



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 5, 2023 – 08:33 AM EDT

PDB ID : 6VBQ
Title : Crystal structure of anti-HIV-1 antibody DH822 bound to gp120 V2 peptide
Authors : Janus, B.M.; Ofek, G.
Deposited on : 2019-12-19
Resolution : 2.12 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 ⓘ 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**
Xtrriage (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

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	
			Total	C	H	N	O				S
1	H	223	3318	1054	1641	283	330	10	0	0	0
1	A	222	3315	1057	1634	285	329	10	0	2	0
1	E	222	3324	1057	1643	285	329	10	0	1	0
1	C	223	3318	1054	1641	283	330	10	0	0	0

- Molecule 2 is a protein called DH822 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	L	208	3078	984	1515	254	320	5	0	0	0
2	B	208	3083	985	1517	254	322	5	0	0	0
2	F	208	3078	984	1515	254	320	5	0	0	0
2	D	208	3089	987	1520	255	322	5	0	1	0

- Molecule 3 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
3	J	15	265	86	138	22	19	0	0	0
3	P	15	274	88	145	22	19	0	0	0
3	I	15	265	86	138	22	19	0	0	0
3	K	13	234	76	123	20	15	0	0	0

- Molecule 4 is water.

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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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.

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

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

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