Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 03:10 AM EDT

PDB ID	:	6VY5
Title	:	Crystal structure of Nipah receptor binding protein head domain in complex with human neutralizing antibody HENV-26
Authors	:	Dong, J.; Crowe, J.E.
Deposited on	:	2020-02-25
Resolution	:	3.40 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 ⓘ 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 ⓘ) 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-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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 4 unique types of molecules in this entry. The entry contains 6252 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 Anti-Hendra receptor binding protein antibody HENV-26 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	218	Total	C	N	O	S	0	0	0
			1575	999	270	299	7			

- Molecule 2 is a protein called Anti-Hendra receptor binding protein antibody HENV-26 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	208	Total	C	N	O	S	0	0	0
			1431	889	248	290	4			

- Molecule 3 is a protein called receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	409	Total	C	N	O	S	0	0	0
			3176	2029	538	589	20			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	603	GLU	-	expression tag	UNP Q9IH62
A	604	ASN	-	expression tag	UNP Q9IH62
A	605	LEU	-	expression tag	UNP Q9IH62
A	606	TYR	-	expression tag	UNP Q9IH62
A	607	PHE	-	expression tag	UNP Q9IH62
A	608	GLN	-	expression tag	UNP Q9IH62
A	609	GLY	-	expression tag	UNP Q9IH62
A	610	HIS	-	expression tag	UNP Q9IH62
A	611	HIS	-	expression tag	UNP Q9IH62
A	612	HIS	-	expression tag	UNP Q9IH62
A	613	HIS	-	expression tag	UNP Q9IH62
A	614	HIS	-	expression tag	UNP Q9IH62

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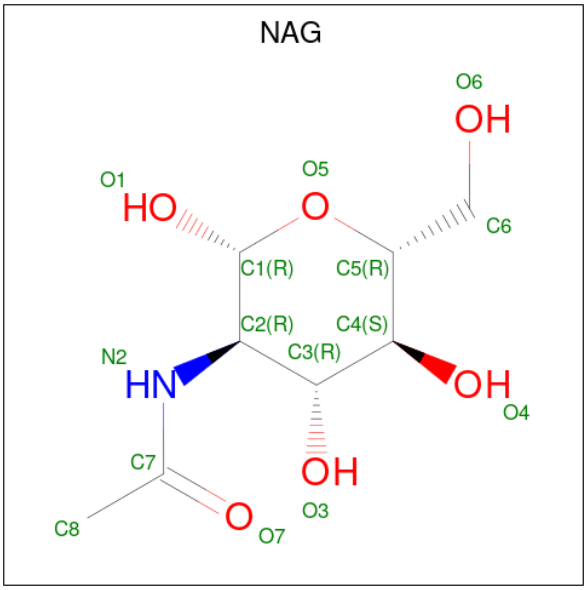
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	HIS	-	expression tag	UNP Q9IH62

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.70Å 186.70Å 81.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.92 – 3.40	Depositor
% Data completeness (in resolution range)	99.9 (44.92-3.40)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.208 , 0.250	Depositor
Wilson B-factor (Å^2)	81.4	Xtriage
Anisotropy	0.421	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
Total number of atoms	6252	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical 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.

4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

5 ligands 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	701	3	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	A	702	3	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	A	704	3	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	A	705	3	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	703	3	14,14,15	0.23	0	17,19,21	0.49	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	A	701	3	-	0/6/23/26	0/1/1/1
4	NAG	A	702	3	-	2/6/23/26	0/1/1/1
4	NAG	A	704	3	-	2/6/23/26	0/1/1/1
4	NAG	A	705	3	-	2/6/23/26	0/1/1/1
4	NAG	A	703	3	-	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 (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	NAG	O5-C5-C6-O6
4	A	702	NAG	C4-C5-C6-O6
4	A	703	NAG	O5-C5-C6-O6
4	A	705	NAG	C4-C5-C6-O6
4	A	704	NAG	C8-C7-N2-C2
4	A	704	NAG	O7-C7-N2-C2
4	A	702	NAG	O5-C5-C6-O6
4	A	703	NAG	C4-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

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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