

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

Feb 5, 2024 – 12:17 AM EST

PDB ID : 1TYX

Title: TITLE OF TAILSPIKE-PROTEIN

Authors: Steinbacher, S.; Huber, R.

Deposited on : 1996-07-26

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
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 (i)) 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)

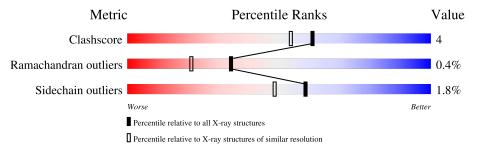
Validation Pipeline (wwPDB-VP) : 2.36

## 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 1.80 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (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 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	A	554	87%	10%			
2	В	8	62% 38%				



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4407 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 TAILSPIKE PROTEIN.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	543	Total 4115	C 2598	N 701	O 802	S 14	0	0	0

• Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-2)-[alpha-D-Abequopyra nose-(1-3)]alpha-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyr anose-(1-2)-[alpha-D-Abequopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace	
2	В	8	Total 83	C 48	O 35	0	0	0

• Molecule 3 is water.

$\mathbf{Mol}$	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
3	A	209	Total O 209 209	0	0

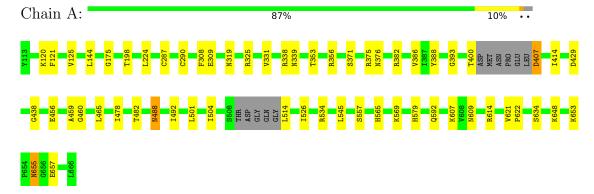


## 3 Residue-property plots (i)

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: TAILSPIKE PROTEIN



• Molecule 2: alpha-D-galactopyranose-(1-2)-[alpha-D-Abequopyranose-(1-3)]alpha-D-mannopyra nose-(1-4)-alpha-L-rhamnopyranose-(1-3)-alpha-D-galactopyranose-(1-2)-[alpha-D-Abequopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-alpha-L-rhamnopyranose





## 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 3	Depositor
Cell constants	120.90Å 120.90Å 120.90Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 - 1.80	Depositor
% Data completeness	(Not available) (8.00-1.80)	Depositor
(in resolution range)	(1100 available) (0.00 1.00)	Берозног
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
$R, R_{free}$	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4407	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	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: GLA, MAN, ABE, RAM

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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.46	0/4198	0.75	0/5692

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	A	4115	0	4038	36	0
2	В	83	0	75	1	0
3	A	209	0	0	3	0
All	All	4407	0	4113	37	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 (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$	
1:A:545:LEU:HD13	3:A:836:HOH:O	1.73	0.88	

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Continued from press		Interatomic	Clash
Atom-1	Atom-2	${\rm distance}\ (\rm \mathring{A})$	overlap (Å)
1:A:609:ASN:HD22	1:A:614:ARG:H	1.45	0.65
1:A:407:ASP:HB2	1:A:414:ILE:HG12	1.82	0.61
1:A:438:GLY:O	1:A:460:GLY:HA3	2.02	0.59
3:A:874:HOH:O	2:B:1:RAM:H1	2.03	0.58
1:A:175:GLY:HA2	1:A:198:THR:HG23	1.87	0.56
1:A:655:ASN:ND2	1:A:657:GLU:H	2.06	0.54
1:A:309:GLU:HG2	3:A:756:HOH:O	2.08	0.54
1:A:290:CYS:H	1:A:319:ASN:HD22	1.56	0.53
1:A:407:ASP:HB2	1:A:414:ILE:CG1	2.39	0.52
1:A:120:LYS:HE3	1:A:121:PHE:CZ	2.46	0.51
1:A:609:ASN:ND2	1:A:614:ARG:H	2.09	0.50
1:A:290:CYS:H	1:A:319:ASN:ND2	2.11	0.48
1:A:579:HIS:HE1	1:A:592:GLN:NE2	2.12	0.48
1:A:356:ARG:HA	1:A:388:TYR:O	2.14	0.47
1:A:459:ALA:HA	1:A:482:THR:OG1	2.15	0.47
1:A:534:ARG:HH11	1:A:534:ARG:HG2	1.81	0.46
1:A:501:LEU:O	1:A:526:ILE:HA	2.14	0.46
1:A:607:LYS:N	1:A:607:LYS:HD2	2.32	0.45
1:A:386:VAL:HG11	1:A:393:GLY:HA2	1.99	0.45
1:A:488:ASN:HA	1:A:514:LEU:O	2.17	0.44
1:A:565:HIS:HD2	1:A:569:LYS:NZ	2.17	0.42
1:A:456:GLU:HA	1:A:478:ILE:O	2.19	0.42
1:A:465:LEU:HD12	1:A:492:ILE:HG12	2.02	0.42
1:A:609:ASN:HD22	1:A:614:ARG:N	2.13	0.42
1:A:287:CYS:HB3	1:A:290:CYS:SG	2.59	0.42
1:A:621:VAL:HA	1:A:622:PRO:HD3	1.93	0.42
1:A:653:LYS:HB2	1:A:655:ASN:ND2	2.35	0.42
1:A:339:ASN:H	1:A:376:ASN:ND2	2.18	0.41
1:A:308:PHE:CD1	1:A:319:ASN:HB3	2.55	0.41
1:A:290:CYS:O	1:A:319:ASN:HA	2.20	0.41
1:A:325:ARG:HA	1:A:353:THR:O	2.20	0.41
1:A:125:VAL:HG23	1:A:144:LEU:HD13	2.03	0.41
1:A:338:ARG:HA	1:A:375:ARG:O	2.20	0.41
1:A:557:SER:HB3	1:A:579:HIS:CD2	2.56	0.40
1:A:382:ARG:HA	1:A:429:ASP:O	2.21	0.40
1:A:653:LYS:HE3	1:A:655:ASN:HD21	1.86	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.

Mo	ol Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	537/554 (97%)	520 (97%)	15 (3%)	2 (0%)	34 21

#### All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ILE
1	A	331	VAL

#### 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	A	442/451 (98%)	434 (98%)	8 (2%)	59 48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	LEU
1	A	371	SER
1	A	400	THR
1	A	407	ASP
1	A	488	ASN
1	A	634	SER
1	A	648	LYS
1	A	655	ASN



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	297	ASN
1	A	319	ASN
1	A	339	ASN
1	A	376	ASN
1	A	416	GLN
1	A	425	ASN
1	A	488	ASN
1	A	489	GLN
1	A	539	ASN
1	A	565	HIS
1	A	579	HIS
1	A	581	ASN
1	A	592	GLN
1	A	609	ASN
1	A	610	HIS
1	A	655	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)

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

### 5.5 Carbohydrates (i)

8 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	Mol Type Chain		in Res 1	Link	Во	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
2	RAM	В	1	2	11,11,11	0.68	0	15,16,16	0.72	0	
2	MAN	В	2	2	11,11,12	0.43	0	15,15,17	0.70	0	
2	GLA	В	3	2	11,11,12	0.48	0	15,15,17	0.57	0	
2	RAM	В	4	2	10,10,11	0.64	0	14,14,16	0.53	0	
2	MAN	В	5	2	11,11,12	0.49	0	15,15,17	0.62	0	
2	GLA	В	6	2	11,11,12	0.56	0	15,15,17	0.60	0	
2	ABE	В	7	2	9,9,10	1.15	1 (11%)	10,12,14	0.82	0	
2	ABE	В	8	2	9,9,10	1.20	1 (11%)	10,12,14	0.61	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	RAM	В	1	2	-	-	0/1/1/1
2	MAN	В	2	2	-	0/2/19/22	0/1/1/1
2	GLA	В	3	2	-	0/2/19/22	0/1/1/1
2	RAM	В	4	2	-	-	0/1/1/1
2	MAN	В	5	2	-	0/2/19/22	0/1/1/1
2	GLA	В	6	2	-	0/2/19/22	0/1/1/1
2	ABE	В	7	2	-	-	0/1/1/1
2	ABE	В	8	2	-	-	0/1/1/1

#### All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
2	В	8	ABE	C1-C2	3.02	1.53	1.51
2	В	7	ABE	C1-C2	2.38	1.53	1.51

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

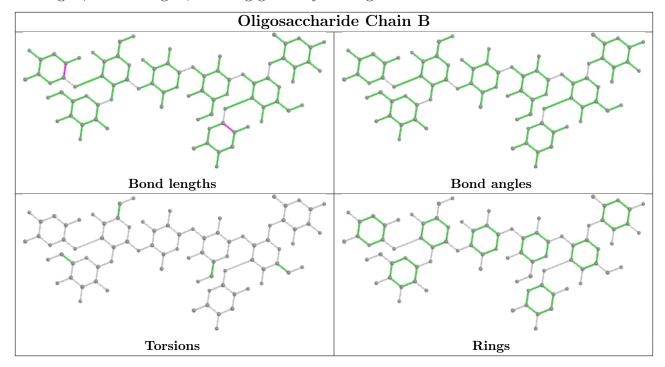
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	1	RAM	1	0

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)

There are no ligands in this entry.

### 5.7 Other polymers (i)

There are no such residues in this entry.

### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	507:ARG	С	508:SER	N	13.11



## 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.

