

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:25 AM EDT

PDB ID : 6VRY

Title: Structure of NCI09 fab in complex with SIV V2 peptide

Authors: Gorman, J.; Ahmadi, M.; Kwong, P.D.

Deposited on : 2020-02-10

Resolution : 1.40 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 : 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: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.40 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.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7693 atoms, of which 3501 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 NCI09 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	L	214	Total 3365	C 1069	H 1668	N 278	O 343	S 7	0	13	0

• Molecule 2 is a protein called SIV V2 peptide.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
2	G	11	Total 202	C 61	H 102	N 18	O 21	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	173	ASN	-	expression tag	UNP P08810

• Molecule 3 is a protein called NCI09 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	Н	225	Total 3409	C 1090	H 1697	N 276	O 338	S 8	0	7	0

• Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	A	4	Total 83	C 28	H 34	N 2	O 19	0	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	300	Total O 300 300	0	0
5	G	26	Total O 26 26	0	0
5	Н	308	Total O 308 308	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	65.76Å 72.09Å 100.83Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	31.26 - 1.40	Depositor	
% Data completeness	88.0 (31.26-1.40)	Depositor	
(in resolution range)	, , ,		
R_{merge}	0.04	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	4.40 (at 1.40Å)	Xtriage	
Refinement program	PHENIX (1.14_3260: ???)	Depositor	
R, R_{free}	0.147 , 0.168	Depositor	
Wilson B-factor (\mathring{A}^2)	13.7	Xtriage	
Anisotropy	0.016	Xtriage	
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	7693	wwPDB-VP	
Average B, all atoms (\mathring{A}^2)	20.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.02% 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.

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)

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).



Mal	Mol Type Chain Res Link				Bo	ond leng	ths	Bond angles		
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1	4,1	14,14,15	0.95	1 (7%)	17,19,21	0.55	0
4	NAG	A	2	4	14,14,15	0.62	1 (7%)	17,19,21	0.64	0
4	BMA	A	3	4	11,11,12	0.82	0	15,15,17	1.06	1 (6%)
4	FUC	A	4	4	10,10,11	0.89	0	14,14,16	1.07	2 (14%)

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	A	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	A	2	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3	4	-	2/2/19/22	0/1/1/1
4	FUC	A	4	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

	Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
	4	A	1	NAG	O5-C1	-3.51	1.38	1.43
Ī	4	A	2	NAG	O5-C1	-2.23	1.40	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$\operatorname{Ideal}(^{o})$
4	A	3	BMA	C1-O5-C5	3.22	116.55	112.19
4	A	4	FUC	C1-O5-C5	2.27	117.92	112.78
4	A	4	FUC	C1-C2-C3	2.25	112.43	109.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3	BMA	C4-C5-C6-O6
4	A	3	BMA	O5-C5-C6-O6

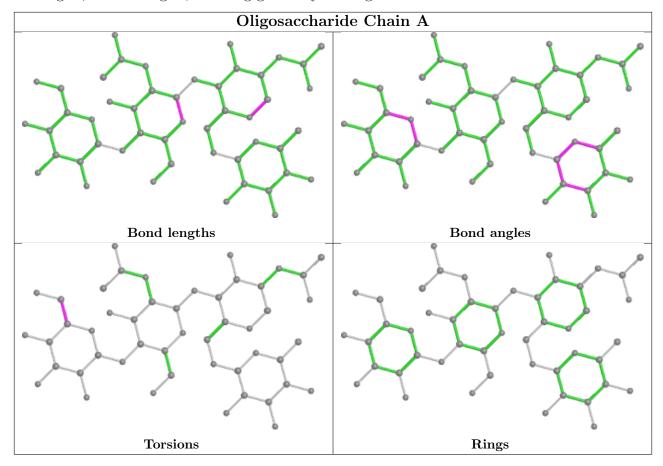
There are no ring outliers.

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)

There are no ligands in this entry.

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.

