



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:05 AM UTC

PDB ID : 7N08 / pdb_00007n08
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

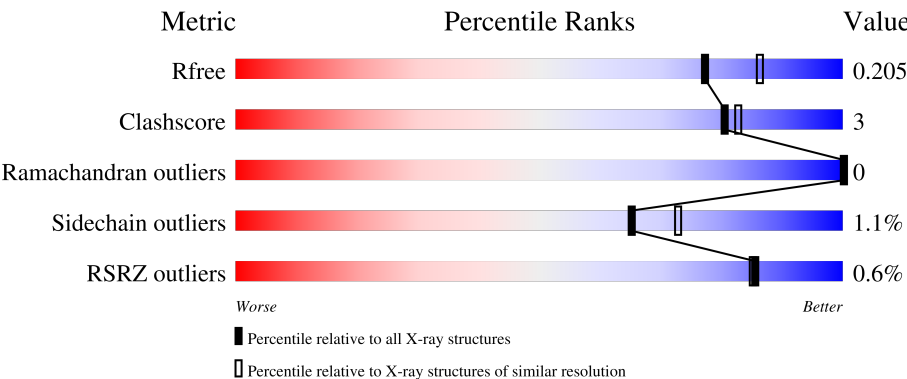
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	% 90% 5%
2	C	247	90% 6%

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Mol	Chain	Length	Quality of chain
2	H	247	% 91% 6%
3	B	212	93% 6%
3	D	212	96%
3	L	212	90% 10%

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
1	G	11	Total	C	H	N	O	0	0	0
			170	55	87	13	15			
1	F	11	Total	C	H	N	O	0	0	0
			170	55	87	13	15			
1	E	11	Total	C	H	N	O	0	0	0
			170	55	87	13	15			

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

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

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

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

- Molecule 4 is water.

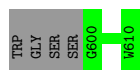
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	10	Total	O	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	242	Total 242	O 242	0	0
4	F	14	Total 14	O 14	0	0
4	E	9	Total 9	O 9	0	0
4	L	194	Total 194	O 194	0	0
4	B	154	Total 154	O 154	0	0
4	A	232	Total 232	O 232	0	0
4	D	173	Total 173	O 173	0	0
4	C	185	Total 185	O 185	0	0

- Molecule 1: HIV-1 gp41 immunodominant region



- TRP
GLY
SER
SER
G600
K601
W610

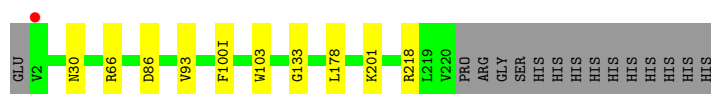
- TRP
GLY
SER
SER
G600
S604
W610

- [illegible]

-
- | Protein | Number of Mutations |
|---------|---------------------|
| E1 | 1 |
| V2 | 1 |
| K64 | 2 |
| G65 | 2 |
| R66 | 2 |
| N82A | 2 |
| D86 | 2 |
| V93 | 2 |
| R96 | 2 |
| F100I | 2 |
| G133 | 3 |
| K201 | 2 |
| V220 | 2 |
| P221 | 3 |

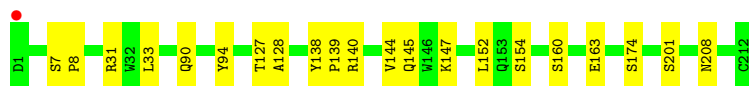
- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

Chain C:  90% • 6%

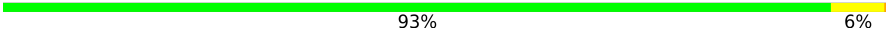


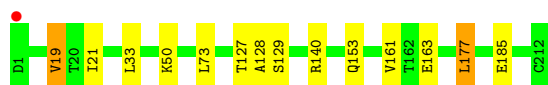
- Molecule 3: Fab 3D6 light chain

Chain L:  90% 10%

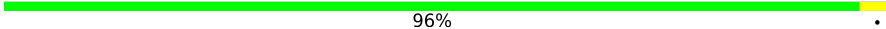


- Molecule 3: Fab 3D6 light chain

Chain B:  93% 6% •



- Molecule 3: Fab 3D6 light chain

Chain D:  96% •



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)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.165 , 0.203 0.169 , 0.205	Depositor DCC
R_{free} test set	2017 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -h,-k,l 0.049 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
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

Xtriage'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

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	E	0.54	0/85	0.59	0/115
1	F	0.56	0/85	0.64	0/115
1	G	0.46	0/85	0.54	0/115
2	A	0.57	2/1779 (0.1%)	0.63	0/2424
2	C	0.47	1/1759 (0.1%)	0.59	0/2396
2	H	0.51	0/1778	0.65	0/2420
3	B	0.46	0/1656	0.62	0/2253
3	D	0.54	0/1652	0.66	0/2251
3	L	0.54	1/1651 (0.1%)	0.65	0/2249
All	All	0.52	4/10530 (0.0%)	0.63	0/14338

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	VAL	N-CA	5.97	1.53	1.46
2	C	201	LYS	CA-C	5.51	1.59	1.52
2	A	201	LYS	CA-C	5.13	1.58	1.52
3	L	208	ASN	CG-OD1	5.04	1.33	1.23

There are no bond angle outliers.

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	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	8	0
2	C	1717	1647	1647	10	0
2	H	1735	1680	1680	4	0
3	B	1617	1546	1548	13	0
3	D	1616	1531	1529	6	1
3	L	1615	1526	1525	13	1
4	A	232	0	0	4	1
4	B	154	0	0	8	0
4	C	185	0	0	4	0
4	D	173	0	0	2	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	53	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 3.

All (53) 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
3:B:50:LYS:NZ	4:B:305:HOH:O	2.29	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:GLN:CD	3:L:152:LEU:HD22	2.29	0.58
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
2:C:66:ARG:NH2	2:C:86:ASP:OD2	2.38	0.53
2:H:20:LEU:HG	2:H:82:MET:HE2	1.94	0.49
3:B:140:ARG:HD3	4:B:304:HOH:O	2.14	0.48
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:D:205:LYS:NZ	4:D:302:HOH:O	2.30	0.46
2:A:66:ARG:HH22	2:A:86:ASP:CG	2.25	0.45
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
2:C:178:LEU:C	2:C:178:LEU:HD23	2.43	0.43
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
3:L:7:SER:HA	3:L:8:PRO:C	2.45	0.40
2:A:64:LYS:NZ	4:A:314:HOH:O	2.53	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%)	191 (100%)	0	100	100
2	C	188/207 (91%)	188 (100%)	0	100	100
2	H	192/207 (93%)	189 (98%)	3 (2%)	55	62
3	B	183/188 (97%)	180 (98%)	3 (2%)	55	62
3	D	182/188 (97%)	180 (99%)	2 (1%)	65	73
3	L	182/188 (97%)	179 (98%)	3 (2%)	55	62
All	All	1145/1221 (94%)	1132 (99%)	13 (1%)	65	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	71	ARG
2	H	85	GLU
2	H	135	THR
1	F	601	LYS
1	E	604	SER
3	L	33	LEU
3	L	144	VAL
3	L	154	SER
3	B	19	VAL
3	B	33	LEU
3	B	177	LEU
3	D	19	VAL
3	D	33	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	81	GLN
2	H	82(A)	ASN
2	H	192	GLN
3	L	136	ASN
3	L	145	GLN
3	L	158	GLN
3	B	92	ASN

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 oligosaccharides 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%)	-0.61	0 100 100	23, 26, 36, 52	0
1	F	11/15 (73%)	-0.65	0 100 100	21, 26, 39, 52	0
1	G	11/15 (73%)	-0.54	0 100 100	26, 30, 45, 50	0
2	A	234/247 (94%)	-0.62	2 (0%) 81 80	14, 29, 46, 77	1 (0%)
2	C	232/247 (93%)	-0.52	1 (0%) 88 88	21, 30, 52, 64	0
2	H	233/247 (94%)	-0.68	3 (1%) 75 74	18, 26, 45, 78	0
3	B	212/212 (100%)	-0.42	1 (0%) 87 87	20, 35, 51, 70	1 (0%)
3	D	212/212 (100%)	-0.48	0 100 100	18, 32, 51, 63	2 (0%)
3	L	212/212 (100%)	-0.58	1 (0%) 87 87	18, 31, 43, 70	1 (0%)
All	All	1368/1422 (96%)	-0.55	8 (0%) 85 85	14, 30, 50, 78	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	1	ASP	4.0
2	C	2	VAL	2.4
2	A	221	PRO	2.3
2	H	221	PRO	2.2
2	H	133	GLY	2.1
2	H	2	VAL	2.0
3	L	1	ASP	2.0
2	A	133	GLY	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 oligosaccharides 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.