W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 12:11 AM BST

PDB ID	:	6PEF
Title	:	Vaccine-elicited NHP FP-targeting antibody DF2F-a.01 in complex with HIV fusion peptide (residue 512-519)
Authors	:	Xu, K.; Liu, K.; Wang, Y.; Kwong, P.D.
Deposited on	:	2019-06-20
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

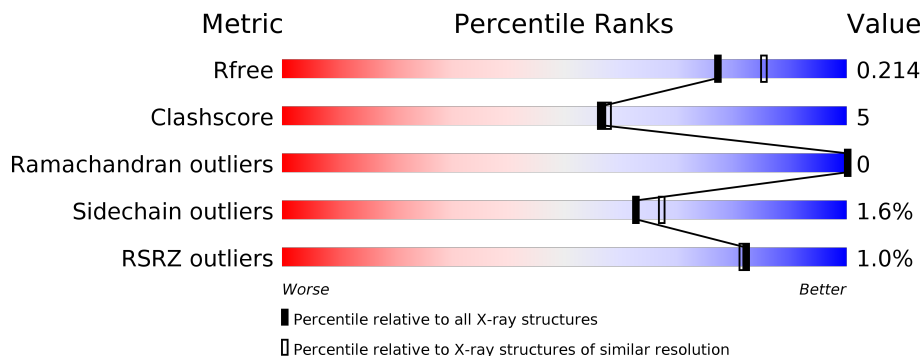|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.214
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		1.0%

Worse ____ Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	226	2% 83% 14% •
1	D	226	% 87% 8% • •
2	B	216	% 86% 11% •
2	E	216	89% 8% •
3	C	8	88% 13%
3	F	8	88% 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7162 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 antibody DF2F-a.01 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total 1628	C 1025	N 272	O 326	S 5	0	0	0
1	D	219	Total 1628	C 1025	N 272	O 326	S 5	0	0	0

- Molecule 2 is a protein called antibody DF2F-a.01 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total 1557	C 978	N 258	O 317	S 4	0	0	0
2	E	210	Total 1551	C 975	N 257	O 315	S 4	0	0	0

- Molecule 3 is a protein called HIV fusion peptide residue 512-519.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total 51	C 35	N 8	O 8	0	0	0
3	F	8	Total 51	C 35	N 8	O 8	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	165	Total 165	O 165	0	0
4	B	173	Total 173	O 173	0	0
4	C	3	Total 3	O 3	0	0
4	D	172	Total 172	O 172	0	0

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	180	Total 180	O 180	0	0
4	F	3	Total 3	O 3	0	0

3 Residue-property plots ⓘ

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.
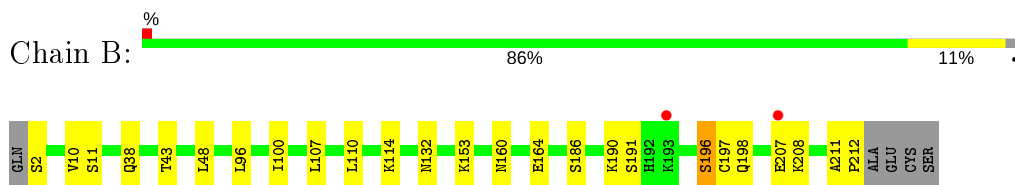
- Molecule 1: antibody DF2F-a.01 heavy chain
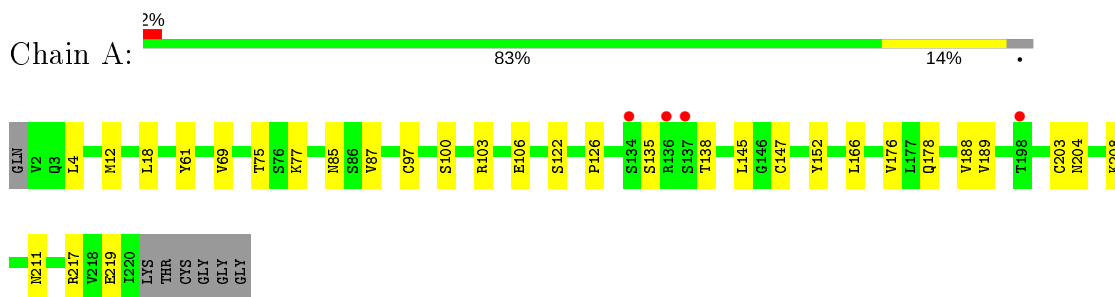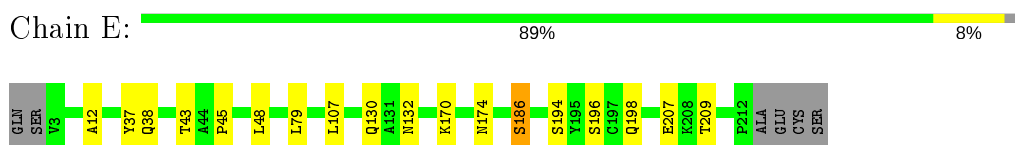

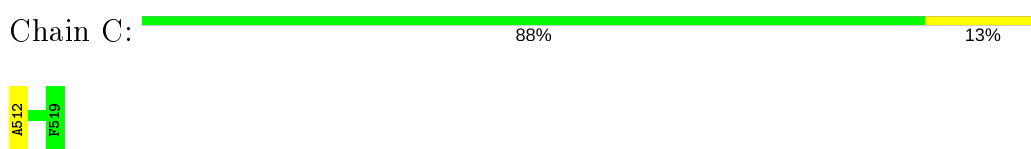- Molecule 1: antibody DF2F-a.01 heavy chain
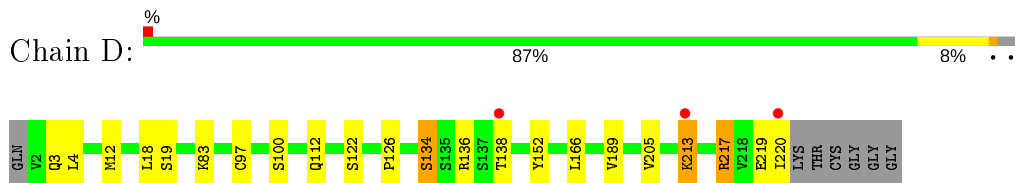
- Molecule 2: antibody DF2F-a.01 light chain

- Molecule 2: antibody DF2F-a.01 light chain

- Molecule 3: HIV fusion peptide residue 512-519

• Molecule 3: HIV fusion peptide residue 512-519

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.57Å 52.50Å 151.72Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	43.17 – 2.00 43.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.17-2.00) 95.1 (43.17-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.183 , 0.214 0.183 , 0.214	Depositor DCC
R_{free} test set	3555 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.2	EDS
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.420 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7162	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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	0.41	0/1666	0.68	5/2273 (0.2%)
1	D	0.43	0/1666	0.64	0/2273
2	B	0.42	0/1593	0.63	1/2175 (0.0%)
2	E	0.36	0/1587	0.57	0/2167
3	C	0.51	0/51	0.46	0/68
3	F	0.44	0/51	0.51	0/68
All	All	0.41	0/6614	0.63	6/9024 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	LEU	CA-CB-CG	7.50	132.55	115.30
1	A	77	LYS	CD-CE-NZ	6.17	125.88	111.70
1	A	77	LYS	CG-CD-CE	-5.83	94.42	111.90
2	B	190	LYS	CB-CG-CD	5.72	126.47	111.60
1	A	188	VAL	CG1-CB-CG2	5.62	119.89	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	217	ARG	Sidechain

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	1628	0	1605	17	0
1	D	1628	0	1605	17	0
2	B	1557	0	1520	21	0
2	E	1551	0	1515	12	0
3	C	51	0	53	1	0
3	F	51	0	53	1	0
4	A	165	0	0	4	1
4	B	173	0	0	4	1
4	C	3	0	0	0	0
4	D	172	0	0	2	0
4	E	180	0	0	4	0
4	F	3	0	0	0	0
All	All	7162	0	6351	64	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 5.

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)
2:E:170:LYS:HE3	2:E:174:ASN:HA	1.49	0.94
2:E:43:THR:OG1	4:E:302:HOH:O	1.89	0.89
1:A:75:THR:OG1	4:A:301:HOH:O	1.93	0.86
2:B:11:SER:HB2	2:B:110:LEU:HD11	1.62	0.80
1:D:217:ARG:HD3	1:D:219:GLU:HG2	1.68	0.74

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)
4:A:442:HOH:O	4:B:427:HOH:O[2_445]	1.90	0.30

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	217/226 (96%)	214 (99%)	3 (1%)	0	100	100
1	D	217/226 (96%)	213 (98%)	4 (2%)	0	100	100
2	B	209/216 (97%)	204 (98%)	5 (2%)	0	100	100
2	E	208/216 (96%)	204 (98%)	4 (2%)	0	100	100
3	C	6/8 (75%)	6 (100%)	0	0	100	100
3	F	6/8 (75%)	6 (100%)	0	0	100	100
All	All	863/900 (96%)	847 (98%)	16 (2%)	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	188/192 (98%)	184 (98%)	4 (2%)	53	57
1	D	188/192 (98%)	185 (98%)	3 (2%)	62	67
2	B	173/177 (98%)	170 (98%)	3 (2%)	60	65
2	E	172/177 (97%)	170 (99%)	2 (1%)	71	76
3	C	4/4 (100%)	4 (100%)	0	100	100
3	F	4/4 (100%)	4 (100%)	0	100	100
All	All	729/746 (98%)	717 (98%)	12 (2%)	62	67

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	191	SER
2	B	196	SER
1	D	213	LYS
2	B	114	LYS
1	D	134	SER

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

Mol	Chain	Res	Type
1	D	3	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 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, 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(Å²)	Q<0.9
1	A	219/226 (96%)	-0.03	4 (1%)	68	66	17, 36, 61, 85	0
1	D	219/226 (96%)	-0.07	3 (1%)	75	74	17, 35, 60, 79	0
2	B	211/216 (97%)	-0.08	2 (0%)	84	83	16, 33, 67, 79	0
2	E	210/216 (97%)	-0.17	0	100	100	17, 33, 64, 79	0
3	C	8/8 (100%)	-0.19	0	100	100	20, 22, 30, 40	0
3	F	8/8 (100%)	-0.32	0	100	100	21, 22, 28, 39	0
All	All	875/900 (97%)	-0.09	9 (1%)	82	81	16, 34, 64, 85	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	SER	3.9
1	A	198	THR	3.2
1	D	213	LYS	2.8
1	D	220	ILE	2.6
1	A	134	SER	2.4

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 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.