



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:32 pm BST

PDB ID : 6DG2
Title : Antigen Binding Fragment of the Pan-ebolavirus Monoclonal Antibody 6D6
Authors : Milligan, J.C.; Saphire, E.O.
Deposited on : 2018-05-16
Resolution : 1.96 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

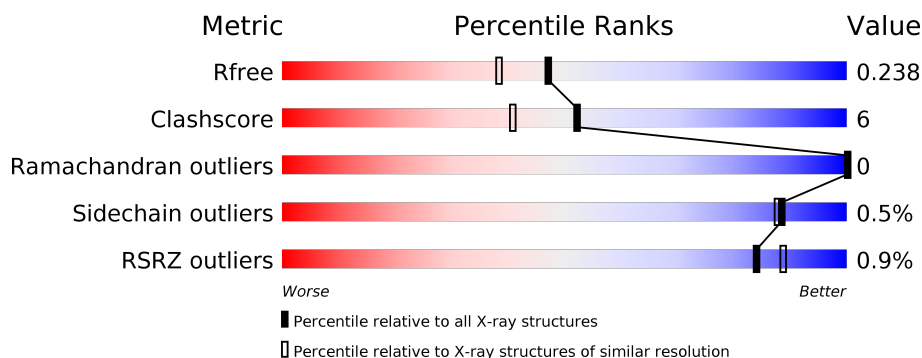
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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	230	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>6%</div> </div> </div>
1	C	230	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
2	B	215	<div> <div></div> <div> <div></div> <div>92%</div> <div>6%</div> </div> </div>
2	D	215	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6846 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 6D6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1632	1035	270	322	5			
1	C	211	Total	C	N	O	S	0	0	0
			1601	1017	264	315	5			

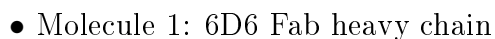
- Molecule 2 is a protein called 6D6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1640	1031	277	326	6			
2	D	211	Total	C	N	O	S	0	0	0
			1636	1029	276	325	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		
3	B	86	Total	O	0	0
			86	86		
3	C	92	Total	O	0	0
			92	92		
3	D	55	Total	O	0	0
			55	55		

- Molecule 1: 6D6 Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.23 Å 72.04 Å 107.15 Å 90.00° 104.20° 90.00°	Depositor
Resolution (Å)	68.08 – 1.96 68.08 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.5 (68.08-1.96) 93.5 (68.08-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 1.95 Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.191 , 0.235 0.196 , 0.238	Depositor DCC
R_{free} test set	1959 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6846	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 4.46% 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

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	0.61	2/1675 (0.1%)	0.67	4/2283 (0.2%)
1	C	0.64	1/1644 (0.1%)	0.75	5/2242 (0.2%)
2	B	0.52	1/1677 (0.1%)	0.66	2/2277 (0.1%)
2	D	0.43	1/1673 (0.1%)	0.71	6/2272 (0.3%)
All	All	0.56	5/6669 (0.1%)	0.70	17/9074 (0.2%)

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
2	B	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	119	ALA	C-N	-17.66	0.93	1.34
2	B	77	SER	C-N	-12.54	1.05	1.34
1	A	201	CYS	C-N	-9.51	1.12	1.34
2	D	208	LYS	C-N	7.79	1.51	1.34
1	A	200	ILE	C-N	6.27	1.48	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	77	SER	O-C-N	-12.47	102.75	122.70
1	C	157	VAL	CB-CA-C	-11.26	90.01	111.40
1	C	157	VAL	N-CA-C	10.95	140.57	111.00
2	B	76	SER	C-N-CA	-7.15	103.83	121.70
2	D	97	TRP	N-CA-CB	6.52	122.33	110.60
2	D	30	SER	N-CA-C	5.98	127.14	111.00
2	D	96	PRO	N-CA-C	-5.71	97.26	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	SER	CB-CA-C	-5.69	99.30	110.10
1	C	158	SER	N-CA-C	5.52	125.91	111.00
1	C	120	SER	O-C-N	-5.42	114.03	122.70
1	A	183	LEU	CA-CB-CG	5.38	127.68	115.30
2	D	29	VAL	N-CA-C	-5.25	96.83	111.00
2	D	30	SER	CB-CA-C	-5.21	100.21	110.10
2	D	209	SER	CA-C-N	-5.19	105.78	117.20
1	C	158	SER	N-CA-CB	-5.18	102.73	110.50
1	A	133	SER	N-CA-C	5.17	124.95	111.00
1	A	129	LEU	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	SER	Mainchain

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	1632	0	1584	17	0
1	C	1601	0	1555	15	0
2	B	1640	0	1594	12	0
2	D	1636	0	1592	27	0
3	A	104	0	0	2	0
3	B	86	0	0	3	0
3	C	92	0	0	3	0
3	D	55	0	0	4	0
All	All	6846	0	6325	71	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 6.

All (71) 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:C:157:VAL:O	1:C:157:VAL:CG1	1.81	1.23
2:D:146:LYS:HB3	2:D:198:THR:HG22	1.41	1.01
1:C:1:GLN:N	3:C:301:HOH:O	1.65	0.96
1:C:157:VAL:O	1:C:157:VAL:HG12	1.03	0.95
2:D:128:SER:OG	3:D:301:HOH:O	1.92	0.87
1:A:125:SER:OG	3:A:301:HOH:O	2.00	0.78
1:A:219:LYS:HG2	1:A:220:SER:N	2.01	0.76
1:A:219:LYS:HG2	1:A:220:SER:H	1.58	0.69
1:A:41:PRO:O	1:A:43:GLN:NE2	2.25	0.67
2:B:106:GLU:OE1	3:B:302:HOH:O	2.15	0.65
1:A:133:SER:OG	1:A:134:LYS:N	2.29	0.65
1:C:54:ARG:NH1	3:C:302:HOH:O	2.31	0.63
1:A:211:LYS:NZ	1:A:213:ASP:OD1	2.32	0.63
2:D:123:ASP:HA	2:D:126:LEU:HD12	1.81	0.62
2:B:156:GLN:HE21	2:B:156:GLN:HA	1.64	0.62
2:B:168:ASP:OD1	2:B:170:LYS:HG2	2.02	0.60
1:C:60:PHE:HB2	1:C:65:LYS:HG2	1.84	0.59
1:C:67:LYS:HE2	1:C:90:ASP:OD2	2.02	0.59
2:B:203:ARG:CD	3:B:301:HOH:O	2.51	0.58
2:D:29:VAL:O	2:D:29:VAL:HG23	2.03	0.58
1:A:140:THR:O	1:A:140:THR:HG23	2.04	0.57
2:D:127:LYS:HA	2:D:184:LYS:NZ	2.21	0.56
2:D:95:PRO:O	2:D:96:PRO:C	2.41	0.56
2:D:127:LYS:HA	2:D:184:LYS:HZ3	1.71	0.56
2:B:186:ASP:OD1	2:B:189:LYS:NZ	2.38	0.53
2:D:47:LEU:O	2:D:48:ILE:HG13	2.08	0.53
2:B:203:ARG:HD3	3:B:301:HOH:O	2.08	0.52
2:D:54:ARG:HG2	2:D:58:VAL:HB	1.93	0.51
2:B:106:GLU:HG2	2:B:107:ILE:N	2.24	0.51
1:C:62:GLU:OE1	1:C:65:LYS:HE3	2.11	0.51
1:C:206:LYS:HG3	3:C:387:HOH:O	2.11	0.51
1:A:62:GLU:OE1	1:A:65:LYS:NZ	2.45	0.50
2:D:83:MET:SD	2:D:83:MET:N	2.84	0.49
2:D:150:LYS:NZ	2:D:196:GLU:OE2	2.44	0.49
2:D:9:LYS:HD2	3:D:316:HOH:O	2.14	0.48
1:C:46:GLU:OE2	1:C:63:LYS:HD3	2.12	0.48
2:D:95:PRO:O	2:D:97:TRP:N	2.46	0.48
1:A:203:VAL:O	1:A:211:LYS:HD2	2.13	0.48
1:C:164:LEU:HD21	1:C:187:VAL:HG21	1.95	0.48
1:A:219:LYS:CG	1:A:220:SER:N	2.76	0.48
2:D:39:LYS:HZ3	2:D:81:GLU:HG2	1.77	0.48
2:D:120:PRO:HB3	2:D:210:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HE3	1:A:80:PHE:CD2	2.50	0.46
2:D:127:LYS:HD2	2:D:127:LYS:C	2.35	0.46
2:D:54:ARG:HH21	2:D:63:THR:HG22	1.79	0.46
2:B:127:LYS:HB3	2:B:127:LYS:HE2	1.72	0.46
2:B:126:LEU:O	2:B:184:LYS:HE2	2.15	0.46
1:A:215:LYS:HG2	1:A:217:GLU:OE2	2.16	0.45
2:B:17:ASP:O	2:B:77:SER:HA	2.17	0.45
1:A:55:ASN:ND2	3:A:307:HOH:O	2.50	0.44
2:D:151:VAL:HG12	2:D:193:TYR:CD1	2.51	0.44
2:B:126:LEU:O	2:B:184:LYS:HD3	2.18	0.44
2:D:10:PHE:HB3	3:D:328:HOH:O	2.17	0.43
1:C:1:GLN:O	1:C:1:GLN:HG3	2.18	0.43
2:D:35:TRP:CE2	2:D:73:PHE:HB2	2.54	0.43
2:D:189:LYS:HB2	2:D:190:HIS:CE1	2.54	0.42
1:C:200:ILE:HG12	1:C:215:LYS:HB2	2.02	0.42
2:D:185:ALA:O	2:D:189:LYS:HE2	2.20	0.42
2:D:46:LEU:O	2:D:47:LEU:HD23	2.20	0.41
2:B:14:SER:HB2	2:B:17:ASP:OD2	2.20	0.41
2:D:187:TYR:O	2:D:193:TYR:OH	2.38	0.41
1:C:12:VAL:HG13	1:C:16:ALA:HB3	2.00	0.41
1:A:219:LYS:CG	1:A:220:SER:H	2.30	0.41
1:C:62:GLU:HA	1:C:65:LYS:HE2	2.02	0.41
1:A:143:LEU:HD12	1:A:143:LEU:C	2.41	0.41
2:D:39:LYS:NZ	2:D:81:GLU:HG2	2.36	0.41
2:D:95:PRO:O	2:D:97:TRP:CD1	2.74	0.41
1:A:215:LYS:HG2	1:A:217:GLU:HG3	2.02	0.40
1:A:10:GLU:HG2	1:A:18:VAL:HG21	2.03	0.40
1:C:55:ASN:HA	1:C:55:ASN:HD22	1.66	0.40
2:D:14:SER:OG	3:D:302:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	213/230 (93%)	207 (97%)	6 (3%)	0	100	100
1	C	207/230 (90%)	200 (97%)	7 (3%)	0	100	100
2	B	210/215 (98%)	201 (96%)	9 (4%)	0	100	100
2	D	209/215 (97%)	191 (91%)	18 (9%)	0	100	100
All	All	839/890 (94%)	799 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	183/198 (92%)	183 (100%)	0	100	100
1	C	181/198 (91%)	180 (99%)	1 (1%)	86	85
2	B	186/189 (98%)	185 (100%)	1 (0%)	88	88
2	D	186/189 (98%)	184 (99%)	2 (1%)	73	71
All	All	736/774 (95%)	732 (100%)	4 (0%)	88	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	156	GLN
1	C	55	ASN
2	D	127	LYS
2	D	146	LYS

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

Mol	Chain	Res	Type
2	B	156	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	201:CYS	C	202:ASN	N	1.12
1	B	77:SER	C	78:VAL	N	1.05
1	C	119:ALA	C	120:SER	N	0.93

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	217/230 (94%)	-0.20	3 (1%) 75 82	29, 42, 74, 117	0
1	C	211/230 (91%)	-0.19	3 (1%) 75 82	28, 45, 92, 118	0
2	B	212/215 (98%)	-0.23	0 100 100	31, 50, 79, 88	0
2	D	211/215 (98%)	-0.12	2 (0%) 84 89	32, 56, 94, 113	0
All	All	851/890 (95%)	-0.19	8 (0%) 84 89	28, 48, 83, 118	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	SER	5.4
1	C	194	LEU	3.8
1	C	133	SER	3.5
2	D	95	PRO	3.0
1	A	133	SER	2.9
2	D	29	VAL	2.7
1	C	195	GLY	2.5
1	A	138	GLY	2.1

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.