

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 - 09:40 pm GMT

PDB ID Title		6TKL Non-cleavable tsetse thrombin inhibitor in complex with human alpha-
		thrombin
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Deposited on	:	2019-11-28
Resolution	:	1.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

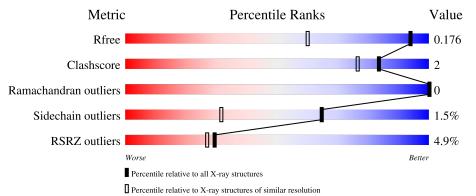
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as $541$ be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.30 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 of 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% 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.

Mol	Chain	Length		Quality of ch	nain	
1	L	36	8%	92%		8%
2	Н	259	4%	92%		
3	Ι	53	<sup>2%</sup> 40%	9%	51%	



#### 6TKL

# 2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 2844 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 Prothrombin.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
1	L	36	Total 287	C 177	N 48	O 61	S 1	17	0	0

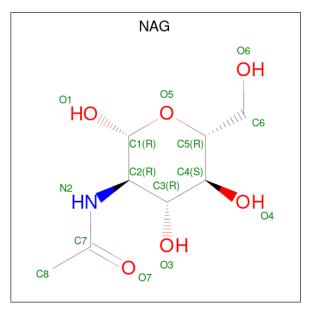
• Molecule 2 is a protein called Prothrombin.

Mo	l Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	Н	251	Total 2078	C 1325	N 368	0 371	S 14	0	7	0

• Molecule 3 is a protein called Tsetse thrombin inhibitor.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
3	Ι	26	Total 202	C 123	N 31	O 46	${S \over 2}$	0	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



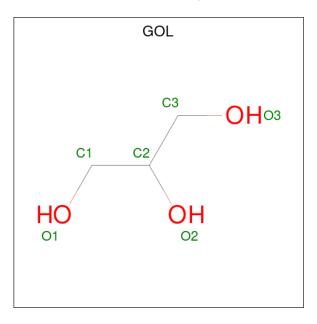


Mol	Chain	Residues	A	tor	ns		ZeroOcc	AltConf
4	Н	1	Total	C 8	N 1	0 5	0	0

• Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	1	Total Na 1 1	0	0

• Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

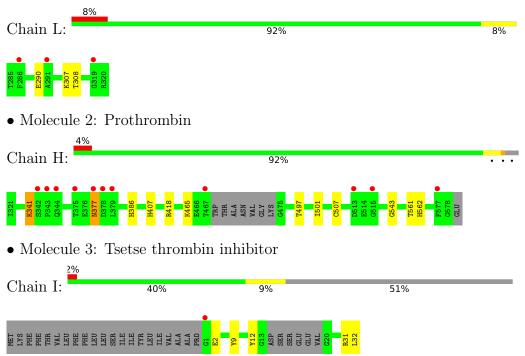
• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	34	$\begin{array}{cc} \text{Total} & \text{O} \\ 34 & 34 \end{array}$	0	0
7	Н	188	Total O 189 189	0	1
7	Ι	33	Total O 33 33	0	0



# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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.



• Molecule 1: Prothrombin



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	46.93Å 81.31Å 86.28Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	43.14 - 1.30	Depositor
	43.14 - 1.30	EDS
% Data completeness	99.5(43.14-1.30)	Depositor
(in resolution range)	99.6(43.14-1.30)	EDS
R <sub>merge</sub>	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.02 (at 1.30 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
$R, R_{free}$	0.145 , $0.176$	Depositor
II, II, <i>free</i>	0.146 , $0.176$	DCC
$R_{free}$ test set	4031 reflections $(4.92%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	19.7	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38, 54.9	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	2844	wwPDB-VP
Average B, all atoms $(Å^2)$	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.85% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: TYS, GOL, MLE, NA, NAG

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		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	L	0.48	0/290	0.66	0/384	
2	Н	0.53	0/2133	0.71	0/2882	
3	Ι	0.47	0/161	0.66	0/214	
All	All	0.53	0/2584	0.70	0/3480	

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	H(model)	H(added)	Clashes	Symm-Clashes
1	L	287	0	275	3	0
2	Н	2078	0	2058	7	0
3	Ι	202	0	177	2	0
4	Н	14	0	13	0	0
5	Н	1	0	0	0	0
6	Н	6	0	8	0	0
7	Н	189	0	0	4	0
7	Ι	33	0	0	1	0
7	L	34	0	0	1	0
All	All	2844	0	2531	12	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 2.

The worst 5 of 12 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)
3:I:2:GLU:HG2	7:I:122:HOH:O	2.03	0.58
1:L:307:LYS:HG3	1:L:308:THR:HG23	1.85	0.57
1:L:307:LYS:HE3	7:H:757:HOH:O	2.05	0.55
2:H:386:HIS:HD2	7:H:819[A]:HOH:O	1.97	0.47
3:I:31:ARG:HA	3:I:32:MLE:HN1	1.71	0.47

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	Perce	ntiles
1	L	34/36~(94%)	33~(97%)	1 (3%)	0	100	100
2	Н	254/259~(98%)	249 (98%)	5 (2%)	0	100	100
3	Ι	20/53~(38%)	$19 \ (95\%)$	1 (5%)	0	100	100
All	All	308/348~(88%)	301 (98%)	7 (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	L	31/31~(100%)	31~(100%)	0	100 100	
2	Н	226/225~(100%)	222~(98%)	4 (2%)	59 24	
3	Ι	16/41~(39%)	16 (100%)	0	100 100	
All	All	273/297~(92%)	269~(98%)	4 (2%)	65 31	

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Н	341	LYS
2	Н	377	ASN
2	Н	507	CYS
2	Н	562	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are 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	Turne	Chain	Res	Res Link Bond lengths			Bond angles			
INIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	TYS	Ι	9	3	15, 16, 17	1.75	3 (20%)	18,22,24	0.93	1 (5%)
3	TYS	Ι	12	3	15,16,17	1.55	3 (20%)	18,22,24	0.92	0
3	MLE	Ι	32	3	9,9,9	0.91	0	9,11,11	0.74	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.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	Ι	9	3	-	2/10/11/13	0/1/1/1
3	TYS	Ι	12	3	-	0/10/11/13	0/1/1/1
3	MLE	Ι	32	3	-	3/10/10/10	-

'-' means no outliers of that kind were identified.

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Ι	9	TYS	O2-S	4.43	1.64	1.45
3	Ι	12	TYS	O2-S	4.22	1.63	1.45
3	Ι	9	TYS	OH-S	-3.30	1.53	1.58
3	Ι	9	TYS	OH-CZ	-3.05	1.37	1.42
3	Ι	12	TYS	OH-CZ	-2.69	1.38	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ι	9	TYS	OH-CZ-CE2	2.01	122.59	118.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Ι	9	TYS	CE1-CZ-OH-S
3	Ι	9	TYS	CE2-CZ-OH-S
3	Ι	32	MLE	OXT-C-CA-CB
3	Ι	32	MLE	O-C-CA-CB
3	Ι	32	MLE	CB-CA-N-CN

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ι	32	MLE	1	0

### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



### 5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	Turne	Chain	Res	Link	Bo	Bond lengths			Bond angles		
	Type		nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
4	NAG	Н	601	2	$14,\!14,\!15$	0.79	1 (7%)	$17,\!19,\!21$	0.75	1 (5%)	
6	GOL	Н	603	-	$5,\!5,\!5$	0.97	0	$5,\!5,\!5$	0.95	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
4	NAG	Н	601	2	-	2/6/23/26	0/1/1/1
6	GOL	Н	603	-	-	0/4/4/4	-

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Н	601	NAG	C1-C2	2.72	1.56	1.52

All (1) bond angle outliers are listed below:

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	601	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Н	601	NAG	O5-C5-C6-O6
4	Н	601	NAG	C4-C5-C6-O6

There are no ring outliers.



No monomer is involved in short contacts.

### 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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	L	33/36~(91%)	0.41	3 (9%) 9 6	21, 28, 58, 68	0
2	Н	251/259~(96%)	0.02	11 (4%) 34 32	16, 24, 50, 63	0
3	Ι	23/53~(43%)	0.02	1 (4%) 35 32	23, 26, 59, 81	0
All	All	307/348~(88%)	0.07	15 (4%) 29 27	16, 25, 52, 81	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	286	PHE	4.8
1	L	319	GLY	4.5
2	Н	379	LEU	4.2
2	Н	343	PRO	4.0
3	Ι	1	GLY	3.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
3	TYS	Ι	12	16/17	0.64	0.24	$76,\!98,\!102,\!103$	0
3	MLE	Ι	32	10/10	0.84	0.12	22,28,36,38	0
3	TYS	Ι	9	16/17	0.88	0.11	33,47,63,63	0

## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	NAG	Н	601	14/15	0.79	0.21	$63,\!79,\!95,\!102$	0
6	GOL	Н	603	6/6	0.81	0.24	56,65,76,82	0
5	NA	Н	602	1/1	1.00	0.06	21,21,21,21	0

### 6.5 Other polymers (i)

There are no such residues in this entry.

