

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

Sep 18, 2021 – 08:02 am BST

PDB ID : 6XTG

Title : Ab 1116NS19.9 bound to CA19-9 Authors : Diskin, R.; Borenstein-Katz, A.

Deposited on : 2020-01-16

Resolution : 1.55 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 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)

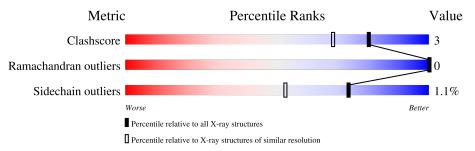
Validation Pipeline (wwPDB-VP) : 2.23.1

## 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 1.55 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	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

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	L	214	96%		•
2	Н	222	91%	6%	<del>.</del>
3	A	4	100%		



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7143 atoms, of which 3348 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 Light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	L	214	Total 3360	C 1065	H 1664	N 279	O 343	S 9	0	7	0

• Molecule 2 is a protein called Heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace			
2	Н	216	Total 3294	C 1047	H 1634	N 276	O 327	S 10	0	10	0

• Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



N	/Iol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
	3	A	4	Total 106	C 31	H 50	N 2	O 23	0	0	0

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

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

• Molecule 5 is water.

$\mathbf{Mol}$	Chain	Residues	${f Atoms}$	ZeroOcc	AltConf
5	L	201	Total O 201 201	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	181	Total O 181 181	0	0

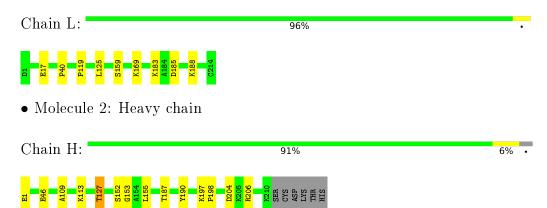


## 3 Residue-property plots (i)

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: Light chain



• Molecule 3: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-[alpha-L-fucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%



# 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 2	Depositor
Cell constants	89.17Å 60.20Å 84.44Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.59 - 1.55	Depositor
% Data completeness	97.3 (44.59-1.55)	Depositor
(in resolution range)	31.0 (41.03 1.00)	Берозгот
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX 1.13_2998	Depositor
$R, R_{free}$	0.174 , 0.201	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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: SIA, NA, FUC, GAL, 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).

Mal	Mol Chain		lengths	Bond angles		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	L	0.34	0/1752	0.51	0/2371	
2	Н	0.37	0/1729	0.54	0/2352	
All	All	0.36	0/3481	0.52	0/4723	

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	1696	1664	1664	7	0
2	Н	1660	1634	1642	11	1
3	A	56	50	49	0	0
4	L	1	0	0	0	0
5	Н	181	0	0	10	1
5	L	201	0	0	6	1
All	All	3795	3348	3355	18	3

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 3.

The worst 5 of 18 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
2:H:152:SER:O	5:H:401:HOH:O	1.96	0.82
2:H:46:GLU:OE2	5:H:402:HOH:O	1.99	0.79
1:L:185:ASP:OD2	5:L:401:HOH:O	2.01	0.77
1:L:17:GLU:OE2	5:L:402:HOH:O	2.05	0.73
1:L:119:PRO:O	5:L:403:HOH:O	2.07	0.72

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$egin{array}{c}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
5:L:425:HOH:O	5:L:466:HOH:O[3_454]	1.67	0.53
2:H:187:THR:O	2:H:206:ARG:NH1[2_565]	2.05	0.15
5:H:556:HOH:O	5:H:556:HOH:O[2_555]	2.05	0.15

#### 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	L	$219/214 \ (102\%)$	216 (99%)	3 (1%)	0	100	100
2	Н	$224/222 \; (101\%)$	219 (98%)	5 (2%)	0	100	100
All	All	443/436 (102%)	435 (98%)	8 (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	197/190 (104%)	196 (100%)	1 (0%)	88 78		
2	Н	191/187 (102%)	188 (98%)	3 (2%)	62 35		
All	All	388/377 (103%)	384 (99%)	4 (1%)	73 57		

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

Mol	Chain	Res	Type
1	L	188	LYS
2	Н	1	GLU
2	Н	127	THR
2	Н	155	LEU

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)

4 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	Chain	Ros	Link		ond leng			ond ang	
				nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
	3	NAG	A	1	3	15,15,15	0.61	1 (6%)	21,21,21	0.74	1 (4%)	



Mol Type Ch		Chain	Res	Link	Bo	nd leng	ths	В	ond ang	les
10101	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GAL	A	2	3	11,11,12	1.19	1 (9%)	15,15,17	1.22	1 (6%)
3	SIA	A	3	3	17,20,21	0.89	1 (5%)	21,28,31	1.42	4 (19%)
3	FUC	A	4	3	10,10,11	0.59	0	14,14,16	0.95	1 (7%)

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	NAG	A	1	3	-	0/6/26/26	0/1/1/1
3	GAL	A	2	3	-	0/2/19/22	0/1/1/1
3	SIA	A	3	3	-	0/14/34/38	0/1/1/1
3	FUC	A	4	3	-	-	0/1/1/1

#### All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	A	2	GAL	O5-C1	-3.02	1.38	1.43
3	A	3	SIA	C6-C5	2.21	1.56	1.53
3	A	1	NAG	O4-C4	-2.10	1.38	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$\mathbf{Ideal}(^o)$
3	A	1	NAG	O4-C4-C5	3.22	117.31	109.30
3	A	3	SIA	C6-O6-C2	2.99	117.74	111.34
3	A	3	SIA	C4-C3-C2	2.68	114.60	109.81
3	A	2	GAL	C1-C2-C3	2.49	112.73	109.67
3	A	4	FUC	C1-C2-C3	2.16	112.32	109.67

There are no chirality outliers.

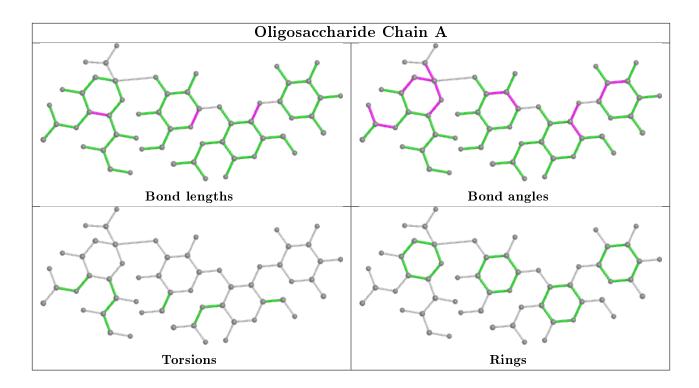
There are no torsion outliers.

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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)

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.

