Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:28 pm BST

PDB ID	:	6IW0
Title	:	Crystal structure of 5A ScFv in complex with YFV-17D sE in postfusion state
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Deposited on	:	2018-12-04
Resolution	:	3.60 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:

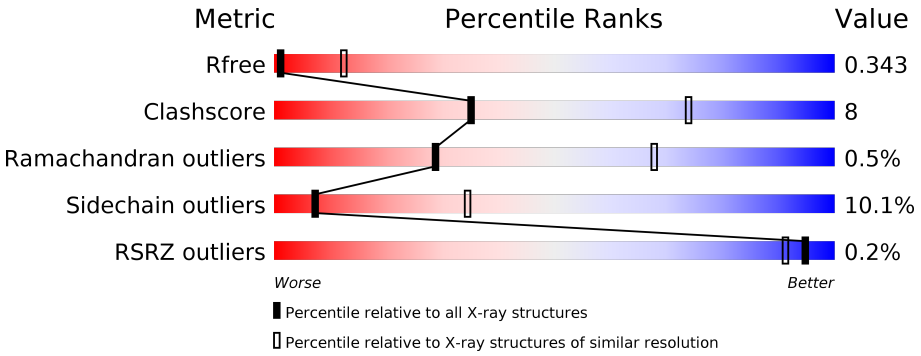
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 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	395	72% 22% • 5%
2	H	145	55% 21% 7% 17%
3	L	107	% 74% 25% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4653 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2895	1818	501	557	19			

- Molecule 2 is a protein called Heavy chain of monoclonal antibody 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	120	Total	C	N	O	S	0	0	0
			948	603	155	187	3			

- Molecule 3 is a protein called Light chain of monoclonal antibody 5A.

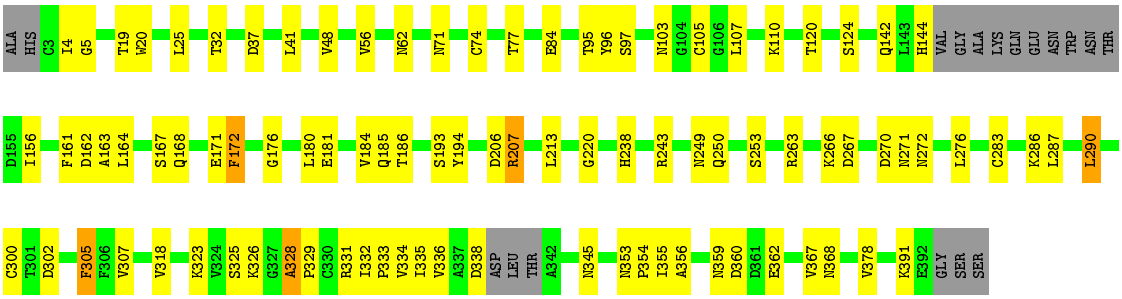
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	106	Total	C	N	O	S	0	0	0
			810	515	131	161	3			

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.

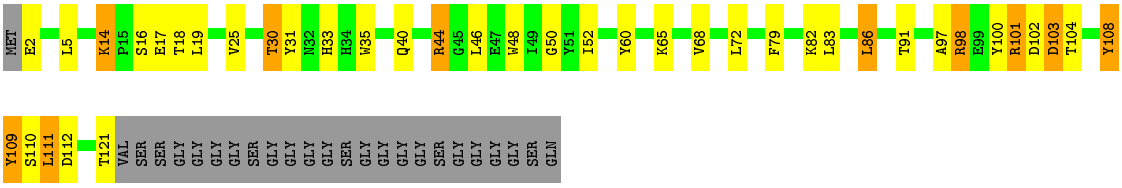
- Molecule 1: Envelope protein E

Chain A:



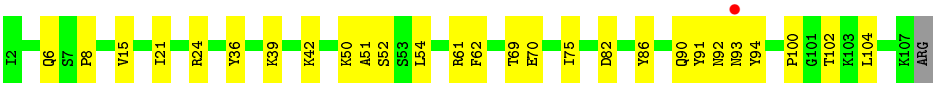
- Molecule 2: Heavy chain of monoclonal antibody 5A

Chain H:



- Molecule 3: Light chain of monoclonal antibody 5A

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	103.99Å 103.99Å 368.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.46 – 3.60 45.46 – 3.56	Depositor EDS
% Data completeness (in resolution range)	90.5 (45.46-3.60) 92.6 (45.46-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.277 , 0.336 0.274 , 0.343	Depositor DCC
R_{free} test set	413 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	1.346	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , -10.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	4653	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.26	0/2950	0.45	0/3998
2	H	0.28	0/976	0.61	3/1335 (0.2%)
3	L	0.25	0/830	0.44	0/1128
All	All	0.26	0/4756	0.49	3/6461 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	111	LEU	N-CA-C	-6.16	94.36	111.00
2	H	112	ASP	N-CA-C	5.39	125.56	111.00
2	H	112	ASP	CB-CA-C	-5.27	99.86	110.40

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	2895	0	2849	38	0
2	H	948	0	896	26	0
3	L	810	0	785	13	0
All	All	4653	0	4530	75	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 8.

All (75) 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:A:267:ASP:O	1:A:271:ASN:ND2	2.22	0.72
2:H:98:ARG:O	2:H:111:LEU:HD23	1.91	0.69
3:L:69:THR:HG23	3:L:70:GLU:HG3	1.79	0.64
2:H:44:ARG:HE	2:H:44:ARG:HA	1.65	0.60
1:A:307:VAL:HG21	1:A:362:GLU:HG2	1.84	0.58
1:A:20:TRP:CD1	1:A:286:LYS:HA	2.39	0.58
1:A:162:ASP:OD1	1:A:163:ALA:N	2.37	0.57
1:A:334:VAL:HG13	1:A:378:VAL:HG22	1.85	0.57
1:A:96:TYR:HB3	1:A:110:LYS:HB3	1.87	0.56
2:H:33:HIS:HA	2:H:101:ARG:HB3	1.87	0.56
3:L:21:ILE:HD13	3:L:102:THR:HB	1.86	0.56
1:A:325:SER:O	1:A:359:ASN:ND2	2.28	0.55
2:H:91:THR:HG23	2:H:121:THR:HA	1.89	0.55
2:H:5:LEU:HD22	2:H:25:VAL:HG22	1.87	0.55
2:H:19:LEU:O	2:H:82:LYS:HA	2.08	0.54
1:A:193:SER:O	1:A:207:ARG:NH1	2.39	0.54
2:H:72:LEU:HD23	2:H:79:PHE:HB3	1.90	0.54
3:L:8:PRO:O	3:L:102:THR:OG1	2.18	0.54
1:A:161:PHE:CZ	1:A:168:GLN:HB2	2.43	0.53
2:H:40:GLN:HB2	2:H:46:LEU:HD23	1.89	0.53
1:A:368:ASN:OD1	1:A:391:LYS:NZ	2.41	0.53
2:H:109:TYR:O	2:H:110:SER:OG	2.27	0.52
1:A:331:ARG:CZ	1:A:353:ASN:HA	2.40	0.52
2:H:52:ILE:HD13	2:H:72:LEU:HB2	1.92	0.52
2:H:30:THR:HA	2:H:35:TRP:CZ2	2.45	0.51
2:H:100:TYR:HB2	2:H:110:SER:HB2	1.92	0.51
2:H:60:TYR:HD1	2:H:65:LYS:HG3	1.76	0.51
3:L:6:GLN:HG3	3:L:100:PRO:HD2	1.91	0.50
1:A:142:GLN:HB3	1:A:156:ILE:HG23	1.94	0.50
2:H:103:ASP:H	2:H:108:TYR:HE1	1.56	0.50
1:A:267:ASP:OD2	1:A:270:ASP:N	2.42	0.50
3:L:24:ARG:HG3	3:L:70:GLU:HG2	1.94	0.49
2:H:19:LEU:HB2	2:H:86:LEU:HD23	1.94	0.49
2:H:103:ASP:HA	2:H:108:TYR:OH	2.14	0.48
1:A:171:GLU:HG3	1:A:172:PHE:N	2.29	0.48
1:A:84:GLU:OE1	1:A:84:GLU:N	2.47	0.48
1:A:331:ARG:NH1	1:A:353:ASN:HA	2.29	0.47
2:H:48:TRP:CZ2	2:H:50:GLY:HA2	2.49	0.47
2:H:14:LYS:O	2:H:17:GLU:HB2	2.14	0.47
2:H:68:VAL:HG22	2:H:83:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:SER:HA	1:A:180:LEU:O	2.14	0.47
1:A:328:ALA:HB1	1:A:329:PRO:HD2	1.95	0.47
1:A:4:ILE:HD13	1:A:355:ILE:HB	1.96	0.47
1:A:56:VAL:O	1:A:220:GLY:N	2.48	0.46
3:L:61:ARG:NE	3:L:82:ASP:OD2	2.46	0.46
2:H:19:LEU:HD23	2:H:83:LEU:HB3	1.97	0.46
2:H:19:LEU:HB3	2:H:83:LEU:H	1.80	0.46
3:L:39:LYS:H	3:L:42:LYS:HE2	1.81	0.45
2:H:5:LEU:HD12	2:H:97:ALA:HA	1.98	0.45
1:A:336:VAL:HG21	1:A:367:VAL:HG11	1.99	0.45
1:A:74:CYS:O	1:A:77:THR:OG1	2.23	0.45
1:A:48:VAL:HG12	1:A:276:LEU:HD23	1.99	0.45
1:A:353:ASN:ND2	1:A:353:ASN:O	2.50	0.45
1:A:249:ASN:OD1	1:A:250:GLN:N	2.50	0.45
3:L:36:TYR:O	3:L:86:TYR:HA	2.18	0.44
1:A:19:THR:HG21	1:A:290:LEU:O	2.17	0.44
3:L:50:LYS:O	3:L:52:SER:N	2.51	0.43
3:L:92:ASN:O	3:L:93:ASN:HB2	2.18	0.43
1:A:103:ASN:HA	2:H:31:TYR:CE2	2.54	0.42
1:A:97:SER:O	1:A:110:LYS:HA	2.20	0.42
3:L:91:TYR:CG	3:L:92:ASN:N	2.88	0.42
1:A:213:LEU:HA	1:A:213:LEU:HD23	1.91	0.42
1:A:331:ARG:NH1	1:A:354:PRO:HD2	2.35	0.42
2:H:82:LYS:HB2	2:H:82:LYS:HE2	1.57	0.41
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.89	0.41
1:A:307:VAL:HG23	1:A:323:LYS:HB2	2.03	0.41
2:H:17:GLU:HB3	2:H:18:THR:H	1.68	0.41
3:L:62:PHE:CD2	3:L:75:ILE:HG12	2.56	0.41
1:A:329:PRO:HA	1:A:356:ALA:O	2.22	0.40
1:A:172:PHE:HB2	1:A:176:GLY:O	2.21	0.40
1:A:5:GLY:HA2	1:A:32:THR:O	2.21	0.40
1:A:302:ASP:OD2	1:A:326:LYS:HD2	2.21	0.40
1:A:332:ILE:HA	1:A:333:PRO:HD3	1.87	0.40
1:A:305:PHE:CE2	1:A:323:LYS:HB3	2.57	0.40
2:H:111:LEU:HB2	3:L:36:TYR:OH	2.22	0.40

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	371/395 (94%)	352 (95%)	18 (5%)	1 (0%)	41 75
2	H	118/145 (81%)	101 (86%)	17 (14%)	0	100 100
3	L	104/107 (97%)	93 (89%)	9 (9%)	2 (2%)	8 42
All	All	593/647 (92%)	546 (92%)	44 (7%)	3 (0%)	29 68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ALA
3	L	15	VAL
3	L	51	ALA

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	317/331 (96%)	282 (89%)	35 (11%)	6 31
2	H	106/116 (91%)	93 (88%)	13 (12%)	4 26
3	L	90/92 (98%)	86 (96%)	4 (4%)	28 63
All	All	513/539 (95%)	461 (90%)	52 (10%)	7 34

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	37	ASP
1	A	41	LEU
1	A	62	ASN
1	A	71	ASN
1	A	95	THR
1	A	105	CYS
1	A	107	LEU
1	A	120	THR
1	A	124	SER
1	A	144	HIS
1	A	164	LEU
1	A	172	PHE
1	A	181	GLU
1	A	184	VAL
1	A	185	GLN
1	A	186	THR
1	A	194	TYR
1	A	206	ASP
1	A	207	ARG
1	A	238	HIS
1	A	243	ARG
1	A	253	SER
1	A	263	ARG
1	A	266	LYS
1	A	272	ASN
1	A	283	CYS
1	A	290	LEU
1	A	300	CYS
1	A	305	PHE
1	A	318	VAL
1	A	335	ILE
1	A	338	ASP
1	A	345	ASN
1	A	360	ASP
2	H	2	GLU
2	H	14	LYS
2	H	16	SER
2	H	30	THR
2	H	44	ARG
2	H	86	LEU
2	H	98	ARG
2	H	101	ARG

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Mol	Chain	Res	Type
2	H	102	ASP
2	H	103	ASP
2	H	104	THR
2	H	108	TYR
2	H	109	TYR
3	L	54	LEU
3	L	90	GLN
3	L	94	TYR
3	L	104	LEU

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

Mol	Chain	Res	Type
1	A	27	GLN
1	A	309	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	A	377/395 (95%)	-0.26	0 100 100	9, 39, 81, 124	0
2	H	120/145 (82%)	-0.19	0 100 100	17, 50, 101, 125	0
3	L	106/107 (99%)	-0.25	1 (0%) 84 73	14, 43, 74, 92	0
All	All	603/647 (93%)	-0.25	1 (0%) 95 91	9, 42, 84, 125	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	93	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.