

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 07:43 AM EDT

PDB ID	:	6U6U
Title	:	IL36R extracellular domain in complex with BI655130 Fab $$
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Deposited on		
Resolution	:	2.31 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



6U6U

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 5225 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 BI00655130 Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	221	Total 1701	C 1075	N 283	O 336	${ m S} 7$	0	5	0

• Molecule 2 is a protein called BI00655130 Fab light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	L	214	Total 1676	C 1047	N 290	0 334	${S \atop 5}$	0	2	0

• Molecule 3 is a protein called Interleukin-1 receptor-like 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
3	R	197	Total 1613	C 1024	N 279	O 299	S 11	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

(Chain	Residue	Modelled	Actual	Comment	Reference	
	R	216	HIS	-	expression tag	UNP Q9HB29	
	R	217	HIS	-	expression tag	UNP Q9HB29	

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

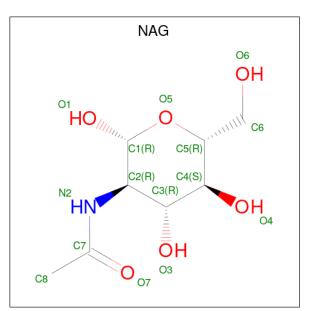
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	А	2	Total 28	C 16	N 2	O 10	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	R	1	Total 14	C 8	N 1	O 5	0	0

• Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Н	84	Total O 85 85	0	1
7	L	49	$\begin{array}{cc} \text{Total} & \text{O} \\ 50 & 50 \end{array}$	0	1
7	R	56	$\begin{array}{cc} \text{Total} & \text{O} \\ 57 & 57 \end{array}$	0	1

MolProbity and EDS failed to run properly - this section is therefore empty.



3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	60.70Å 70.66Å 233.27Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.99 - 2.31	Depositor
% Data completeness	99.9 (36.99-2.31)	Depositor
(in resolution range)		-
R _{merge}	0.09	Depositor
R _{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$2.30 (at 2.31 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.9_{1692}	Depositor
R, R_{free}	0.179 , 0.202	Depositor
Wilson B-factor $(Å^2)$	48.1	Xtriage
Anisotropy	0.497	Xtriage
L-test for $twinning^2$	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5225	wwPDB-VP
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.48% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts (i)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains (i)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA (i)

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 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).



Mal	Mol Type Chain Res		Dag	Link	Bo	ond leng	\mathbf{ths}	Bond angles		
IVIOI	туре	Chain	n nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	NAG	А	1	3,4	$14,\!14,\!15$	0.64	1 (7%)	$17,\!19,\!21$	0.63	0
4	NAG	А	2	4	14,14,15	0.31	0	17,19,21	0.57	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	А	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	А	2	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	1	NAG	O5-C1	-2.04	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

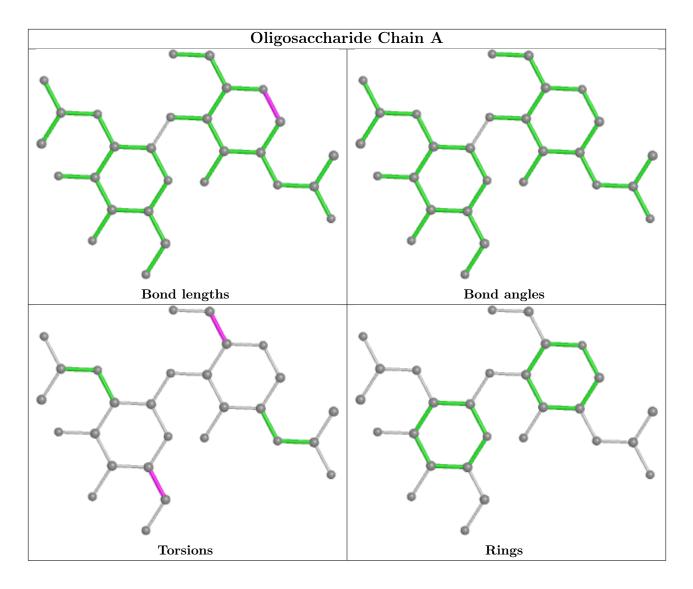
Mol	Chain	Res	Type	Atoms
4	А	2	NAG	O5-C5-C6-O6
4	А	2	NAG	C4-C5-C6-O6
4	А	1	NAG	C4-C5-C6-O6
4	А	1	NAG	O5-C5-C6-O6

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.





4.6 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).

ſ	Mol	Type	Chain	Res	Link	Bo	ond leng	\mathbf{ths}	В	ond ang	les
	WIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
	6	NAG	R	303	3	14,14,15	0.39	0	17,19,21	0.87	1 (5%)

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
6	NAG	R	303	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	R	303	NAG	C1-O5-C5	2.91	116.13	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	303	NAG	C4-C5-C6-O6
6	R	303	NAG	C8-C7-N2-C2
6	R	303	NAG	O7-C7-N2-C2
6	R	303	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

