



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2017 – 03:11 PM EST

PDB ID : 4G6F
Title : Crystal Structure of 10E8 Fab in Complex with an HIV-1 gp41 Peptide
Authors : Ofek, G.; Huang, J.; Connors, M.; Kwong, P.D.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

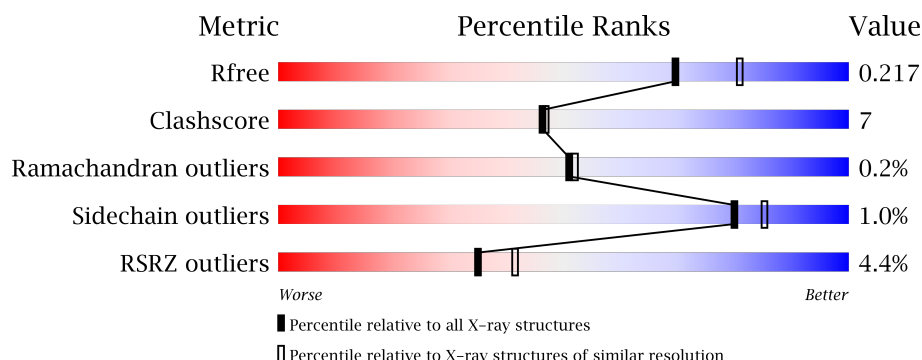
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	B	236	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 84% 14% • </div> </div>
1	H	236	<div> <div style="width: 6%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 6% 83% 14% • </div> </div>
2	D	215	<div> <div style="width: 5%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 5% 86% 11% •• </div> </div>
2	L	215	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 0% 86% 13% • </div> </div>
3	F	34	<div> <div style="width: 24%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green;"></div> <div style="width: 100%; height: 10px; background-color: yellow;"></div> <div style="width: 100%; height: 10px; background-color: grey;"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 24% 71% 6% • 21% </div> </div>

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Mol	Chain	Length	Quality of chain
3	P	34	<div><div></div><div></div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7728 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 10E8 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	232	Total	C	N	O	S	0	0	0
			1763	1122	294	340	7			
1	B	235	Total	C	N	O	S	0	0	0
			1783	1132	297	346	8			

- Molecule 2 is a protein called 10E8 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1590	988	276	322	4			
2	D	211	Total	C	N	O	S	0	0	0
			1581	983	275	319	4			

- Molecule 3 is a protein called gp41 MPER Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	29	Total	C	N	O	0	0	0
			268	180	42	46			
3	F	27	Total	C	N	O	0	0	0
			259	175	44	40			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	109	Total	O	0	0
			109	109		
4	B	161	Total	O	0	0
			161	161		
4	L	104	Total	O	0	0
			104	104		
4	D	98	Total	O	0	0
			98	98		

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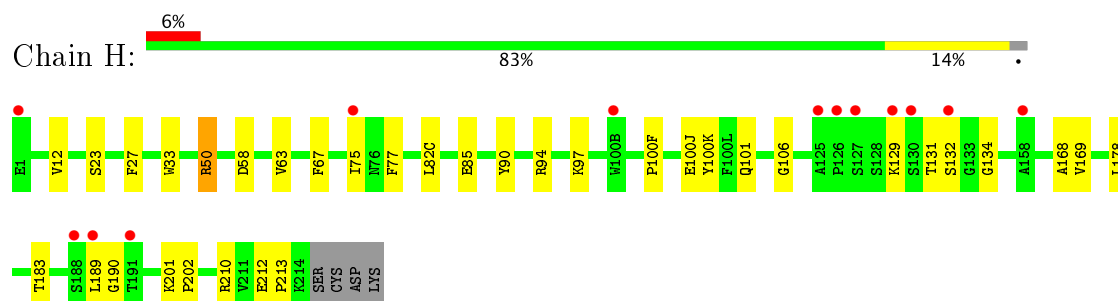
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	7	Total	O	0	0
			7	7		
4	F	5	Total	O	0	0
			5	5		

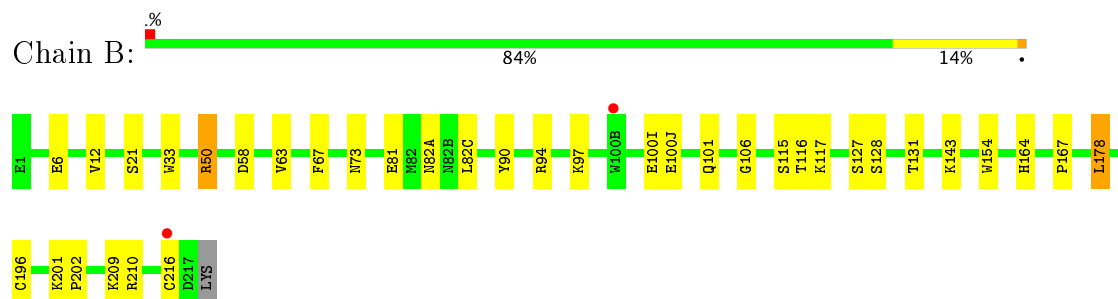
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

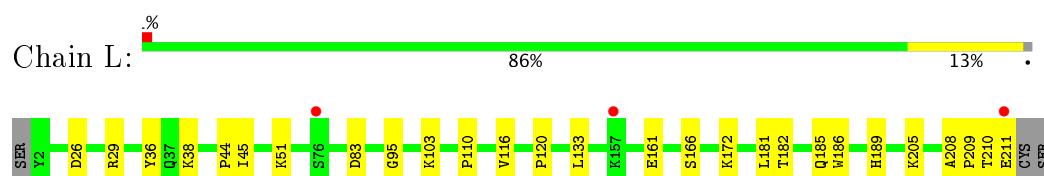
- Molecule 1: 10E8 Heavy Chain



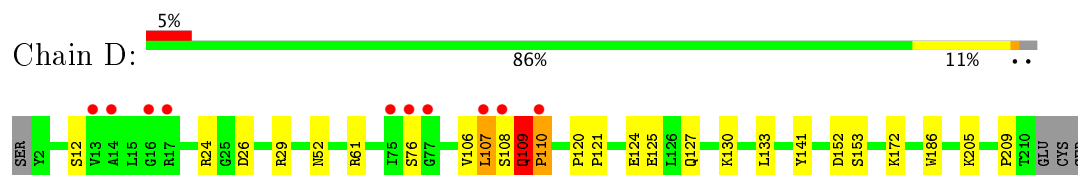
- Molecule 1: 10E8 Heavy Chain



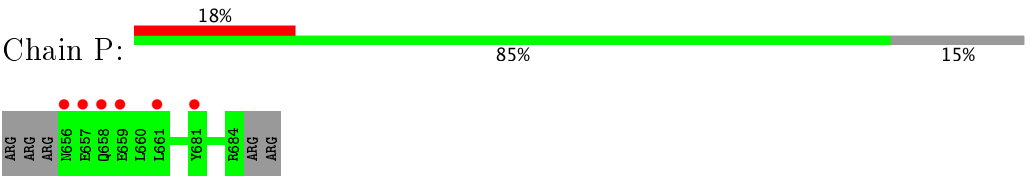
- Molecule 2: 10E8 Light Chain



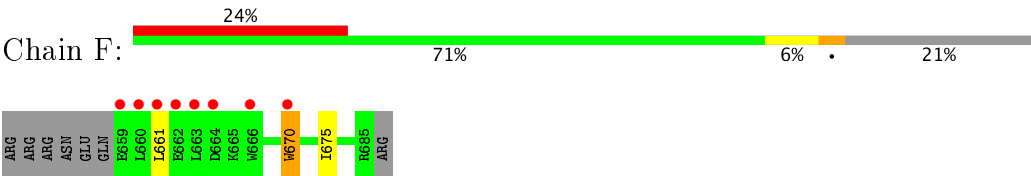
- Molecule 2: 10E8 Light Chain



- Molecule 3: gp41 MPER Peptide



• Molecule 3: gp41 MPER Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.02Å 71.43Å 129.24Å 90.00° 104.50° 90.00°	Depositor
Resolution (Å)	42.59 – 2.10 42.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.4 (42.59-2.10) 84.4 (42.59-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.180 , 0.218 0.183 , 0.217	Depositor DCC
R_{free} test set	1919 reflections (3.25%)	DCC
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% 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	B	0.43	0/1834	0.58	0/2499
1	H	0.36	0/1814	0.52	0/2472
2	D	0.40	1/1616 (0.1%)	0.55	1/2198 (0.0%)
2	L	0.37	0/1625	0.52	0/2210
3	F	0.31	0/270	0.41	0/369
3	P	0.28	0/279	0.36	0/383
All	All	0.38	1/7438 (0.0%)	0.53	1/10131 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	110	PRO	N-CD	5.36	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	109	GLN	C-N-CD	5.57	140.09	128.40

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	B	1783	0	1714	28	0
1	H	1763	0	1700	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1581	0	1542	26	0
2	L	1590	0	1548	23	0
3	F	259	0	245	5	0
3	P	268	0	241	0	0
4	B	161	0	0	9	0
4	D	98	0	0	9	0
4	F	5	0	0	0	0
4	H	109	0	0	5	0
4	L	104	0	0	2	0
4	P	7	0	0	0	0
All	All	7728	0	6990	102	0

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 7.

The worst 5 of 102 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)
4:H:387:HOH:O	2:L:166:SER:HB3	1.64	0.94
1:B:178:LEU:HD12	1:B:178:LEU:C	1.95	0.86
1:H:50:ARG:NH2	1:H:58:ASP:OD2	2.11	0.82
1:B:209:LYS:NZ	2:D:124:GLU:OE2	2.11	0.80
1:H:210:ARG:HD3	1:H:212:GLU:OE2	1.87	0.74

There are no symmetry-related clashes.

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	B	233/236 (99%)	230 (99%)	3 (1%)	0	100	100
1	H	230/236 (98%)	221 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	209/215 (97%)	205 (98%)	2 (1%)	2 (1%)	18	12
2	L	210/215 (98%)	205 (98%)	5 (2%)	0	100	100
3	F	25/34 (74%)	25 (100%)	0	0	100	100
3	P	27/34 (79%)	27 (100%)	0	0	100	100
All	All	934/970 (96%)	913 (98%)	19 (2%)	2 (0%)	51	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	52	ASN
2	D	109	GLN

5.3.2 Protein sidechains ⓘ

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	B	197/198 (100%)	193 (98%)	4 (2%)	60	66
1	H	194/198 (98%)	193 (100%)	1 (0%)	91	94
2	D	175/180 (97%)	173 (99%)	2 (1%)	78	83
2	L	176/180 (98%)	176 (100%)	0	100	100
3	F	26/33 (79%)	25 (96%)	1 (4%)	38	38
3	P	27/33 (82%)	27 (100%)	0	100	100
All	All	795/822 (97%)	787 (99%)	8 (1%)	80	85

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	164	HIS
3	F	670	TRP
2	D	107	LEU
1	B	100(I)	GLU
1	B	178	LEU

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

Mol	Chain	Res	Type
2	D	79	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 carbohydrates 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	B	235/236 (99%)	-0.26	2 (0%) 84 86	26, 37, 60, 103	0
1	H	232/236 (98%)	0.25	13 (5%) 25 31	33, 51, 95, 127	0
2	D	211/215 (98%)	0.12	10 (4%) 32 38	26, 49, 79, 113	0
2	L	212/215 (98%)	-0.10	3 (1%) 75 79	30, 47, 78, 106	0
3	F	27/34 (79%)	1.66	8 (29%) 1 1	41, 67, 121, 129	0
3	P	29/34 (85%)	0.98	6 (20%) 1 1	51, 67, 131, 136	0
All	All	946/970 (97%)	0.08	42 (4%) 35 41	26, 47, 86, 136	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	108	SER	9.2
3	F	661	LEU	7.5
3	F	660	LEU	6.0
1	B	216	CYS	5.8
1	H	129	LYS	5.8

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.