

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 07:04 am BST

PDB ID : 1MS6

Title: Dipeptide Nitrile Inhibitor Bound to Cathepsin S.

Authors: Ward, Y.D.; Thomson, D.S.; Frye, L.L.; Cywin, C.L.; Morwick, T.; Emmanuel,

M.J.; Zindell, R.; McNeil, D.; Bekkali, Y.; Giradot, M.; Hrapchak, M.; DeTuri, M.; Crane, K.; White, D.; Pav, S.; Wang, Y.; Hao, M.H.; Grygon, C.A.; Labadia, M.E.; Freeman, D.M.; Davidson, W.; Hopkins, J.L.; Brown, M.L.;

Spero, D.M.

Deposited on : 2002-09-19

Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp 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:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : NOT EXECUTED

EDS: NOT EXECUTED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

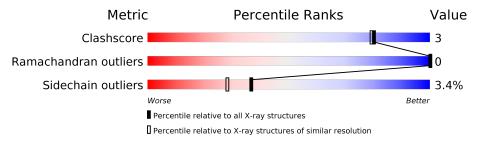
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 1.90 Å.

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	Similar resolution	
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$	
Clashscore	141614	6847 (1.90-1.90)	
Ramachandran outliers	138981	6760 (1.90-1.90)	
Sidechain outliers	138945	6760 (1.90-1.90)	

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain		
1	٨	000			
T	Α	222	91%	7%	•



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1714 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

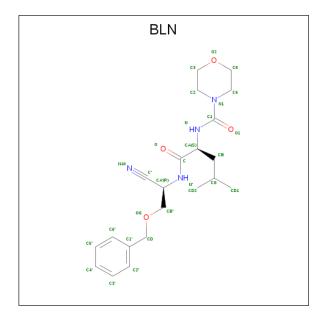
• Molecule 1 is a protein called Cathepsin S.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	217	Total	С	N	О	S	0	0	0
1	A	211	1685	1064	286	323	12	0	U	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	HIS	_	EXPRESSION TAG	UNP P25774
A	219	HIS	-	EXPRESSION TAG	UNP P25774
A	220	HIS	-	EXPRESSION TAG	UNP P25774
A	221	HIS	-	EXPRESSION TAG	UNP P25774
A	222	HIS	-	EXPRESSION TAG	UNP P25774

• Molecule 2 is MORPHOLINE-4-CARBOXYLIC ACID [1S-(2-BENZYLOXY-1R-CYANO -ETHYLCARBAMOYL)-3-METHYL-BUTYL]AMIDE (three-letter code: BLN) (formula: $C_{21}H_{30}N_4O_4$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C 21	N 4	O 4	0	0

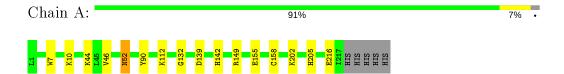


3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Cathepsin S





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants	85.29Å 85.29Å 150.07Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 1.90	Depositor
% Data completeness	(Not available) (50.00-1.90)	Depositor
(in resolution range)	(1100 available) (90.00 1.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.155 , 0.197	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1714	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP



5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BLN

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	A	0.49	0/1727	0.63	0/2335	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	$\mathbf{H}(\mathbf{model})$	$\mathbf{H}(\mathbf{added})$	Clashes	Symm-Clashes
1	A	1685	0	1606	9	0
2	A	29	0	30	0	0
All	All	1714	0	1636	9	0

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 3.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1 Atom-2		$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	Clash overlap (Å)	
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.49	0.77	
1:A:139:ASP:OD2	1:A:142:HIS:HE1	1.88	0.55	

Continued on next page...



$\alpha \cdots$	· ·	•	
Continued	trom	mromanne	maaa
-	110116	DICUIUU	Du_iu_{C}

Atom-1	Atom-2	$egin{array}{ll} ext{Interatomic} \ ext{distance} \ (ext{\AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$
1:A:7:TRP:CE3	1:A:10:LYS:HD2	2.46	0.50
1:A:155:GLU:H	1:A:205:HIS:CE1	2.31	0.48
1:A:7:TRP:CZ2	1:A:132:GLY:HA2	2.51	0.46
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.24	0.44
1:A:52:ASN:C	1:A:52:ASN:HD22	2.23	0.42
1:A:149:ARG:HG3	1:A:149:ARG:NH1	2.25	0.40
1:A:112:LYS:HE3	1:A:216:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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	215/222 (97%)	211 (98%)	4 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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	178/183 (97%)	172 (97%)	6 (3%)	37 28	

All (6) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	44	LYS
1	A	46	VAL
1	A	52	ASN
1	A	90	TYR
1	A	158	CYS
1	A	202	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	${f Res}$	Type
1	A	67	ASN
1	A	97	GLN
1	A	142	HIS
1	A	160	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mo	l Type	Chain	Chain	Chain	Chain	Res Li	Link	Bond lengths			Bond angles		
IVIC	Type		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2			
2	BLN	A	281	1	29,30,30	1.88	2 (6%)	33,38,38	6.66	3 (9%)			

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	BLN	A	281	1	-	0/26/36/36	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	A	281	BLN	C'-N40	9.41	1.33	1.14
2	A	281	BLN	CA'-C'	2.58	1.52	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	${f Atoms}$	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
2	A	281	BLN	CA'-C'-N40	-38.00	124.32	177.95
2	A	281	BLN	C6-N1-C2	2.47	117.37	112.62
2	A	281	BLN	C-CA-N	-2.10	105.45	111.16

There are no chirality outliers.

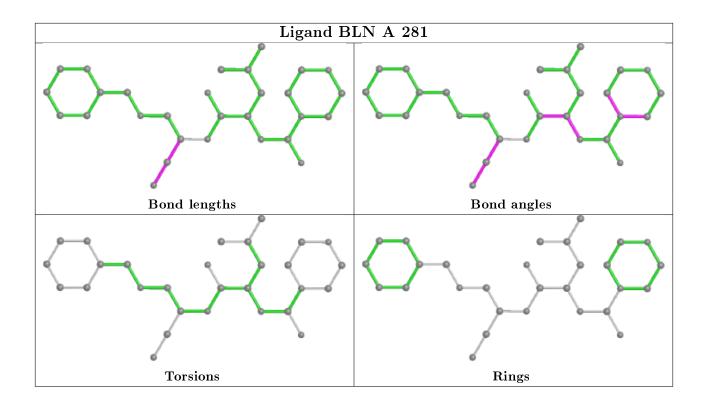
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

