



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 01:20 AM UTC

PDB ID : 6VBQ / pdb_00006vbq
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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

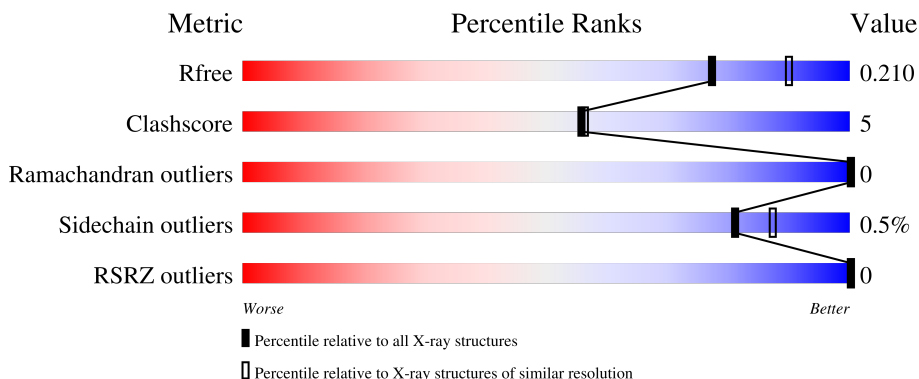
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	 87% 9% .
1	C	230	 90% 7% .
1	E	230	 87% 10% .
1	H	230	 93% . .
2	B	214	 82% 15% .

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Mol	Chain	Length	Quality of chain
2	D	214	 90% 7%
2	F	214	 86% 11%
2	L	214	 92% 6%
3	I	22	 68% 32%
3	J	22	 55% 9% 5% 32%
3	K	22	 55% 5% 41%
3	P	22	 55% 14% 32%

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.

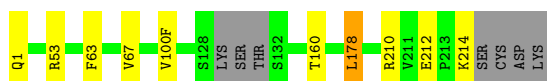
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	138	Total 138	O 138	0	0
4	L	81	Total 81	O 81	0	0
4	B	59	Total 59	O 59	0	0
4	F	56	Total 56	O 56	0	0
4	D	73	Total 73	O 73	0	0
4	A	118	Total 118	O 118	0	0
4	E	111	Total 111	O 111	0	0
4	C	142	Total 142	O 142	0	0
4	J	4	Total 4	O 4	0	0
4	P	3	Total 3	O 3	0	0
4	I	4	Total 4	O 4	0	0
4	K	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DH822 heavy chain

Chain H:  93%



- Molecule 1: DH822 heavy chain

Chain A:  87%




- Molecule 1: DH822 heavy chain

Chain E:  87%



- Molecule 1: DH822 heavy chain

Chain C:  90%




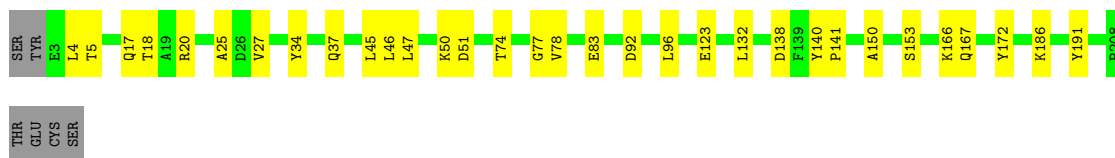
- Molecule 2: DH822 light chain

Chain L:  92%




- Molecule 2: DH822 light chain

Chain B:  82% 15%



- Molecule 2: DH822 light chain

Chain F:  86% 11%



- Molecule 2: DH822 light chain

Chain D:  90% 7%



- Molecule 3: Envelope glycoprotein gp160

Chain J:  55% 9% 5% 32%



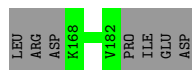
- Molecule 3: Envelope glycoprotein gp160

Chain P:  55% 14% 32%



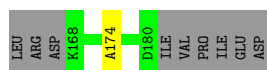
- Molecule 3: Envelope glycoprotein gp160

Chain I:  68% 32%



- Molecule 3: Envelope glycoprotein gp160

Chain K:  55% 5% 41%



4 Data and refinement statistics i

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 40.68 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.68-2.12) 97.5 (40.68-2.12)	Depositor EDS
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 0.182 , 0.210	Depositor DCC
R_{free} test set	1999 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtrriage
Anisotropy	0.304	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.5	EDS
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
F_o, F_c correlation	0.97	EDS
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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/1728	0.52	0/2355
1	C	0.34	0/1716	0.52	0/2338
1	E	0.35	0/1721	0.54	0/2345
1	H	0.34	0/1716	0.52	0/2338
2	B	0.26	0/1605	0.46	0/2196
2	D	0.31	0/1608	0.53	0/2201
2	F	0.26	0/1602	0.47	0/2192
2	L	0.31	0/1602	0.52	0/2192
3	I	0.32	0/129	0.56	0/170
3	J	0.32	0/129	0.59	0/170
3	K	0.27	0/113	0.50	0/148
3	P	0.27	0/131	0.52	0/173
All	All	0.31	0/13800	0.51	0/18818

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1681	1634	1636	21	0
1	C	1677	1641	1641	19	0
1	E	1681	1643	1642	21	0
1	H	1677	1641	1641	7	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1566	1517	1516	25	0
2	D	1569	1520	1519	13	0
2	F	1563	1515	1514	15	2
2	L	1563	1515	1514	7	0
3	I	127	138	137	0	0
3	J	127	138	137	3	0
3	K	111	123	122	1	0
3	P	129	145	144	2	0
4	A	118	0	0	6	1
4	B	59	0	0	8	0
4	C	142	0	0	11	1
4	D	73	0	0	7	0
4	E	111	0	0	9	3
4	F	56	0	0	2	0
4	H	138	0	0	3	4
4	I	4	0	0	0	0
4	J	4	0	0	1	0
4	K	2	0	0	0	0
4	L	81	0	0	1	1
4	P	3	0	0	1	0
All	All	14262	13170	13163	124	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 124 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ASN:OD1	4:C:301:HOH:O	1.88	0.90
1:A:1:GLN:N	4:A:301:HOH:O	1.98	0.89
2:B:186:LYS:NZ	4:B:302:HOH:O	2.07	0.88
2:L:186:LYS:NZ	4:L:301:HOH:O	2.08	0.85
1:H:1:GLN:NE2	4:H:302:HOH:O	2.10	0.83

The worst 5 of 7 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:388:HOH:O	4:A:346:HOH:O[3_864]	2.00	0.20
4:E:335:HOH:O	4:C:400:HOH:O[3_864]	2.00	0.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:410:HOH:O	4:E:383:HOH:O[1_455]	2.01	0.19
1:H:160:THR:OG1	2:F:53:GLU:OE2[1_455]	2.04	0.16
4:H:321:HOH:O	4:E:302:HOH:O[1_455]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/230 (96%)	219 (100%)	1 (0%)	0	100	100
1	C	219/230 (95%)	215 (98%)	4 (2%)	0	100	100
1	E	219/230 (95%)	217 (99%)	2 (1%)	0	100	100
1	H	219/230 (95%)	215 (98%)	4 (2%)	0	100	100
2	B	206/214 (96%)	196 (95%)	10 (5%)	0	100	100
2	D	207/214 (97%)	198 (96%)	9 (4%)	0	100	100
2	F	206/214 (96%)	198 (96%)	8 (4%)	0	100	100
2	L	206/214 (96%)	200 (97%)	6 (3%)	0	100	100
3	I	13/22 (59%)	13 (100%)	0	0	100	100
3	J	13/22 (59%)	11 (85%)	2 (15%)	0	100	100
3	K	11/22 (50%)	11 (100%)	0	0	100	100
3	P	13/22 (59%)	11 (85%)	2 (15%)	0	100	100
All	All	1752/1864 (94%)	1704 (97%)	48 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	192/198 (97%)	191 (100%)	1 (0%)	81	87
1	C	191/198 (96%)	191 (100%)	0	100	100
1	E	191/198 (96%)	190 (100%)	1 (0%)	81	87
1	H	191/198 (96%)	190 (100%)	1 (0%)	81	87
2	B	177/184 (96%)	175 (99%)	2 (1%)	65	74
2	D	177/184 (96%)	177 (100%)	0	100	100
2	F	176/184 (96%)	176 (100%)	0	100	100
2	L	176/184 (96%)	175 (99%)	1 (1%)	78	85
3	I	13/21 (62%)	13 (100%)	0	100	100
3	J	13/21 (62%)	12 (92%)	1 (8%)	12	9
3	K	11/21 (52%)	11 (100%)	0	100	100
3	P	14/21 (67%)	14 (100%)	0	100	100
All	All	1522/1612 (94%)	1515 (100%)	7 (0%)	81	87

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	153	SER
1	A	1	GLN
3	J	181	ILE
1	E	153	SER
2	B	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3	GLN
1	E	171	GLN
2	F	194	GLN
2	F	126	GLN
1	A	171	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	222/230 (96%)	-1.28	0 100 100	23, 42, 68, 83	1 (0%)
1	C	223/230 (96%)	-1.31	0 100 100	24, 41, 83, 122	0
1	E	222/230 (96%)	-1.30	0 100 100	24, 43, 71, 98	1 (0%)
1	H	223/230 (96%)	-1.32	0 100 100	23, 41, 82, 125	0
2	B	208/214 (97%)	-1.19	0 100 100	31, 59, 88, 107	0
2	D	208/214 (97%)	-1.31	0 100 100	26, 46, 72, 98	1 (0%)
2	F	208/214 (97%)	-1.20	0 100 100	32, 59, 87, 96	0
2	L	208/214 (97%)	-1.27	0 100 100	27, 47, 71, 95	0
3	I	15/22 (68%)	-1.03	0 100 100	36, 48, 90, 91	0
3	J	15/22 (68%)	-1.07	0 100 100	38, 46, 93, 105	0
3	K	13/22 (59%)	-1.29	0 100 100	38, 46, 75, 84	0
3	P	15/22 (68%)	-1.17	0 100 100	38, 49, 96, 111	0
All	All	1780/1864 (95%)	-1.27	0 100 100	23, 46, 83, 125	3 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.