

Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 – 03:02 pm GMT

PDB ID : 7A0E

Title: The Crystal Structure of Bovine Thrombin in complex with Hirudin

(C6U/C14U) at 1.9 Angstroms Resolution

Authors: Hidmi, T.; Mousa, R.; Pomyalov, S.; Lansky, S.; Khouri, L.; Metanis, N.;

Shoham, G.

Deposited on : 2020-08-07

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 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 as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

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

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

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

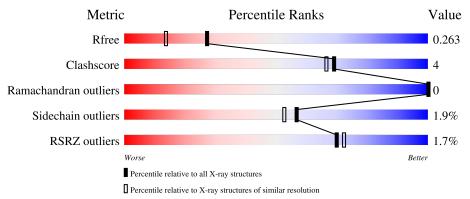
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-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 $(\# \mathrm{Entries})$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$		
R_{free}	130704	6207 (1.90-1.90)		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (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 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 chain		
1	ННН	259	89%	9%	•
2	III	65	5% 86%	12%	
3	LLL	49	78%	18%	_



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3092 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	Atoms			ZeroOcc	AltConf	Trace		
1	ННН	256	Total 2064	C 1321	N 364	O 367	S 12	0	2	0

• Molecule 2 is a protein called Hirudin variant-1.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace				
2	III	64	Total 469	C 280	N 78	O 105	S 4	Se 2	0	0	0	

There are 2 discrepancies between the modelled and reference sequences:

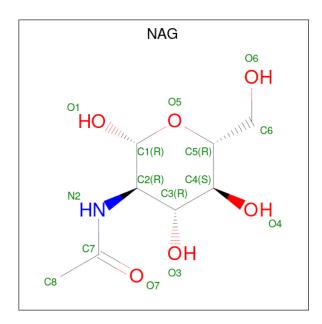
Chain	Residue	Modelled	Actual	Comment	Reference
III	6	SEC	CYS	conflict	UNP P01050
III	14	SEC	CYS	conflict	UNP P01050

• Molecule 3 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	LLL	40	Total 329	C 211	N 51	O 66	S 1	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	Atoms				ZeroOcc	AltConf
4	ННН	1	Total 14	C 8	N 1	O 5	0	0

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

Mo	l Chair	n Residues	Atoms	ZeroOcc	AltConf
5	ННН	1	Total Na	0	0

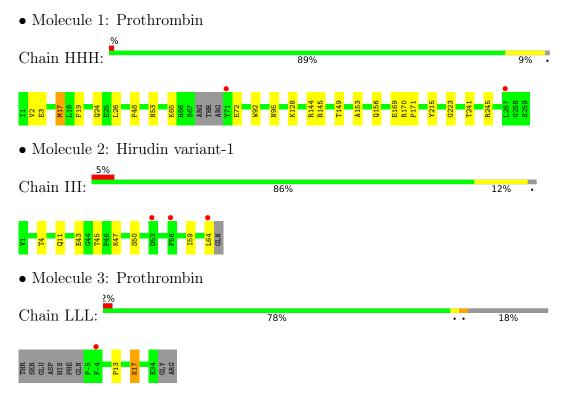
• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	ННН	155	Total O 155 155	0	0
6	III	34	Total O 34 34	0	0
6	LLL	26	Total O 26 26	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.





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	58.10Å 102.00Å 144.04Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.02 - 1.90	Depositor
Resolution (A)	72.02 - 1.90	EDS
% Data completeness	97.9 (72.02-1.90)	Depositor
(in resolution range)	97.9 (72.02-1.90)	EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) > 1$	0.98 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.214 , 0.263	Depositor
it, it free	0.214 , 0.263	DCC
R_{free} test set	1572 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	$0.35\;,38.2$	EDS
L-test for twinning ²	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.017 for 1/2 +h-1/2 +k,-3/2 +h-1/2 +k,-l	Xtriage
Estimated twinning fraction	0.035 for 1/2 *h + 1/2 *k, 3/2 *h - 1/2 *k, -1	Alliage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3092	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.08% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities 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: SEC, 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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	ННН	0.35	0/2123	0.75	0/2875	
2	III	0.36	0/461	0.72	0/620	
3	LLL	0.39	0/336	0.73	0/448	
All	All	0.36	0/2920	0.75	0/3943	

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	ННН	2064	0	2054	16	0
2	III	469	0	414	4	0
3	LLL	329	0	310	1	0
4	ННН	14	0	13	1	0
5	ННН	1	0	0	0	0
6	ННН	155	0	0	3	0
6	III	34	0	0	0	0
6	LLL	26	0	0	0	0
All	All	3092	0	2791	20	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 4.

All (20) 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:HHH:53:ASN:HD21	4:HHH:301:NAG:C1	1.32	1.42
1:HHH:170:ARG:HB2	1:HHH:171:PRO:HD3	1.60	0.82
1:HHH:65:LYS:HG3	1:HHH:72:GLU:OE1	1.83	0.78
1:HHH:245:ARG:HD2	6:HHH:537:HOH:O	2.07	0.54
1:HHH:169:GLU:HB3	1:HHH:171:PRO:HD2	1.91	0.51
3:LLL:13:PRO:HA	3:LLL:17:LYS:HB2	1.92	0.50
1:HHH:149:THR:HB	6:HHH:474:HOH:O	2.10	0.50
1:HHH:17:MET:HE3	1:HHH:26:LEU:HD13	1.94	0.49
1:HHH:48:PRO:HG2	1:HHH:92:TRP:CE2	2.50	0.47
2:III:43:GLU:OE1	2:III:43:GLU:HA	2.15	0.46
1:HHH:48:PRO:HA	6:HHH:473:HOH:O	2.16	0.45
1:HHH:128:LYS:HD2	1:HHH:215:TYR:CE2	2.52	0.45
1:HHH:24:GLN:NE2	2:III:59:ILE:HG12	2.32	0.44
1:HHH:153:ALA:HA	1:HHH:156:GLN:OE1	2.17	0.44
1:HHH:170:ARG:CB	1:HHH:171:PRO:HD3	2.41	0.44
1:HHH:2:VAL:HG12	1:HHH:3:GLU:HG2	2.01	0.43
1:HHH:144:ARG:O	1:HHH:145:ARG:HG3	2.20	0.42
2:III:11:GLN:HA	2:III:45:THR:O	2.21	0.41
1:HHH:223:GLY:HA2	1:HHH:241:THR:O	2.21	0.41
2:III:4:THR:OG1	2:III:47:LYS:NZ	2.50	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	Perce	entiles
1	ННН	254/259 (98%)	243 (96%)	11 (4%)	0	100	100
2	III	60/65~(92%)	54 (90%)	6 (10%)	0	100	100

Continued on next page...



Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
3	LLL	38/49 (78%)	37 (97%)	1 (3%)	0	100	100
All	All	352/373~(94%)	334 (95%)	18 (5%)	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	ННН	223/226~(99%)	219 (98%)	4 (2%)	59 55		
2	III	52/54 (96%)	50 (96%)	2 (4%)	33 24		
3	LLL	35/43 (81%)	34 (97%)	1 (3%)	42 35		
All	All	310/323 (96%)	303 (98%)	7 (2%)	57 45		

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	ННН	17	MET
1	ННН	19	PHE
1	ННН	95[A]	ASN
1	ННН	95[B]	ASN
2	III	50	SER
2	III	64	LEU
3	LLL	17	LYS

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)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	Pog	Link	Bond lengths			Bond angles		
MIOI	туре		nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	ННН	301	1	14,14,15	0.42	0	17,19,21	1.59	4 (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
4	NAG	ННН	301	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\mathbf{Ideal}(^{o})$
4	ННН	301	NAG	O5-C1-C2	-2.79	106.88	111.29
4	ННН	301	NAG	C3-C4-C5	2.21	114.19	110.24
4	ННН	301	NAG	C8-C7-N2	2.15	119.75	116.10
4	ННН	301	NAG	C1-O5-C5	-2.02	109.45	112.19

There are no chirality outliers.



All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	ННН	301	NAG	O5-C5-C6-O6
4	ННН	301	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	ННН	301	NAG	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 (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	<rsrz></rsrz>	$\#\mathrm{RS}$	RZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	ННН	256/259 (98%)	-0.20	2 (0%)	86 87	23, 35, 59, 88	0
2	III	62/65 (95%)	0.09	3 (4%)	30 33	27, 39, 81, 92	0
3	LLL	40/49 (81%)	-0.18	1 (2%)	57 60	30, 37, 71, 76	0
All	All	358/373 (95%)	-0.15	6 (1%)	70 72	23, 36, 71, 92	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	ННН	257	LEU	3.4
2	III	53	ASP	3.1
1	ННН	71	TYR	2.6
2	III	56	PHE	2.5
3	LLL	-4	PHE	2.5
2	III	64	LEU	2.3

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

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

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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
4	NAG	ННН	301	14/15	0.86	0.12	56,72,87,91	0
5	NA	ННН	302	1/1	0.97	0.08	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.

