



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 06:30 AM EDT

PDB ID : 7N08
Title : Crystal structure of the 3D6 antibody fragment bound to the HIV-1 gp41 immunodominant region
Authors : Cook, J.D.; Lee, J.E.
Deposited on : 2021-05-25
Resolution : 2.00 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35.1
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

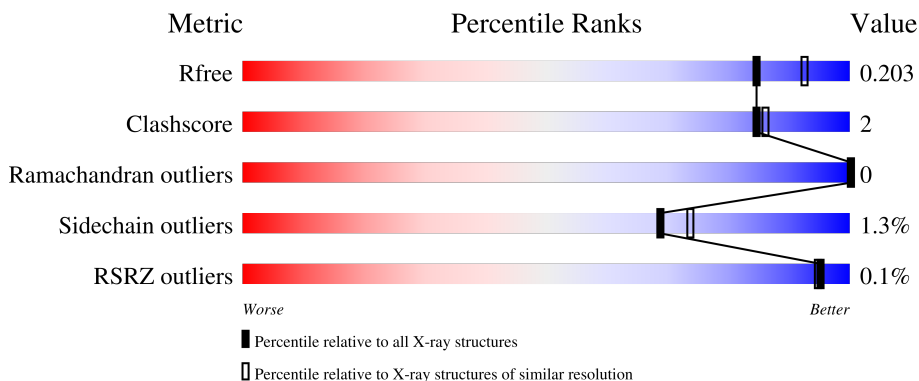
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-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.




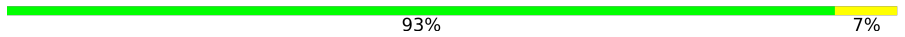
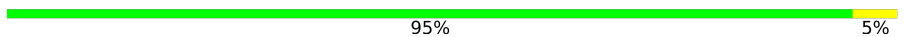

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 $\leq 5\%$. 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	E	15	 67% 7% 27%
1	F	15	 60% 13% 27%
1	G	15	 73% 27%
2	A	247	 91% 5% 5%
2	C	247	 90% 6% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	247	 92% .. 6%
3	B	212	 93% 7%
3	D	212	 95% 5%
3	L	212	 91% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21356 atoms, of which 9858 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 HIV-1 gp41 immunodominant region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	G	11	170	55	87	13	15	0	0	0
1	F	11	170	55	87	13	15	0	0	0
1	E	11	170	55	87	13	15	0	0	0

- Molecule 2 is a protein called Fab 3D6 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	233	3415	1096	1680	291	339	9	0	0	0
2	A	234	3403	1096	1667	289	342	9	0	1	0
2	C	232	3364	1084	1647	287	337	9	0	0	0

- Molecule 3 is a protein called Fab 3D6 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	212	3141	1008	1526	268	333	6	0	1	0
3	B	212	3163	1012	1546	270	329	6	0	1	0
3	D	212	3147	1010	1531	268	332	6	0	2	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	10	Total	O	0	0
			10	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	242	Total O 242 242	0	0
4	F	14	Total O 14 14	0	0
4	E	9	Total O 9 9	0	0
4	L	194	Total O 194 194	0	0
4	B	154	Total O 154 154	0	0
4	A	232	Total O 232 232	0	0
4	D	173	Total O 173 173	0	0
4	C	185	Total O 185 185	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: HIV-1 gp41 immunodominant region

Chain G:  73% 27%



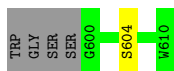
- Molecule 1: HIV-1 gp41 immunodominant region

Chain F:  60% 13% 27%



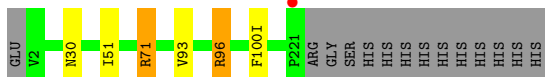
- Molecule 1: HIV-1 gp41 immunodominant region

Chain E:  67% 7% 27%



- Molecule 2: Fab 3D6 heavy chain

Chain H:  92% .. 6%




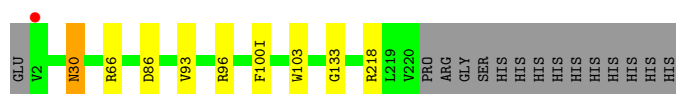
- Molecule 2: Fab 3D6 heavy chain

Chain A:  91% • 5%



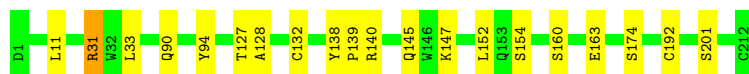
- Molecule 2: Fab 3D6 heavy chain

Chain C:  90% 6%



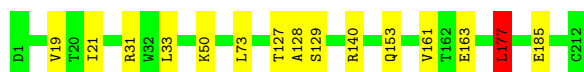
- Molecule 3: Fab 3D6 light chain

Chain L:  91% 9%



- Molecule 3: Fab 3D6 light chain

Chain B:  93% 7%



- Molecule 3: Fab 3D6 light chain

Chain D:  95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	77.83Å 77.83Å 218.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.49 – 2.00 42.49 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (42.49-2.00) 97.9 (42.49-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.00Å)	Xtrriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.165 , 0.203 0.167 , 0.203	Depositor DCC
R_{free} test set	2017 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.009 for -h,-k,l 0.049 for h,-h-k,-l 0.025 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21356	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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 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	E	0.67	0/85	0.62	0/115
1	F	0.65	0/85	0.72	0/115
1	G	0.54	0/85	0.54	0/115
2	A	0.58	0/1779	0.71	2/2424 (0.1%)
2	C	0.51	0/1759	0.67	2/2396 (0.1%)
2	H	0.56	0/1778	0.72	2/2420 (0.1%)
3	B	0.52	0/1656	0.67	1/2253 (0.0%)
3	D	0.57	1/1652 (0.1%)	0.70	0/2251
3	L	0.58	2/1651 (0.1%)	0.69	1/2249 (0.0%)
All	All	0.56	3/10530 (0.0%)	0.69	8/14338 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	192	CYS	CB-SG	-5.79	1.72	1.81
3	L	132	CYS	CB-SG	-5.67	1.72	1.81
3	L	192	CYS	CB-SG	-5.15	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	96	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	A	96	ARG	NE-CZ-NH2	-7.69	116.45	120.30
2	C	96	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	H	96	ARG	NE-CZ-NH1	6.43	123.51	120.30
2	C	96	ARG	NE-CZ-NH1	6.13	123.36	120.30
2	A	96	ARG	NE-CZ-NH1	6.08	123.34	120.30
3	B	177	LEU	CA-CB-CG	5.74	128.51	115.30
3	L	11	LEU	CA-CB-CG	5.61	128.20	115.30

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	E	83	87	87	0	0
1	F	83	87	87	1	0
1	G	83	87	87	0	0
2	A	1736	1667	1667	6	0
2	C	1717	1647	1647	9	0
2	H	1735	1680	1680	3	0
3	B	1617	1546	1548	13	0
3	D	1616	1531	1529	5	1
3	L	1615	1526	1525	12	1
4	A	232	0	0	3	1
4	B	154	0	0	8	0
4	C	185	0	0	4	0
4	D	173	0	0	1	2
4	E	9	0	0	0	0
4	F	14	0	0	1	0
4	G	10	0	0	0	0
4	H	242	0	0	1	1
4	L	194	0	0	6	0
All	All	11498	9858	9857	47	3

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.

All (47) 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)
3:L:174:SER:OG	4:L:301:HOH:O	1.90	0.88
2:C:218:ARG:NH2	4:C:301:HOH:O	1.95	0.86
2:A:221:PRO:O	4:A:302:HOH:O	1.97	0.82
3:B:185:GLU:OE2	4:B:301:HOH:O	1.98	0.80
3:B:163:GLU:OE2	4:B:302:HOH:O	2.10	0.69
2:C:133:GLY:O	4:C:303:HOH:O	2.11	0.69
3:B:19:VAL:HA	4:B:409:HOH:O	1.93	0.68
3:L:140:ARG:NE	4:L:302:HOH:O	2.13	0.68
2:A:66:ARG:NH2	2:A:86:ASP:OD2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:140:ARG:NE	4:B:304:HOH:O	2.27	0.64
3:D:127[A]:THR:OG1	4:D:301:HOH:O	1.91	0.63
3:L:163:GLU:OE2	4:L:303:HOH:O	2.16	0.63
3:L:31:ARG:NH2	4:L:304:HOH:O	2.22	0.60
2:A:82(A):ASN:ND2	4:A:301:HOH:O	1.89	0.60
3:L:160:SER:HB3	4:L:301:HOH:O	2.02	0.59
1:F:600:GLY:N	4:F:701:HOH:O	2.36	0.57
3:B:140:ARG:CD	4:B:304:HOH:O	2.53	0.57
3:L:140:ARG:CD	4:L:302:HOH:O	2.52	0.56
3:L:145:GLN:CD	3:L:152:LEU:HD22	2.29	0.53
2:C:66:ARG:NH2	2:C:86:ASP:OD2	2.38	0.53
3:B:140:ARG:HD3	4:B:304:HOH:O	2.14	0.48
3:B:50:LYS:NZ	4:B:305:HOH:O	2.29	0.47
2:C:93:VAL:CG1	2:C:100(I):PHE:HB3	2.45	0.47
2:A:96:ARG:HD3	4:A:422:HOH:O	2.14	0.47
3:D:43:VAL:CG1	2:C:103:TRP:HB2	2.45	0.47
3:B:21:ILE:HD11	3:B:73:LEU:HD23	1.97	0.47
3:L:145:GLN:CG	3:L:152:LEU:HD22	2.46	0.46
3:B:140:ARG:CZ	3:B:161:VAL:HG21	2.45	0.46
3:L:147:LYS:HG2	3:L:152:LEU:HD23	1.97	0.45
3:L:90:GLN:O	3:L:94:TYR:HA	2.17	0.44
2:H:51:ILE:HD13	2:H:71:ARG:HG2	2.00	0.44
3:L:127[A]:THR:HG22	3:L:128:ALA:N	2.33	0.43
3:L:138:TYR:CG	3:L:139:PRO:HA	2.54	0.43
3:D:43:VAL:HG11	2:C:103:TRP:HB2	2.02	0.42
2:C:30:ASN:HB2	4:C:360:HOH:O	2.18	0.42
2:C:93:VAL:HG11	2:C:100(I):PHE:HB3	2.01	0.42
2:H:96:ARG:HD3	4:H:395:HOH:O	2.19	0.42
2:C:66:ARG:HD3	4:C:390:HOH:O	2.19	0.42
3:B:129:SER:HA	3:B:177:LEU:O	2.20	0.41
3:B:140:ARG:NH2	3:B:161:VAL:HG21	2.35	0.41
3:D:184:TYR:HA	3:D:190:TYR:OH	2.19	0.41
3:B:127[B]:THR:HG22	3:B:128:ALA:N	2.36	0.41
3:D:127[B]:THR:HG22	3:D:128:ALA:N	2.36	0.40
2:A:220:VAL:O	2:A:220:VAL:HG13	2.21	0.40
3:B:153:GLN:OE1	4:B:303:HOH:O	2.21	0.40
2:H:93:VAL:CG1	2:H:100(I):PHE:HB3	2.52	0.40
2:A:93:VAL:CG1	2:A:100(I):PHE:HB3	2.51	0.40

All (3) 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)
3:L:201:SER:OG	3:D:1:ASP:OD2[1_565]	2.08	0.12
4:A:301:HOH:O	4:D:418:HOH:O[2_434]	2.10	0.10
4:H:342:HOH:O	4:D:396:HOH:O[1_665]	2.17	0.03

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	E	9/15 (60%)	9 (100%)	0	0	100	100
1	F	9/15 (60%)	9 (100%)	0	0	100	100
1	G	9/15 (60%)	9 (100%)	0	0	100	100
2	A	233/247 (94%)	229 (98%)	4 (2%)	0	100	100
2	C	230/247 (93%)	227 (99%)	3 (1%)	0	100	100
2	H	231/247 (94%)	225 (97%)	6 (3%)	0	100	100
3	B	211/212 (100%)	206 (98%)	5 (2%)	0	100	100
3	D	212/212 (100%)	207 (98%)	5 (2%)	0	100	100
3	L	211/212 (100%)	205 (97%)	6 (3%)	0	100	100
All	All	1355/1422 (95%)	1326 (98%)	29 (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	E	9/12 (75%)	8 (89%)	1 (11%)	6	3
1	F	9/12 (75%)	8 (89%)	1 (11%)	6	3
1	G	9/12 (75%)	9 (100%)	0	100	100
2	A	191/207 (92%)	190 (100%)	1 (0%)	88	92
2	C	188/207 (91%)	187 (100%)	1 (0%)	88	92
2	H	192/207 (93%)	190 (99%)	2 (1%)	76	81
3	B	183/188 (97%)	180 (98%)	3 (2%)	62	67
3	D	182/188 (97%)	179 (98%)	3 (2%)	62	67
3	L	182/188 (97%)	179 (98%)	3 (2%)	62	67
All	All	1145/1221 (94%)	1130 (99%)	15 (1%)	69	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	30	ASN
2	H	71	ARG
1	F	601	LYS
1	E	604	SER
3	L	31	ARG
3	L	33	LEU
3	L	154	SER
3	B	31	ARG
3	B	33	LEU
3	B	177	LEU
2	A	30	ASN
3	D	19	VAL
3	D	31	ARG
3	D	33	LEU
2	C	30	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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(Å ²)	Q<0.9
1	E	11/15 (73%)	-0.64	0 100 100	21, 23, 32, 49	0
1	F	11/15 (73%)	-0.36	0 100 100	19, 23, 33, 48	0
1	G	11/15 (73%)	-0.51	0 100 100	25, 27, 40, 47	0
2	A	234/247 (94%)	-0.50	0 100 100	16, 26, 41, 68	0
2	C	232/247 (93%)	-0.49	1 (0%) 92 92	19, 28, 47, 57	0
2	H	233/247 (94%)	-0.42	1 (0%) 92 92	17, 24, 38, 71	0
3	B	212/212 (100%)	-0.38	0 100 100	18, 32, 46, 64	0
3	D	212/212 (100%)	-0.48	0 100 100	18, 29, 47, 59	0
3	L	212/212 (100%)	-0.51	0 100 100	18, 28, 38, 64	0
All	All	1368/1422 (96%)	-0.47	2 (0%) 95 95	16, 27, 46, 71	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	221	PRO	2.5
2	C	2	VAL	2.0

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 monosaccharides 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.