

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	4ORG
Title	:	Crystal structure of human Fab CAP256-VRC26.04, a potent V1V2-directed
		HIV-1 neutralizing antibody
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Deposited on	:	2014-02-11
Resolution	:	3.12 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 (i) 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 (1)) 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	:	2.35.1
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)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.12 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.



Motric	Whole archive	Similar resolution
IVIETIC	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 <=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	В	216	93%	• •
1	D	216	93%	
1	F	216	% • 93%	
1	L	216	% 93%	5% •
2	А	256	% 84%	7% 9%



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Mol	Chain	Length	Quality of chain		
2	С	256	% • 86%	6%	7%
2	E	256	2% 82%	0%	8%
2	Н	256	% 8 2%	1.0%	704
2	Н	256	82%	10%	7

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TYS	Н	100(H)	-	-	-	Х
2	TYS	Н	100(I)	-	-	-	Х



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26405 atoms, of which 13008 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.

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
1	т	911	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
		211	3093	979	1529	264	317	4	0		0
1	1 B	208	Total	С	Η	Ν	0	S	0	0	0
		200	3061	970	1513	261	313	4	0	0	0
1	П	208	Total	С	Η	Ν	0	S	0	0	0
T		208	3047	967	1505	258	313	4	0	0	0
1	Б	200	Total	С	Η	Ν	0	S	0	0	0
	F	209	3062	972	1511	259	316	4	0	0	0

• Molecule 1 is a protein called CAP256-VRC26.04 light chain.

• Molecule 2 is a protein called CAP256-VRC26.04 heavy chain.

Mol	Chain	Residues			Atom	\mathbf{s}			ZeroOcc	AltConf	Trace
9	п	028	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	11	230	3565	1146	1751	314	345	9	0	0	0
0	Δ	020	Total	С	Н	Ν	0	S	0	0	0
	А	232	3484	1117	1714	306	338	9	0		0
0	C	227	Total	С	Н	Ν	0	S	0	0	0
		231	3547	1136	1743	312	347	9	0	0	0
0	F	225	Total	С	Н	Ν	0	S	0	0	0
	E	233	3546	1136	1742	310	348	10	0	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: CAP256-VRC26.04 light chain







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	68.02Å 85.47 Å 103.27 Å	Deperitor
a, b, c, α , β , γ	97.90° 107.72° 91.67°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	35.63 - 3.12	Depositor
Resolution (A)	35.63 - 3.12	EDS
% Data completeness	92.7 (35.63-3.12)	Depositor
(in resolution range)	92.8 (35.63 - 3.12)	EDS
R _{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.58 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
D D	0.275 , 0.289	Depositor
Λ, Λ_{free}	0.279 , 0.287	DCC
R_{free} test set	1811 reflections (5.02%)	wwPDB-VP
Wilson B-factor $(Å^2)$	60.6	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.31, 27.4	EDS
L-test for twinning ²	$< L > = 0.42, < L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26405	wwPDB-VP
Average B, all atoms $(Å^2)$	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 84.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6411e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TYS

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).

Mal	Chain	Bond	lengths	Bond	angles
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	В	0.21	0/1585	0.40	0/2167
1	D	0.22	0/1579	0.41	0/2160
1	F	0.21	0/1588	0.40	0/2172
1	L	0.21	0/1602	0.40	0/2192
2	А	0.21	0/1813	0.40	0/2462
2	С	0.22	0/1837	0.39	0/2493
2	Ε	0.22	0/1831	0.40	0/2485
2	Н	0.22	0/1848	0.39	0/2508
All	All	0.22	0/13683	0.40	0/18639

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	В	1548	1513	1515	5	0
1	D	1542	1505	1507	5	0
1	F	1551	1511	1513	5	0
1	L	1564	1529	1531	8	0
2	А	1770	1714	1718	10	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes					
2	С	1804	1743	1746	8	0					
2	Ε	1804	1742	1746	15	0					
2	Н	1814	1751	1753	17	0					
All	All	13397	13008	13029	64	0					

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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.

The worst 5 of 64 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:L:61:ARG:NH1	1:L:77:GLY:O	2.21	0.73
2:H:200:HIS:ND1	2:H:203:SER:OG	2.29	0.66
1:B:124:GLU:OE2	2:A:143:LYS:NZ	2.30	0.65
2:C:52:SER:O	2:C:71:ARG:NH1	2.31	0.64
1:D:124:GLU:OE2	2:C:143:LYS:NZ	2.31	0.64

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	Perce	entiles
1	В	204/216~(94%)	187 (92%)	17 (8%)	0	100	100
1	D	204/216~(94%)	187 (92%)	17 (8%)	0	100	100
1	F	205/216~(95%)	186 (91%)	19 (9%)	0	100	100
1	L	209/216~(97%)	184 (88%)	25 (12%)	0	100	100
2	А	226/256~(88%)	201 (89%)	23 (10%)	2(1%)	17	51
2	С	230/256~(90%)	207~(90%)	21 (9%)	2(1%)	17	51
2	Е	229/256~(90%)	205 (90%)	22 (10%)	2 (1%)	17	51



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Н	232/256~(91%)	211 (91%)	19 (8%)	2(1%)	17 51
All	All	1739/1888~(92%)	1568 (90%)	163 (9%)	8 (0%)	29 63

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5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Н	100(J)	ASP
2	А	126	PRO
2	А	144	ASP
2	С	144	ASP
2	Е	125	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	175/181~(97%)	175 (100%)	0	100	100
1	D	174/181~(96%)	174 (100%)	0	100	100
1	F	175/181~(97%)	175 (100%)	0	100	100
1	L	176/181~(97%)	176~(100%)	0	100	100
2	А	194/215~(90%)	192~(99%)	2(1%)	76	89
2	С	198/215~(92%)	196~(99%)	2(1%)	76	89
2	Ε	197/215~(92%)	191~(97%)	6 (3%)	41	70
2	Н	197/215~(92%)	197 (100%)	0	100	100
All	All	1486/1584~(94%)	1476 (99%)	10 (1%)	84	93

5 of 10 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
2	Е	186	SER
2	Е	188	SER
2	Е	205	THR
2	С	146	PHE



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Mol	Chain	Res	Type
2	Ε	124	LEU

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

Mol	Chain	Res	Type
1	F	184	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)

5 non-standard protein/DNA/RNA residues 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).

Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm sths}$	B	ond ang	gles
	Type	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TYS	С	100(H)	2	$3,\!4,\!17$	0.90	0	2,4,24	1.00	0
2	TYS	Е	100(H)	2	$15,\!16,\!17$	1.25	3 (20%)	18,22,24	0.80	0
2	TYS	C	100(I)	2	$3,\!4,\!17$	0.88	0	2,4,24	1.49	1 (50%)
2	TYS	Н	100(I)	2	3,4,17	0.86	0	2,4,24	1.04	0
2	TYS	H	100(H)	2	3,4,17	0.91	0	2,4,24	1.29	0

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
2	TYS	С	100(H)	2	-	0/0/2/13	-
2	TYS	Е	100(H)	2	-	7/10/11/13	0/1/1/1
2	TYS	С	100(I)	2	-	0/0/2/13	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TYS	Н	100(I)	2	-	0/0/2/13	-
2	TYS	Н	100(H)	2	-	0/0/2/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	100(H)	TYS	OH-CZ	-2.82	1.38	1.42
2	Е	100(H)	TYS	OH-S	-2.53	1.54	1.58
2	E	100(H)	TYS	O3-S	2.21	1.64	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	100(I)	TYS	O-C-CA	-2.10	117.62	124.28

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Е	100(H)	TYS	C-CA-CB-CG
2	Е	100(H)	TYS	CZ-OH-S-O1
2	Е	100(H)	TYS	CZ-OH-S-O2
2	Е	100(H)	TYS	CZ-OH-S-O3
2	Е	100(H)	TYS	N-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Н	100(I)	TYS	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	В	208/216~(96%)	-0.00	0 100 100	35, 55, 75, 85	0
1	D	208/216~(96%)	-0.00	1 (0%) 91 82	33, 59, 77, 93	0
1	F	209/216~(96%)	-0.04	2 (0%) 82 69	24, 45, 64, 78	0
1	L	211/216~(97%)	-0.03	2 (0%) 84 71	15, 52, 80, 90	0
2	А	232/256~(90%)	-0.05	3 (1%) 77 60	30, 52, 73, 84	0
2	С	235/256~(91%)	-0.09	2 (0%) 84 71	27, 55, 72, 82	0
2	Е	234/256~(91%)	-0.01	6 (2%) 56 33	33, 56, 73, 86	0
2	Н	236/256~(92%)	0.01	2 (0%) 86 74	35, 54, 83, 93	0
All	All	1773/1888 (93%)	-0.03	18 (1%) 82 69	15, 54, 74, 93	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
2	С	10	GLY	5.5
1	F	95	LEU	4.9
2	Е	64	TRP	4.0
2	Е	9	GLY	2.9
1	L	95(B)	SER	2.8

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	TYS	Н	100(I)	5/17	0.66	0.52	81,93,108,111	0



	3	1	1 5					
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
2	TYS	Н	100(H)	5/17	0.77	0.44	74,93,108,112	0
2	TYS	E	100(H)	16/17	0.81	0.26	44,71,92,95	0
2	TYS	С	100(I)	5/17	0.82	0.22	68,79,91,98	0
2	TYS	С	100(H)	5/17	0.92	0.33	75,76,90,91	0

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6.3 Carbohydrates (i)

There are no monosaccharides 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.

