



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:43 PM GMT

PDB ID : 2GDE  
Title : Thrombin in complex with inhibitor  
Authors : Xue, Y.  
Deposited on : 2006-03-16  
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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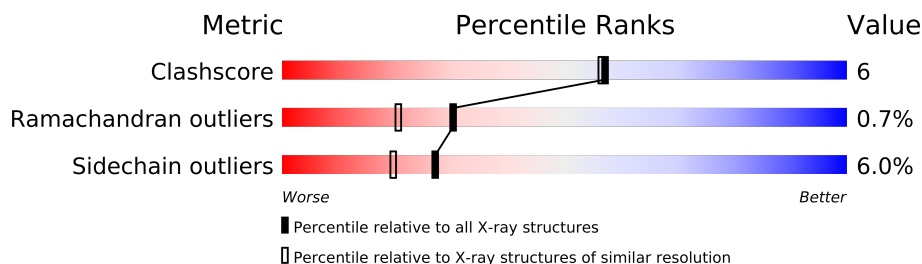
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	D	10	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2450 atoms, of which 0 are hydrogen and 0 are deuterium.

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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	27	Total	C	N	O	S	0	0	0
			222	140	36	45	1			

- Molecule 2 is a protein called Thrombin heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	249	Total	C	N	O	S	0	0	0
			2014	1283	357	360	14			

- Molecule 3 is a protein called Hirudin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	S	0	0	0
			90	56	10	23	1			

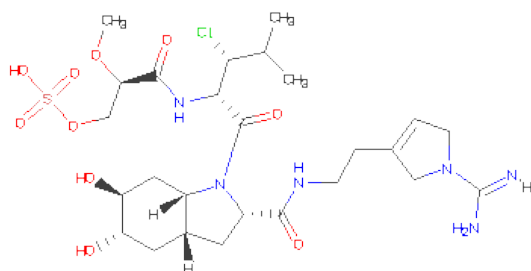
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	361	GLY	GLU	CONFLICT	UNP P28504

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is (R)-3-((2S,3R)-1-((2S,3AR,5S,6S,7AS)-2-(2-(1-CARBAMIMIDOYL-2,5-DIHYDRO-1H-PYRROL-3-YL)ETHYLCARBAMOYL)-5,6-DIHYDROXYOCTAHYDRO-1H-INDOL-1-YL)-3-CHLORO-4-METHYL-1-OXOPENTAN-2-YLAMINO)-2-METHOXY-3-OXOPROPYLHYDROGEN SULFATE (three-letter code: SN3) (formula: C<sub>26</sub>H<sub>43</sub>ClN<sub>6</sub>O<sub>10</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
5	H	1	44	26	1	6	10	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	6	Total	O	0	0
			6	6		
6	H	73	Total	O	0	0
			73	73		

### 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.

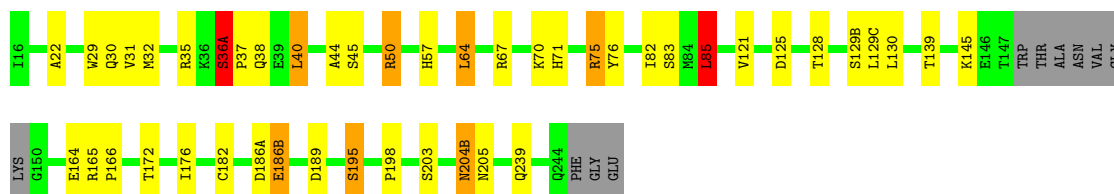
- Molecule 1: Thrombin light chain

Chain L: 



- Molecule 2: Thrombin heavy chain

Chain H: 



- Molecule 3: Hirudin

Chain D: 



## 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, $\alpha$ , $\beta$ , $\gamma$	70.08Å 72.17Å 70.36Å 90.00° 99.06° 90.00°	Depositor
Resolution (Å)	69.50 – 2.00	Depositor
% Data completeness (in resolution range)	97.7 (69.50-2.00)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.209 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	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: NA, SN3, 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	L	0.70	0/224	0.77	0/298
2	H	0.65	0/2065	0.75	3/2790 (0.1%)
3	D	0.56	0/74	0.71	0/96
All	All	0.65	0/2363	0.75	3/3184 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36(A)	SER	C-N-CD	7.02	143.15	128.40
2	H	85	LEU	CA-CB-CG	5.88	128.82	115.30
2	H	125	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	222	0	225	1	0
2	H	2014	0	1992	28	0
3	D	90	0	70	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	H	44	0	42	1	0
6	H	73	0	0	3	0
6	L	6	0	0	0	0
All	All	2450	0	2329	30	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (30) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:36(A):SER:OG	2:H:37:PRO:HD2	1.66	0.96
2:H:165:ARG:HG3	6:H:451:HOH:O	1.71	0.89
2:H:50:ARG:HD3	6:H:446:HOH:O	1.80	0.81
2:H:36(A):SER:OG	2:H:37:PRO:CD	2.29	0.81
2:H:64:LEU:HD12	2:H:85:LEU:HD11	1.64	0.80
2:H:75:ARG:NE	2:H:76:TYR:O	2.18	0.76
2:H:32:MET:HG3	2:H:40:LEU:HD12	1.70	0.73
1:L:5:PRO:HA	1:L:9:LYS:HD3	1.83	0.59
2:H:30:GLN:NE2	2:H:139:THR:OG1	2.36	0.59
2:H:75:ARG:CD	2:H:76:TYR:O	2.54	0.55
2:H:186(A):ASP:OD1	2:H:186(B):GLU:N	2.40	0.54
2:H:35:ARG:O	2:H:38:GLN:HA	2.09	0.53
2:H:75:ARG:HD2	2:H:76:TYR:O	2.09	0.52
3:D:363:TYS:O	3:D:364:LEU:HB2	2.10	0.52
2:H:172:THR:HG21	2:H:176:ILE:HD11	1.92	0.51
2:H:75:ARG:HD2	2:H:76:TYR:N	2.26	0.51
2:H:75:ARG:CZ	2:H:76:TYR:O	2.59	0.50
2:H:50:ARG:CD	6:H:446:HOH:O	2.51	0.49
2:H:164:GLU:HB3	2:H:166:PRO:HD2	1.97	0.47
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.31	0.46
2:H:31:VAL:HB	2:H:44:ALA:HB3	1.97	0.46
2:H:22:ALA:O	2:H:71:HIS:HE1	2.01	0.44
2:H:189:ASP:OD1	5:H:401:SN3:N21	2.43	0.42
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.88	0.42
2:H:30:GLN:HE22	2:H:198:PRO:HD2	1.85	0.42
2:H:57:HIS:CE1	2:H:195:SER:OG	2.73	0.41
2:H:128:THR:HG22	2:H:129(C):LEU:HD12	2.03	0.41
2:H:67:ARG:HG2	2:H:82:ILE:HG12	2.02	0.41
2:H:29:TRP:CG	2:H:121:VAL:HB	2.56	0.41
2:H:45:SER:HB3	2:H:198:PRO:HG3	2.03	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	L	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
2	H	245/259 (95%)	234 (96%)	9 (4%)	2 (1%)	27	17
3	D	7/10 (70%)	7 (100%)	0	0	100	100
All	All	277/305 (91%)	264 (95%)	11 (4%)	2 (1%)	30	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	36(A)	SER
2	H	186(B)	GLU

### 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	L	25/31 (81%)	24 (96%)	1 (4%)	42	36
2	H	218/225 (97%)	204 (94%)	14 (6%)	25	17
3	D	8/8 (100%)	8 (100%)	0	100	100
All	All	251/264 (95%)	236 (94%)	15 (6%)	27	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14(D)	ARG

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Mol	Chain	Res	Type
2	H	40	LEU
2	H	50	ARG
2	H	64	LEU
2	H	75	ARG
2	H	83	SER
2	H	85	LEU
2	H	129(B)	SER
2	H	130	LEU
2	H	145	LYS
2	H	182	CYS
2	H	195	SER
2	H	204(B)	ASN
2	H	205	ASN
2	H	239	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	30	GLN
2	H	62	ASN
2	H	71	HIS
2	H	204(B)	ASN
2	H	209	GLN
2	H	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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
3	TYS	D	363	3	16,16,17	3.98	4 (25%)	20,22,24	0.94	1 (5%)

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	TYS	D	363	3	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	363	TYS	O-C	13.64	1.20	1.11
3	D	363	TYS	OH-S	-5.86	1.53	1.63
3	D	363	TYS	OH-CZ	-5.04	1.36	1.42
3	D	363	TYS	CA-C	2.11	1.52	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	363	TYS	C-CA-N	-2.02	111.82	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
5	SN3	H	401	-	46,46,46	1.38	4 (8%)	67,67,67	1.66	13 (19%)

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
5	SN3	H	401	-	-	1/46/83/83	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	401	SN3	C20-N22	6.13	1.37	1.33
5	H	401	SN3	C20-N21	3.64	1.38	1.33
5	H	401	SN3	C6-C1	2.74	1.56	1.52
5	H	401	SN3	O41-S39	2.19	1.53	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	401	SN3	C19-C18-N17	5.83	105.99	101.93
5	H	401	SN3	O40-S39-O42	3.85	123.51	108.82
5	H	401	SN3	C10-C9-N8	3.63	106.60	103.20
5	H	401	SN3	C18-N17-C16	-3.39	105.61	112.07
5	H	401	SN3	O38-C37-C34	3.15	113.56	107.69
5	H	401	SN3	C15-C16-N17	3.02	107.29	103.39
5	H	401	SN3	C10-C3-C2	-2.80	109.57	116.42
5	H	401	SN3	O35-C34-C37	2.38	113.00	107.04
5	H	401	SN3	C3-C2-C1	2.30	117.52	113.47
5	H	401	SN3	O25-C24-N8	-2.30	117.33	121.69
5	H	401	SN3	C3-C10-C9	-2.25	101.39	104.34
5	H	401	SN3	C2-C1-C6	2.21	113.19	110.37
5	H	401	SN3	C9-N8-C4	-2.04	109.07	112.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	401	SN3	N22-C20-N17-C18

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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.