

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 08:33 AM EDT

PDB ID : 6VBQ

Title : Crystal structure of anti-HIV-1 antibody DH822 bound to gp120 V2 peptide

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Deposited on : 2019-12-19

Resolution : 2.12 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 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 2.12 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 27432 atoms, of which 13170 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 DH822 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Н	223	Total	С	Н	N	О	S	0	0	0
	11		3318	1054	1641	283	330	10			
1	A	222	Total	С	Н	N	О	S	0	2	0
			3315	1057	1634	285	329	10			
1	E	222	Total	С	Н	N	О	S	0	1	0
1	12		3324	1057	1643	285	329	10	0	1	U
1	С	223	Total	С	Н	N	О	S	0	0	0
			3318	1054	1641	283	330	10			

• Molecule 2 is a protein called DH822 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	208	Total	С	Н	N	О	S	0	0	0
			3078	984	1515	254	320	5			
2	В	208	Total	С	Н	N	О	S	0	0	0
	Ъ		3083	985	1517	254	322	5			
2	F	208	Total	С	Н	N	О	S	0	0	0
2			3078	984	1515	254	320	5			
2	D	208	Total	С	Н	N	О	S	0	1	0
			3089	987	1520	255	322	5			

• Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	15	Total	С	Н	N	О	0	0	0
3			265	86	138	22	19			
3	P	15	Total	С	Н	N	О	0	0	0
3	Г		274	88	145	22	19			
3	Т	15	Total	С	Н	N	О	0	0	0
3	1		265	86	138	22	19	0		
3	К	13	Total	С	Н	N	О	0	0	0
			234	76	123	20	15			



• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	138	Total O 138 138	0	0
4	L	81	Total O 81 81	0	0
4	В	59	Total O 59 59	0	0
4	F	56	Total O 56 56	0	0
4	D	73	Total O 73 73	0	0
4	A	118	Total O 118 118	0	0
4	Е	111	Total O 111 111	0	0
4	С	142	Total O 142 142	0	0
4	J	4	Total O 4 4	0	0
4	Р	3	Total O 3 3	0	0
4	I	4	Total O 4 4	0	0
4	К	2	Total O 2 2	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 31	Depositor	
Cell constants	75.07Å 75.07Å 312.87Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	40.68 - 2.12	Depositor	
% Data completeness	99.6 (40.68-2.12)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.77 (at 2.12Å)	Xtriage	
Refinement program	PHENIX 1.14_3228	Depositor	
R, R_{free}	0.181 , 0.211	Depositor	
Wilson B-factor (Å ²)	34.4	Xtriage	
Anisotropy	0.304	Xtriage	
L-test for twinning ²	$< L > = 0.46, < L^2> = 0.28$	Xtriage	
	0.042 for -h,-k,l		
Estimated twinning fraction	0.467 for h,-h-k,-l	Xtriage	
	0.046 for -k,-h,-l		
Total number of atoms	27432	wwPDB-VP	
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.67% 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)

There are no monosaccharides in this entry.

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.

