

wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 - 08:30 PM EDT

PDB ID	:	1NL1
Title	:	BOVINE PROTHROMBIN FRAGMENT 1 IN COMPLEX WITH CALCIUM
		ION
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Deposited on		
Resolution	:	1.90 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:

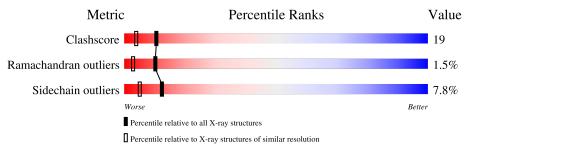
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain			
1	А	147	68%	25% 5% •		
2	В	2	50%	50%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 1424 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	А	147	Total 1216	C 733	N 214	O 258	S 11	0	5	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	7	CGU	GLU	modified residue	UNP P00735
А	8	CGU	GLU	modified residue	UNP P00735
А	15	CGU	GLU	modified residue	UNP P00735
А	17	CGU	GLU	modified residue	UNP P00735
А	20	CGU	GLU	modified residue	UNP P00735
А	21	CGU	GLU	modified residue	UNP P00735
А	26	CGU	GLU	modified residue	UNP P00735
А	27	CGU	GLU	modified residue	UNP P00735
А	30	CGU	GLU	modified residue	UNP P00735
А	33	CGU	GLU	modified residue	UNP P00735

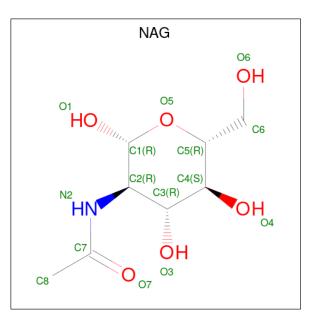
• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
2	В	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
3	А	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	7	Total Ca 7 7	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	159	Total O 159 159	0	0

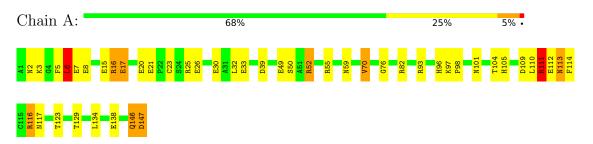


3 Residue-property plots (i)

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. 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: Prothrombin



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:	50%	50%
NAG1 NAG2		



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	39.19Å 53.44Å 128.17Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.60 - 1.90	Depositor
% Data completeness	95.0 (31.60-1.90)	Depositor
(in resolution range)	35.0 (51.00-1.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.219 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1424	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	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: CA, CGU, 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	
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.92	1/1122~(0.1%)	1.30	9/1505~(0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	97	LYS	CE-NZ	5.05	1.61	1.49

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	116	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	А	116	ARG	NE-CZ-NH1	15.42	128.01	120.30
1	А	16	ARG	NE-CZ-NH2	-13.94	113.33	120.30
1	А	16	ARG	NE-CZ-NH1	12.52	126.56	120.30
1	А	111	ARG	NE-CZ-NH1	-8.77	115.91	120.30

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	А	1216	0	1079	43	0
2	В	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	А	14	0	13	1	0
4	А	7	0	0	0	0
5	А	159	0	0	5	0
All	All	1424	0	1117	43	0

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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 19.

The worst 5 of 43 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:5[B]:PHE:O	1:A:6:LEU:HB2	1.56	1.06
1:A:52:ARG:HB3	1:A:52:ARG:HH11	1.25	0.98
1:A:109:ASP:OD1	1:A:111:ARG:NH1	2.06	0.89
1:A:146:GLN:HG3	1:A:147:ASP:H	1.40	0.86
1:A:16:ARG:HD2	1:A:17:CGU:OE22	1.76	0.83

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	А	140/147~(95%)	131 (94%)	7~(5%)	2(1%)	11 3

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	146	GLN
1	А	6	LEU



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	120/116~(103%)	110~(92%)	10 (8%)	11 4

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	129	THR
1	А	134	LEU
1	А	147	ASP
1	А	52	ARG
1	А	70	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	59	ASN
1	А	105	HIS
1	А	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 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).



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Mol	Trune	Chain	Res	Link	В	ond leng	gths	В	ond ang	gles
IVIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CGU	А	27	1,4	9,11,12	1.26	0	9,14,16	0.26	0
1	CGU	А	21	1,4	9,11,12	1.07	1 (11%)	9,14,16	1.10	1 (11%)
1	CGU	А	17	1,4	9,11,12	1.14	0	9,14,16	1.28	1 (11%)
1	CGU	А	20	1,4	9,11,12	1.69	2 (22%)	9,14,16	1.55	1 (11%)
1	CGU	А	8	1,4	9,11,12	1.38	1 (11%)	9,14,16	1.00	0
1	CGU	А	30	1,4	9,11,12	1.05	0	9,14,16	1.19	1 (11%)
1	CGU	А	7	1,4	9,11,12	1.34	1 (11%)	9,14,16	1.01	1 (11%)
1	CGU	А	26	1,4	9,11,12	1.36	2 (22%)	9,14,16	1.34	1 (11%)
1	CGU	А	15	1,4	9,11,12	1.37	2 (22%)	9,14,16	1.55	3 (33%)
1	CGU	А	33	1	9,11,12	1.07	0	9,14,16	1.10	2 (22%)

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
1	CGU	А	27	1,4	-	5/13/14/16	-
1	CGU	А	21	1,4	-	1/13/14/16	-
1	CGU	А	17	1,4	-	4/13/14/16	-
1	CGU	А	20	1,4	-	0/13/14/16	-
1	CGU	А	8	1,4	-	3/13/14/16	-
1	CGU	А	30	1,4	-	1/13/14/16	-
1	CGU	А	7	1,4	-	7/13/14/16	-
1	CGU	А	26	1,4	-	1/13/14/16	-
1	CGU	А	15	1,4	-	1/13/14/16	-
1	CGU	А	33	1	_	1/13/14/16	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	20	CGU	OE21-CD2	3.15	1.31	1.22
1	А	15	CGU	OE22-CD2	-2.39	1.22	1.30
1	А	21	CGU	CG-CD2	-2.27	1.49	1.52
1	А	7	CGU	OE12-CD1	-2.23	1.23	1.30
1	А	20	CGU	OE22-CD2	-2.19	1.23	1.30

The worst 5 of 11 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	20	CGU	CB-CG-CD2	3.34	119.89	113.11
1	А	26	CGU	CB-CG-CD2	3.15	119.52	113.11
1	А	15	CGU	CB-CG-CD2	3.08	119.36	113.11
1	А	30	CGU	CB-CG-CD2	2.48	118.14	113.11
1	А	17	CGU	OE11-CD1-CG	-2.38	112.15	120.14

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	7	CGU	O-C-CA-CB
1	А	17	CGU	O-C-CA-CB
1	А	27	CGU	CA-CB-CG-CD1
1	А	33	CGU	CA-CB-CG-CD2
1	А	26	CGU	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	17	CGU	2	0

5.5 Carbohydrates (i)

2 monosaccharides 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	Type	Chain	Res	Link	Bo	Bond lengths			Bond angles		
IVIOI					Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2	
2	NAG	В	1	2,1	14,14,15	0.57	0	$17,\!19,\!21$	0.93	1 (5%)	
2	NAG	В	2	2	14,14,15	0.64	0	17,19,21	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
2	NAG	В	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	В	2	2	-	4/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	1	NAG	C2-N2-C7	-3.30	118.21	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

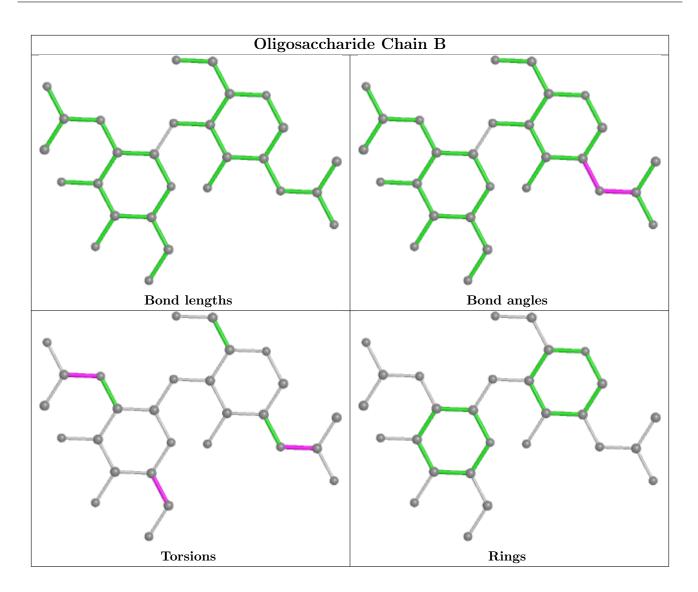
Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C8-C7-N2-C2
2	В	2	NAG	O7-C7-N2-C2
2	В	1	NAG	C8-C7-N2-C2
2	В	1	NAG	O7-C7-N2-C2
2	В	2	NAG	O5-C5-C6-O6

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 oligosaccharide.





5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are 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
3	NAG	А	311	1	14,14,15	0.70	0	17,19,21	0.78	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.

Mo	bl	Type	Chain	Res	Link	Chirals	Torsions	Rings
3		NAG	А	311	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	311	NAG	C8-C7-N2-C2
3	А	311	NAG	O7-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	311	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)

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.

