



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:54 AM BST

PDB ID : 6DB6
Title : Crystal structure of anti-HIV-1 V3 Fab 311-11D in complex with a HIV-1 gp120 V3 peptide from MN strain
Authors : Chan, K.-W.; Kong, X.-P.
Deposited on : 2018-05-02
Resolution : 1.98 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

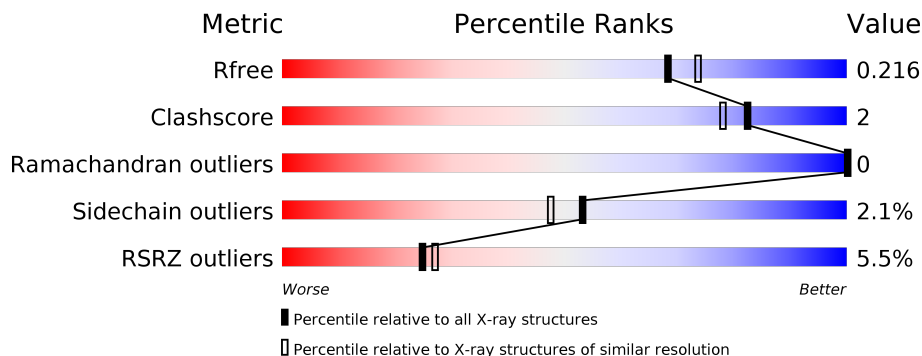
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 on 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	H	230	
2	L	214	
3	P	23	
4	A	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MAN	A	4	-	-	-	X

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 3820 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 Human monoclonal anti-HIV-1 gp120 V3 antibody 311-11D Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	226	1689	1057	288	336	8	0	0	0

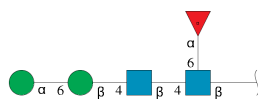
- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody 311-11D Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	1605	1003	264	332	6	0	0	0

- Molecule 3 is a protein called HIV-1 gp120 V3 peptide from MN strain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	14	118	76	26	16	0	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	A	5	60	34	2	24	0	0	0

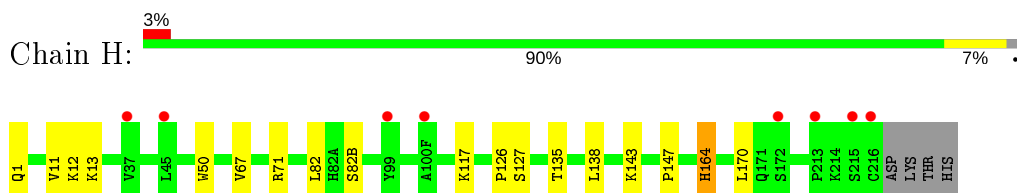
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	192	Total 192	O 192	0	0
5	L	146	Total 146	O 146	0	0
5	P	10	Total 10	O 10	0	0

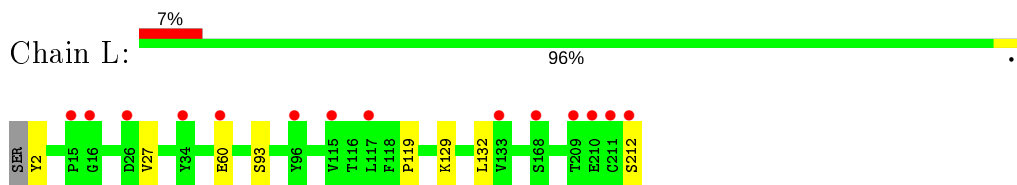
3 Residue-property plots [i](#)

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: Human monoclonal anti-HIV-1 gp120 V3 antibody 311-11D Fab heavy chain



- Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody 311-11D Fab light chain



- Molecule 3: HIV-1 gp120 V3 peptide from MN strain



- Molecule 4: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.57Å 69.16Å 141.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.22 – 1.98 28.22 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.22-1.98) 98.8 (28.22-1.98)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.173 , 0.216 0.173 , 0.216	Depositor DCC
R_{free} test set	1999 reflections (6.16%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtrriage
Anisotropy	0.240	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3820	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FCA, BMA, NAG, MAN

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	H	0.38	0/1729	0.59	0/2352
2	L	0.36	0/1645	0.55	0/2247
3	P	0.36	0/121	0.51	0/160
All	All	0.37	0/3495	0.57	0/4759

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

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	H	1689	0	1640	13	0
2	L	1605	0	1541	4	0
3	P	118	0	123	0	0
4	A	60	0	52	2	0
5	H	192	0	0	6	1
5	L	146	0	0	0	1
5	P	10	0	0	1	0
All	All	3820	0	3356	17	1

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 2.

All (17) 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:H:67:VAL:HG12	1:H:82:LEU:HD13	1.75	0.69
1:H:11:VAL:HB	1:H:147:PRO:HG3	1.82	0.62
1:H:126:PRO:HD2	5:H:534:HOH:O	1.99	0.61
1:H:127:SER:HB2	2:L:212:SER:HB2	1.84	0.59
1:H:82(B):SER:OG	5:H:401:HOH:O	2.18	0.56
1:H:126:PRO:HD3	1:H:138:LEU:HB3	1.93	0.51
1:H:1:GLN:N	5:H:412:HOH:O	2.43	0.50
1:H:67:VAL:CG1	1:H:82:LEU:HD13	2.43	0.47
5:P:401:HOH:O	4:A:5:FCA:H62	2.14	0.47
2:L:119:PRO:HA	2:L:132:LEU:HD23	1.97	0.46
1:H:11:VAL:O	1:H:12:LYS:HD2	2.17	0.45
2:L:2:TYR:CZ	2:L:27:VAL:HG22	2.54	0.43
1:H:164:HIS:HE1	5:H:571:HOH:O	2.02	0.42
1:H:13:LYS:NZ	5:H:423:HOH:O	2.52	0.42
4:A:3:BMA:H61	4:A:4:MAN:O2	2.19	0.41
1:H:143:LYS:NZ	2:L:129:LYS:HD2	2.36	0.41
1:H:117:LYS:NZ	5:H:405:HOH:O	2.33	0.41

All (1) 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)
5:H:401:HOH:O	5:L:409:HOH:O[3_644]	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	H	224/230 (97%)	217 (97%)	7 (3%)	0	100	100
2	L	211/214 (99%)	207 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	12/23 (52%)	11 (92%)	1 (8%)	0	100	100
All	All	447/467 (96%)	435 (97%)	12 (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	H	188/192 (98%)	183 (97%)	5 (3%)	44	35
2	L	183/184 (100%)	181 (99%)	2 (1%)	73	70
3	P	11/19 (58%)	10 (91%)	1 (9%)	9	2
All	All	382/395 (97%)	374 (98%)	8 (2%)	53	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	TRP
1	H	71	ARG
1	H	135	THR
1	H	164	HIS
1	H	170	LEU
2	L	60	GLU
2	L	93	SER
3	P	306	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	164	HIS

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](#)

5 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1	1,4	14,14,15	0.62	1 (7%)	17,19,21	0.57	0
4	NAG	A	2	4	14,14,15	0.52	0	17,19,21	0.53	0
4	BMA	A	3	4	11,11,12	1.03	0	15,15,17	1.15	1 (6%)
4	MAN	A	4	4	11,11,12	1.49	2 (18%)	15,15,17	1.74	3 (20%)
4	FCA	A	5	4	10,10,11	1.84	3 (30%)	14,14,16	1.13	1 (7%)

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	1,4	-	2/6/23/26	0/1/1/1
4	NAG	A	2	4	-	2/6/23/26	0/1/1/1
4	BMA	A	3	4	-	0/2/19/22	0/1/1/1
4	MAN	A	4	4	-	1/2/19/22	1/1/1/1
4	FCA	A	5	4	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5	FCA	O5-C1	4.45	1.50	1.43
4	A	4	MAN	C1-C2	3.21	1.59	1.52
4	A	4	MAN	O5-C5	2.71	1.48	1.43
4	A	5	FCA	O5-C5	2.42	1.48	1.43
4	A	5	FCA	C2-C3	-2.24	1.49	1.52
4	A	1	NAG	O5-C1	-2.12	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	MAN	C1-O5-C5	4.17	117.84	112.19
4	A	4	MAN	C3-C4-C5	-2.69	105.44	110.24
4	A	4	MAN	O2-C2-C3	-2.57	105.00	110.14
4	A	3	BMA	C1-C2-C3	-2.47	106.63	109.67
4	A	5	FCA	C1-O5-C5	-2.21	107.76	112.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C4-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	4	MAN	O5-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3	BMA	1	0
4	A	5	FCA	1	0
4	A	4	MAN	1	0

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

6.1 Protein, DNA and RNA chains

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	H	226/230 (98%)	0.37	8 (3%) 44 46	18, 25, 39, 87	0
2	L	213/214 (99%)	0.52	14 (6%) 18 20	18, 29, 43, 70	0
3	P	14/23 (60%)	1.24	3 (21%) 0 0	22, 32, 55, 55	0
All	All	453/467 (97%)	0.47	25 (5%) 25 27	18, 26, 41, 87	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	216	CYS	14.0
2	L	211	CYS	7.7
3	P	304	ARG	5.7
1	H	215	SER	5.6
2	L	212	SER	4.0
2	L	209	THR	3.8
3	P	319	THR	3.2
2	L	210	GLU	3.1
3	P	318	TYR	3.0
2	L	96	TYR	2.8
1	H	213	PRO	2.7
1	H	37	VAL	2.7
1	H	99	TYR	2.3
1	H	45	LEU	2.2
2	L	60	GLU	2.2
1	H	172	SER	2.2
2	L	168	SER	2.2
2	L	16	GLY	2.2
2	L	117	LEU	2.1
1	H	100(F)	ALA	2.1
2	L	34	TYR	2.1
2	L	133	VAL	2.1
2	L	15	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	115	VAL	2.0
2	L	26	ASP	2.0

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MAN	A	4	11/12	0.58	0.43	65,68,72,72	0
4	BMA	A	3	11/12	0.64	0.32	60,64,69,72	0
4	NAG	A	2	14/15	0.76	0.34	47,56,60,61	0
4	FCA	A	5	10/11	0.79	0.33	46,51,57,59	0
4	NAG	A	1	14/15	0.88	0.16	30,38,46,51	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.