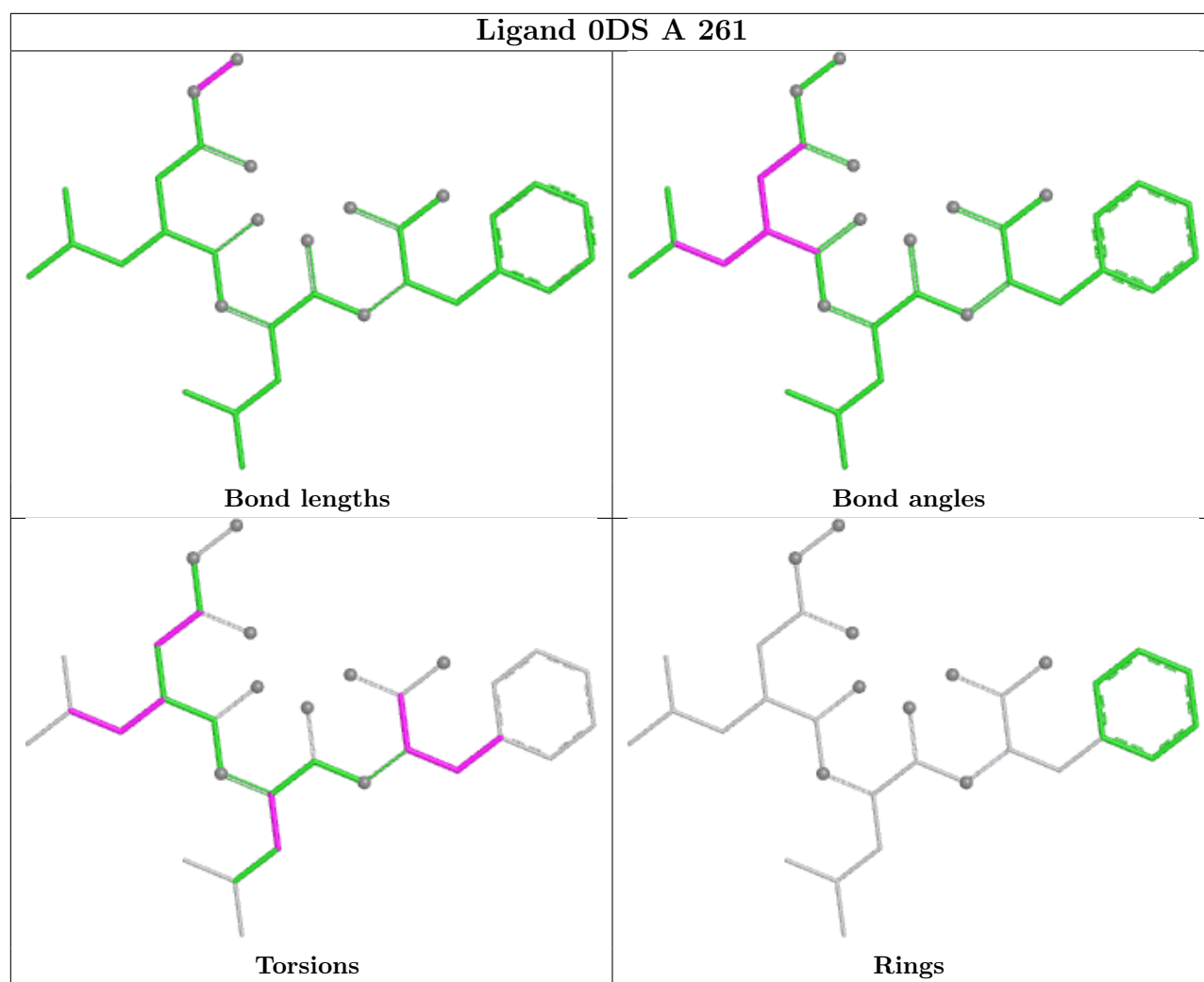
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	261	0DS	C2-C3-C4	2.90	109.56	115.60
4	A	261	0DS	C2-C11-C21	2.43	117.11	112.33

There are no chirality outliers.

There are no torsion outliers.

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