



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z71  
Title : thrombin and P2 pyridine N-oxide inhibitor complex structure  
Authors : Nantermet, P.G.; Burgey, C.S.; Robinson, K.A.; Pellicore, J.M.; Newton, C.L.; Deng, J.Z.; Lyle, T.A.; Selnick, H.G.; Lewis, S.D.; Lucas, B.J.; Krueger, J.A.; Miller-Stein, C.; White, R.B.; Wong, B.; McMasters, D.R.; Wallace, A.A.; Lynch Jr., J.J.; Yan, Y.; Chen, Z.; Kuo, L.; Gardell, S.J.; Shafer, J.A.; Vacca, J.P.  
Deposited on : 2005-03-23  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

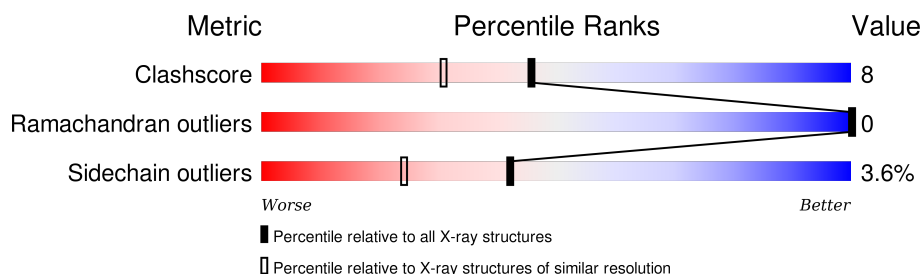
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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 (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	287	 77% 18% . .
2	B	11	 100%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2564 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 thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2237	1424	393	405	15			

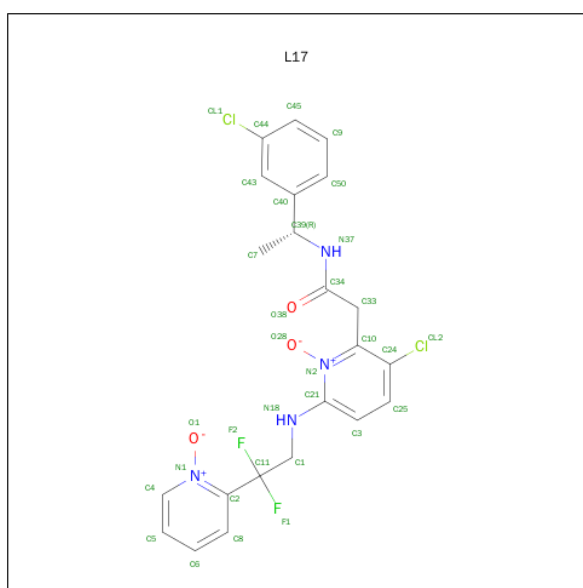
- Molecule 2 is a protein called Hirudin IIIB'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	S	0	0	0
			100	62	11	26	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	365	ALA	GLN	SEE REMARK 999	UNP P28511

- Molecule 3 is L17 (three-letter code: L17) (formula: C<sub>22</sub>H<sub>20</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			33	22	2	2	4	3		

- Molecule 4 is water.

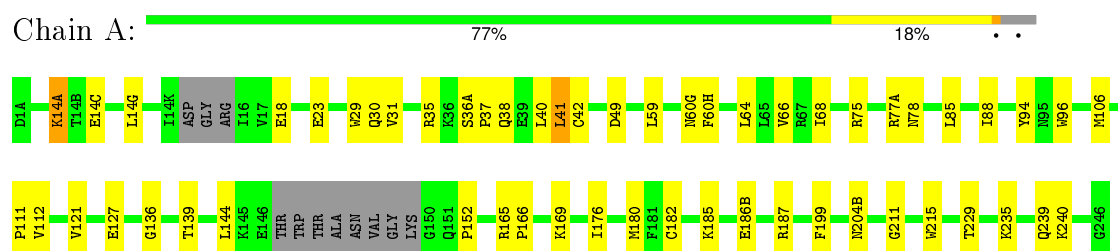
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: thrombin



- Molecule 2: Hirudin IIIB'



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.97 Å   71.49 Å   72.26 Å 90.00°   100.50°   90.00°	Depositor
Resolution (Å)	50.00 – 1.80	Depositor
% Data completeness (in resolution range)	98.0 (50.00-1.80)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2564	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L17, TYS

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	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/2291	0.61	0/3088
2	B	0.41	0/84	0.41	0/110
All	All	0.35	0/2375	0.60	0/3198

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

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	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2237	0	2208	36	0
2	B	100	0	78	0	0
3	A	33	0	20	1	0
4	A	191	0	0	0	0
4	B	3	0	0	0	0
All	All	2564	0	2306	36	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 8.

All (36) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HB2	1:A:41:LEU:HD23	1.61	0.80
1:A:169:LYS:HA	1:A:176:ILE:HD12	1.70	0.73
1:A:14(A):LYS:HG3	1:A:23:GLU:OE2	1.95	0.66
1:A:18:GLU:HG3	1:A:187:ARG:HG3	1.80	0.63
1:A:144:LEU:HD21	1:A:152:PRO:HB3	1.86	0.57
1:A:235:LYS:O	1:A:239:GLN:HG3	2.06	0.54
1:A:31:VAL:HG13	1:A:66:VAL:HG13	1.89	0.53
1:A:85:LEU:HD13	1:A:106:MET:HE2	1.89	0.53
1:A:66:VAL:HG23	1:A:85:LEU:HD21	1.91	0.53
1:A:68:ILE:HD12	1:A:112:VAL:HG21	1.89	0.52
1:A:41:LEU:HG	1:A:64:LEU:CD2	2.44	0.47
1:A:169:LYS:HA	1:A:176:ILE:CD1	2.41	0.47
1:A:77(A):ARG:O	1:A:78:ASN:HB2	2.15	0.47
1:A:94:TYR:CZ	1:A:96:TRP:HB3	2.50	0.47
1:A:185:LYS:HB2	1:A:186(B):GLU:HG3	1.96	0.46
1:A:165:ARG:HB2	1:A:166:PRO:HD3	1.98	0.46
1:A:35:ARG:CB	1:A:41:LEU:HD23	2.41	0.45
1:A:14(C):GLU:O	1:A:14(G):LEU:HD23	2.16	0.45
1:A:14(A):LYS:HE3	1:A:23:GLU:HG3	2.00	0.44
1:A:30:GLN:NE2	1:A:139:THR:OG1	2.50	0.44
1:A:211:GLY:HA2	1:A:229:THR:O	2.16	0.44
1:A:41:LEU:HG	1:A:64:LEU:HD21	2.01	0.43
1:A:35:ARG:HA	1:A:64:LEU:HD23	1.99	0.43
1:A:35:ARG:O	1:A:38:GLN:HA	2.18	0.43
1:A:36(A):SER:HA	1:A:37:PRO:HA	1.84	0.43
1:A:29:TRP:CG	1:A:121:VAL:HB	2.54	0.43
1:A:41:LEU:HD11	1:A:60(H):PHE:CE2	2.54	0.42
1:A:136:GLY:HA3	1:A:199:PHE:CZ	2.54	0.42
1:A:169:LYS:CA	1:A:176:ILE:HD12	2.47	0.41
1:A:35:ARG:HG2	1:A:37:PRO:O	2.21	0.41
1:A:215:TRP:CE3	3:A:1001:L17:H8	2.55	0.41
1:A:41:LEU:HD21	1:A:60(H):PHE:CZ	2.56	0.41
1:A:75:ARG:HA	1:A:75:ARG:HD3	1.90	0.41
1:A:49:ASP:OD2	1:A:111:PRO:HB3	2.21	0.41
1:A:59:LEU:HD13	1:A:88:ILE:HG21	2.04	0.40
1:A:240:LYS:HB2	1:A:240:LYS:HE3	1.87	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 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 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	270/287 (94%)	261 (97%)	9 (3%)	0	100	100
2	B	8/11 (73%)	8 (100%)	0	0	100	100
All	All	278/298 (93%)	269 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 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 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	242/251 (96%)	233 (96%)	9 (4%)	41	23
2	B	9/9 (100%)	9 (100%)	0	100	100
All	All	251/260 (96%)	242 (96%)	9 (4%)	42	24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14(A)	LYS
1	A	40	LEU
1	A	41	LEU
1	A	42	CYS
1	A	60(G)	ASN
1	A	127	GLU
1	A	180	MET
1	A	182	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	204(B)	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	60(G)	ASN
1	A	156	GLN
1	A	204(B)	ASN
1	A	239	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TYS	B	363	2	15,16,17	3.69	2 (13%)	16,22,24	0.75	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
2	TYS	B	363	2	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	363	TYS	OH-CZ	-10.78	1.25	1.42
2	B	363	TYS	OH-S	-9.24	1.46	1.63

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	L17	A	1001	-	34,35,35	2.42	19 (55%)	42,50,50	1.83	10 (23%)

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
3	L17	A	1001	-	-	0/21/24/24	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	L17	F1-C11	-3.12	1.35	1.37
3	A	1001	L17	F2-C11	-2.75	1.35	1.37
3	A	1001	L17	C3-C21	2.12	1.44	1.40
3	A	1001	L17	C4-N1	2.22	1.39	1.36
3	A	1001	L17	C24-C10	2.24	1.43	1.40
3	A	1001	L17	O1-N1	2.37	1.36	1.31
3	A	1001	L17	C4-C5	2.49	1.44	1.38
3	A	1001	L17	C9-C45	2.59	1.44	1.38
3	A	1001	L17	C6-C8	2.72	1.44	1.38
3	A	1001	L17	O28-N2	2.84	1.38	1.31
3	A	1001	L17	C9-C50	2.85	1.44	1.38
3	A	1001	L17	C6-C5	2.86	1.45	1.38
3	A	1001	L17	C21-N18	3.34	1.42	1.35
3	A	1001	L17	C43-C40	3.38	1.44	1.39
3	A	1001	L17	C8-C2	3.86	1.45	1.39
3	A	1001	L17	C43-C44	3.86	1.44	1.38
3	A	1001	L17	C50-C40	3.92	1.45	1.39
3	A	1001	L17	C2-N1	4.03	1.41	1.37
3	A	1001	L17	C45-C44	4.14	1.46	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	L17	C5-C4-N1	-3.91	117.44	120.84
3	A	1001	L17	F1-C11-C1	-3.56	104.30	108.69
3	A	1001	L17	C39-N37-C34	-3.04	118.43	122.90
3	A	1001	L17	C50-C9-C45	-2.49	116.68	120.24
3	A	1001	L17	O1-N1-C2	-2.45	118.00	120.08
3	A	1001	L17	O1-N1-C4	-2.36	116.87	119.82
3	A	1001	L17	C7-C39-C40	-2.29	107.60	112.16
3	A	1001	L17	C10-C24-CL2	-2.23	119.51	123.05
3	A	1001	L17	C25-C24-C10	4.10	121.79	120.12
3	A	1001	L17	C4-N1-C2	4.56	125.10	120.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	L17	1	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.