



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:50 AM GMT

PDB ID : 3JUY
Title : Crystal Structure of a 3B3 Variant, a Broadly Neutralizing HIV-1 scFv Antibody
Authors : Clark, K.R.; Walsh, S.T.
Deposited on : 2009-09-15
Resolution : 2.50 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

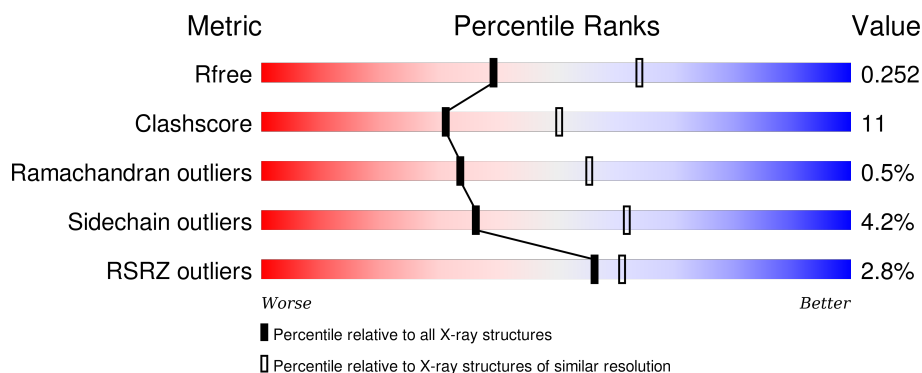
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	A	256	<div> <div>68%</div> <div>22%</div> <div>9%</div> </div>
1	B	256	<div> <div>3%</div> <div>67%</div> <div>25%</div> <div>6%</div> </div>
1	C	256	<div> <div>2%</div> <div>76%</div> <div>15%</div> <div>8%</div> </div>
1	D	256	<div> <div>2%</div> <div>70%</div> <div>22%</div> <div>9%</div> </div>
1	E	256	<div> <div>4%</div> <div>71%</div> <div>19%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	256	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '4%', a large green segment labeled '67%', a yellow segment labeled '22%', and a small grey segment at the end labeled '9%'.

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11275 atoms, of which 0 are hydrogens and 0 are deuteriums.

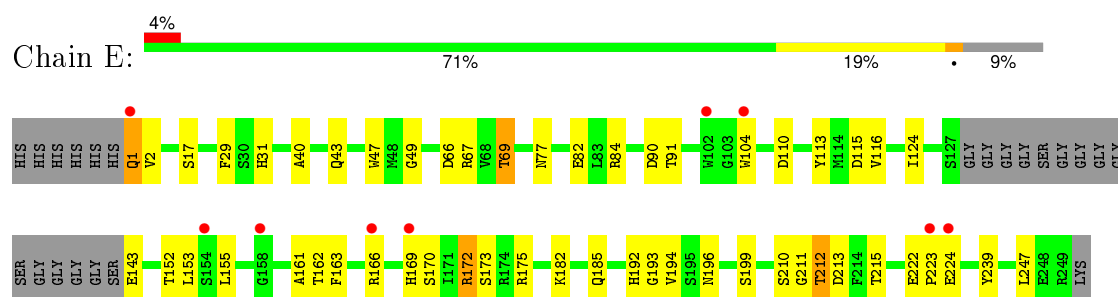
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3B3 single chain variant HIV-1 antibody.

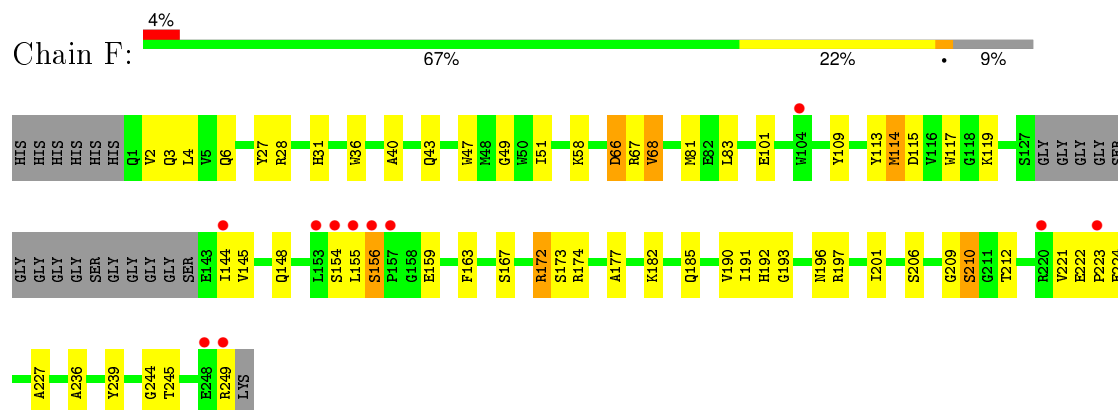
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	240	Total	C	N	O	S	0	0	0
			1856	1165	333	351	7			
1	A	233	Total	C	N	O	S	0	0	0
			1836	1157	327	345	7			
1	C	236	Total	C	N	O	S	0	0	0
			1839	1155	328	349	7			
1	E	234	Total	C	N	O	S	0	0	0
			1824	1148	324	345	7			
1	F	234	Total	C	N	O	S	0	0	0
			1827	1150	327	343	7			
1	D	234	Total	C	N	O	S	0	0	0
			1818	1146	321	344	7			

- Molecule 2 is water.

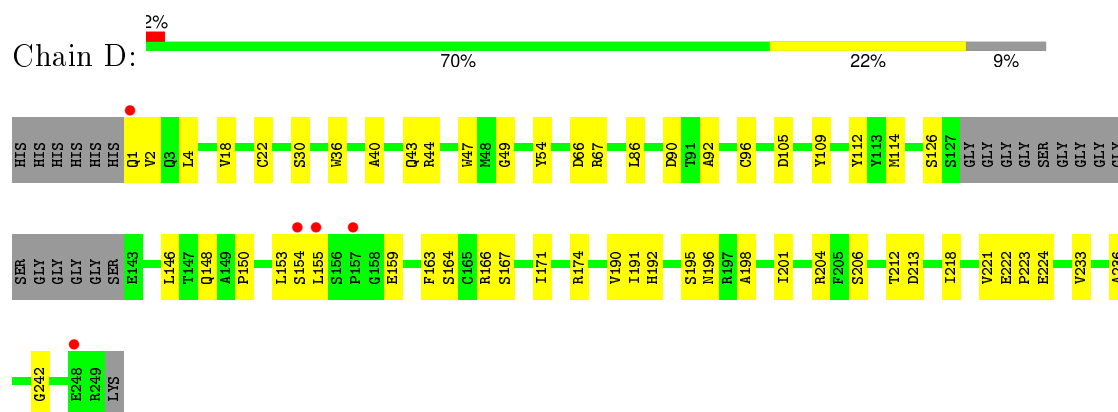
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	54	Total	O	0	0
			54	54		
2	B	56	Total	O	0	0
			56	56		
2	C	50	Total	O	0	0
			50	50		
2	D	36	Total	O	0	0
			36	36		
2	E	45	Total	O	0	0
			45	45		
2	F	34	Total	O	0	0
			34	34		



- Molecule 1: 3B3 single chain variant HIV-1 antibody



- Molecule 1: 3B3 single chain variant HIV-1 antibody



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.17Å 115.13Å 92.37Å 90.00° 111.76° 90.00°	Depositor
Resolution (Å)	29.75 – 2.50 29.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	87.7 (29.75-2.50) 87.4 (29.75-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.195 , 0.260 0.188 , 0.252	Depositor DCC
R_{free} test set	5937 reflections (10.09%)	DCC
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 61604 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11275	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.48	0/1886	0.60	0/2558
1	B	0.50	0/1904	0.62	0/2580
1	C	0.48	0/1887	0.60	0/2559
1	D	0.45	0/1866	0.56	0/2533
1	E	0.47	0/1872	0.60	0/2539
1	F	0.45	0/1875	0.59	0/2543
All	All	0.47	0/11290	0.60	0/15312

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	A	1836	0	1743	43	0
1	B	1856	0	1754	48	0
1	C	1839	0	1739	24	0
1	D	1818	0	1709	31	0
1	E	1824	0	1727	46	0
1	F	1827	0	1730	50	0
2	A	54	0	0	0	0
2	B	56	0	0	1	0
2	C	50	0	0	2	0
2	D	36	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	45	0	0	2	0
2	F	34	0	0	4	0
All	All	11275	0	10402	231	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 11.

The worst 5 of 231 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:B:13:LYS:H	1:B:13:LYS:HD3	1.17	1.03
1:B:13:LYS:N	1:B:13:LYS:HD3	1.93	0.83
1:B:6:GLN:NE2	1:B:121:THR:HG23	1.95	0.81
1:C:126:SER:O	1:C:127:SER:HB3	1.81	0.81
1:E:172:ARG:HE	1:E:173:SER:H	1.29	0.78

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	A	229/256 (90%)	217 (95%)	11 (5%)	1 (0%)	39	61
1	B	236/256 (92%)	222 (94%)	12 (5%)	2 (1%)	24	41
1	C	232/256 (91%)	217 (94%)	14 (6%)	1 (0%)	39	61
1	D	230/256 (90%)	211 (92%)	19 (8%)	0	100	100
1	E	230/256 (90%)	215 (94%)	13 (6%)	2 (1%)	21	37
1	F	230/256 (90%)	217 (94%)	12 (5%)	1 (0%)	39	61
All	All	1387/1536 (90%)	1299 (94%)	81 (6%)	7 (0%)	34	55

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	211	GLY
1	B	159	GLU
1	C	211	GLY
1	E	104	TRP
1	F	210	SER

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	A	193/205 (94%)	186 (96%)	7 (4%)	42	69
1	B	192/205 (94%)	183 (95%)	9 (5%)	32	56
1	C	193/205 (94%)	184 (95%)	9 (5%)	32	56
1	D	188/205 (92%)	182 (97%)	6 (3%)	46	74
1	E	191/205 (93%)	182 (95%)	9 (5%)	32	56
1	F	190/205 (93%)	182 (96%)	8 (4%)	36	62
All	All	1147/1230 (93%)	1099 (96%)	48 (4%)	36	62

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	153	LEU
1	E	31	HIS
1	D	114	MET
1	C	212	THR
1	C	240	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	ASN
1	E	1	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	A	233/256 (91%)	-0.18	2 (0%) 85 88	7, 19, 42, 58	0
1	B	240/256 (93%)	-0.12	7 (2%) 55 60	5, 17, 43, 63	0
1	C	236/256 (92%)	-0.10	6 (2%) 61 65	6, 19, 43, 61	0
1	D	234/256 (91%)	0.06	5 (2%) 67 71	9, 25, 57, 68	0
1	E	234/256 (91%)	-0.00	9 (3%) 44 49	7, 23, 53, 62	0
1	F	234/256 (91%)	0.04	11 (4%) 35 40	9, 27, 59, 69	0
All	All	1411/1536 (91%)	-0.05	40 (2%) 56 61	5, 22, 53, 69	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	154	SER	4.2
1	B	128	GLY	4.0
1	E	104	TRP	3.4
1	B	142	SER	3.3
1	F	223	PRO	3.0

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](#)

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.