



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 05:17 am GMT

PDB ID : 1RZI
Title : Crystal structure of human anti-HIV-1 gp120-reactive antibody 47e fab
Authors : Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.
Deposited on : 2003-12-24
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

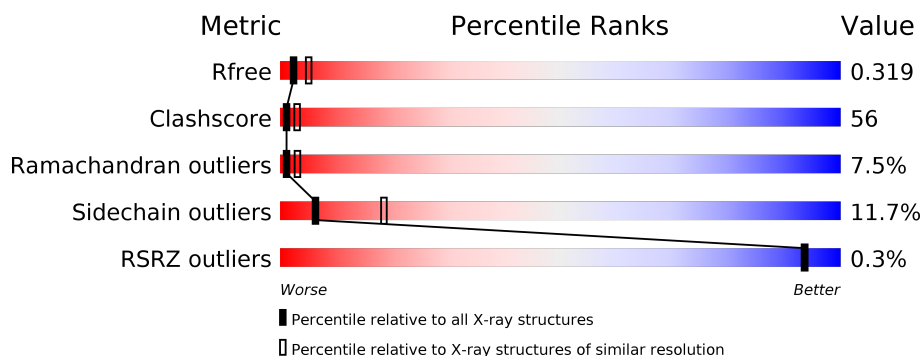
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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. 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	212	<div> <div>29%</div> <div>60%</div> <div>9%</div> <div>.</div> </div>
1	C	212	<div> <div>30%</div> <div>53%</div> <div>16%</div> <div>.</div> </div>
1	E	212	<div> <div>28%</div> <div>59%</div> <div>10%</div> <div>.</div> </div>
1	G	212	<div> <div>32%</div> <div>56%</div> <div>11%</div> <div>.</div> </div>
1	I	212	<div> <div>30%</div> <div>58%</div> <div>11%</div> <div>.</div> </div>
1	K	212	<div> <div>29%</div> <div>57%</div> <div>13%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	212	<div><div></div><div>34%53%11%</div><div></div></div>
1	O	212	<div><div></div><div>26%59%12%</div><div></div></div>
2	B	230	<div><div></div><div>25%56%10%</div><div></div></div>
2	D	230	<div><div></div><div>%32%55%6%6%</div><div></div></div>
2	F	230	<div><div></div><div>30%53%11%6%</div><div></div></div>
2	H	230	<div><div></div><div>22%58%13%6%</div><div></div></div>
2	J	230	<div><div></div><div>%29%52%13%6%</div><div></div></div>
2	L	230	<div><div></div><div>25%58%10%7%</div><div></div></div>
2	N	230	<div><div></div><div>38%48%8%6%</div><div></div></div>
2	P	230	<div><div></div><div>32%51%9%6%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25973 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 Fab 47e light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	C	212	Total	C	N	O	S	0	0	0
			1628	1016	273	334	5			
1	E	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	G	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	I	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	K	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	M	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			
1	O	211	Total	C	N	O	S	0	0	0
			1620	1012	272	331	5			

- Molecule 2 is a protein called Fab 47e heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	D	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	F	217	Total	C	N	O	S	0	0	0
			1586	998	265	316	7			
2	H	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	J	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	L	215	Total	C	N	O	S	0	0	0
			1572	990	262	313	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	P	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			

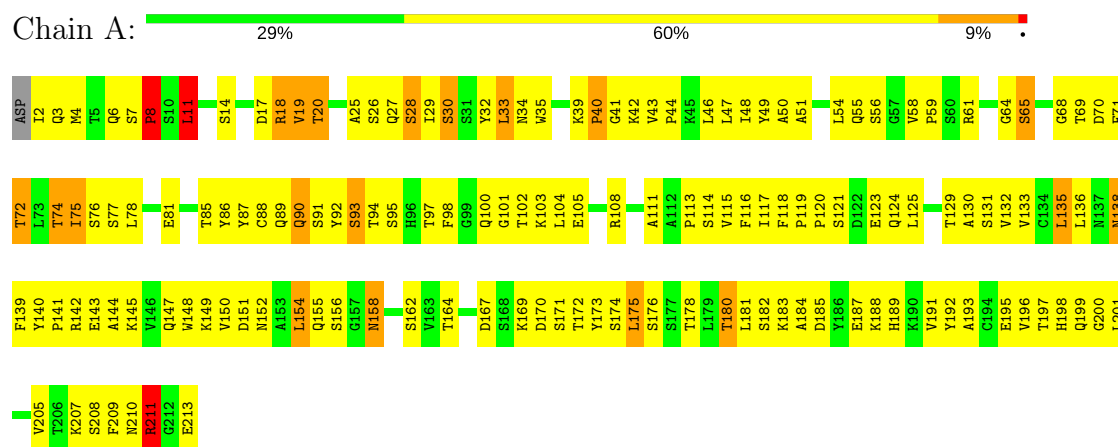
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	29	Total	O	0	0
			29	29		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		
3	E	26	Total	O	0	0
			26	26		
3	F	18	Total	O	0	0
			18	18		
3	G	23	Total	O	0	0
			23	23		
3	H	31	Total	O	0	0
			31	31		
3	I	21	Total	O	0	0
			21	21		
3	J	17	Total	O	0	0
			17	17		
3	K	21	Total	O	0	0
			21	21		
3	L	20	Total	O	0	0
			20	20		
3	M	23	Total	O	0	0
			23	23		
3	N	31	Total	O	0	0
			31	31		
3	O	22	Total	O	0	0
			22	22		
3	P	23	Total	O	0	0
			23	23		

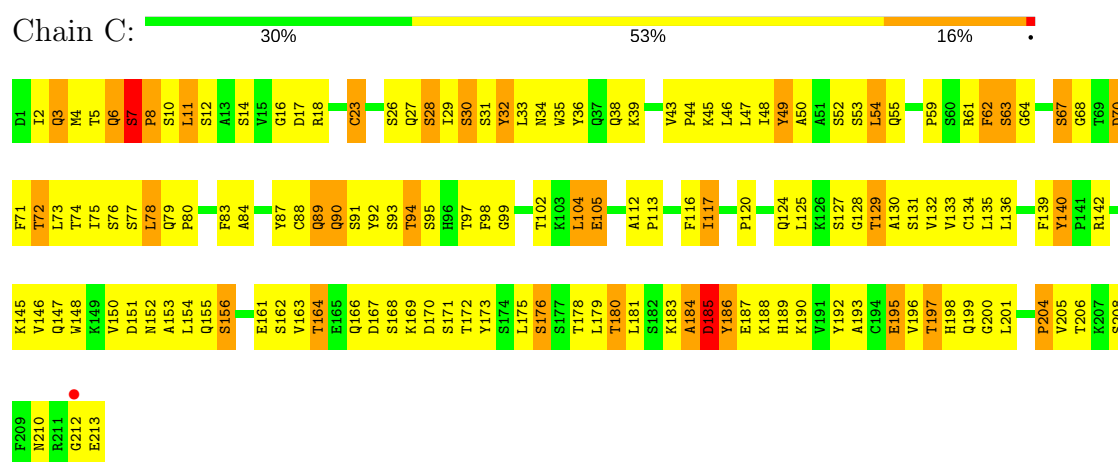
3 Residue-property plots

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.

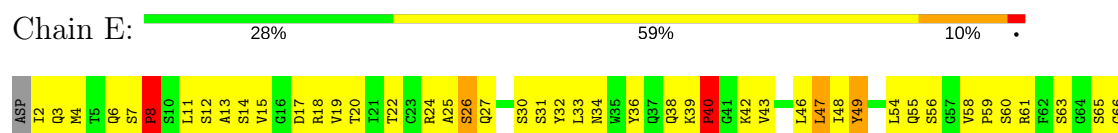
• Molecule 1: Fab 47e light chain

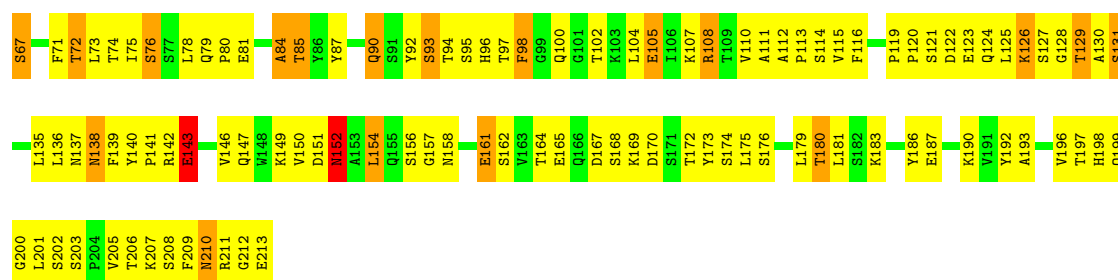


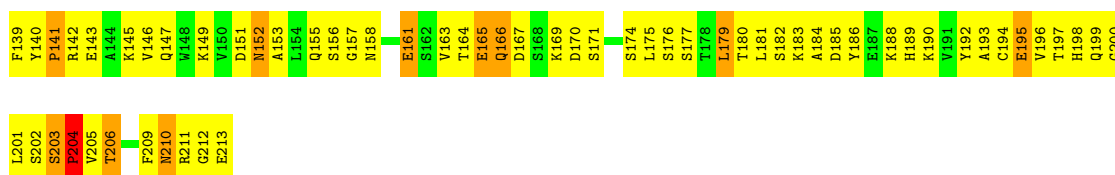
• Molecule 1: Fab 47e light chain



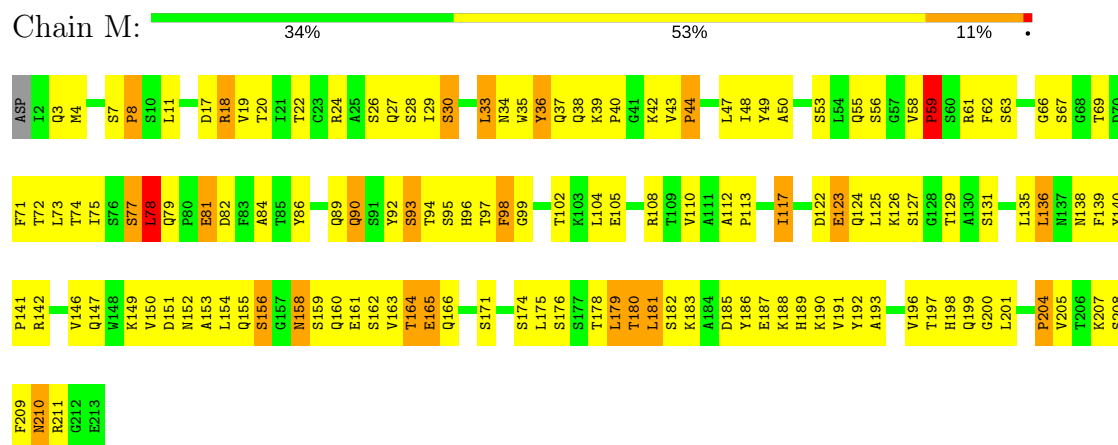
• Molecule 1: Fab 47e light chain



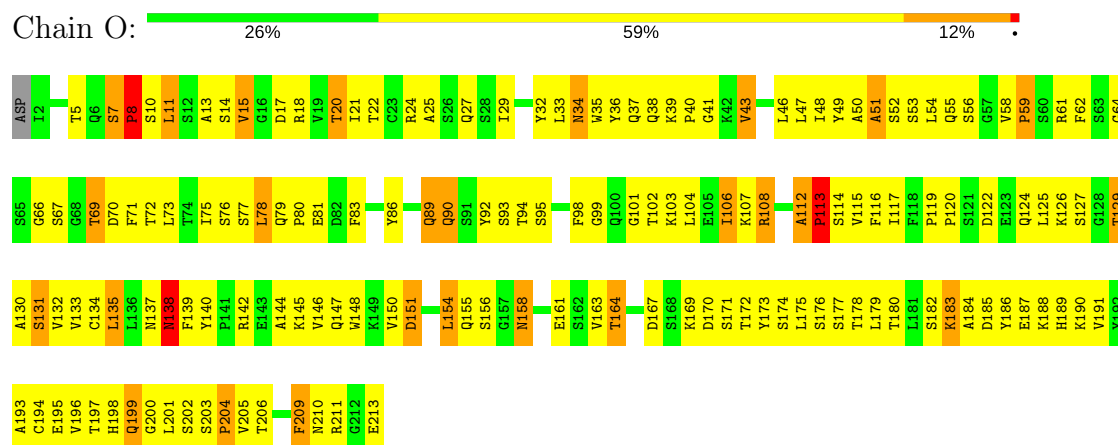




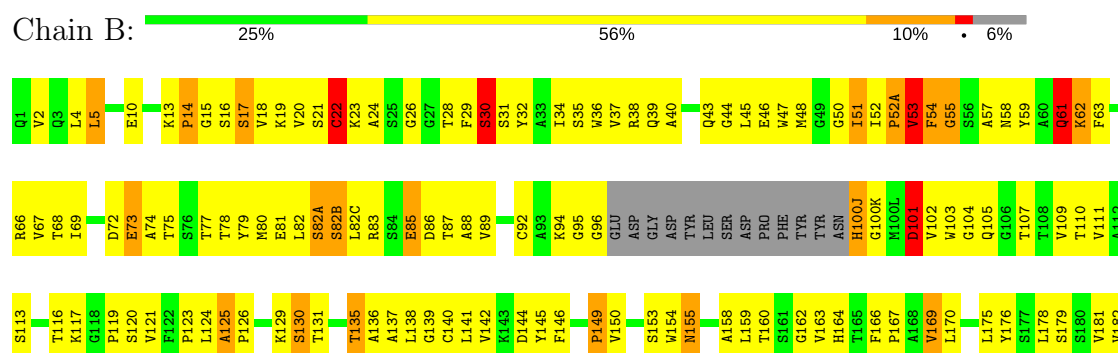
• Molecule 1: Fab 47e light chain



• Molecule 1: Fab 47e light chain



• Molecule 2: Fab 47e heavy chain



T183
V184
P185
S186
S187
S188
L189
G190
T191
Q192
T193
Y194
I195
C196
N197
V198
H199
H200
K201
P202
S203
N204
T205
K206
V207
D208
K209
K210
V211
E212
P213
LYS

• Molecule 2: Fab 47e heavy chain

Chain D: 

G1
V2
Q3
L4
L5
S187
S188
L189
G190
T191
Q192
T193
Y194
I195
C196
N197
V198
H199
H200
K201
P202
S203
N204
T205
K206
V207
D208
K209
K210
V211
E212
P213
LYS

V67
T70
A71
D72
E73
P119
A74
T75
S76
T77
T78
Y79
G80
E81
L82
S82A
S82B
L82C
R83
S84
E85
D86
T87
A88
V89
Y90
A93
K94
G95
S95
GLU
ASP
GLY
ASP
TYR
LEU
SER
ASP
PRO
PHE
TYR
ASN
H100J
I51
M100L
D101
V102
V103
G104
Q105
T107
T108
V109
T110
V111
A112
S113

A114
S115
T116
K117
G118
P119
S120
V121
P122
P123
P126
S127
S128
A129
T131
A137
L138
G139
D140
L141
D144
Y145
T151
V152
S153
W154
L159
T160
S161
G162
V163
H164
T165
P167
Q171
L175
Y176
S177
L178
S179
S180
V181
V182
T183
V184
P185
S188
L189
G190
T191

Q192
T193
Y194
I195
C196
N197
V198
K201
P202
S203
N204
T205
D208
K209
K210
V211
E212
P213
LYS

• Molecule 2: Fab 47e heavy chain

Chain F: 

Q1
V2
Q3
L4
L5
Q6
S7
V11
K12
K13
S16
S17
V18
K19
S20
C22
K23
A24
S25
G26
G27
T28
F29
S30
S31
Y32
A33
I34
S35
W36
V37
R38
Q39
A40
Q43
E46
V47
M48
Q49
G50
I51
I52
P52A
V53
F54
G55
S56
A57
N58
Y59
Q61
K62
F63
Q64

G55
R66
V67
T68
I69
T70
A71
S76
T77
T78
Y79
E81
S82A
S82B
L82C
R83
S84
E85
D86
T87
A88
V89
C92
A93
K94
G95
S95
GLU
ASP
GLY
ASP
TYR
LEU
SER
ASN
H100J
I51
M100L
D101
V102
V103
G104
Q105
T107
T108
V109
T110
V111
A112
S113

A114
S115
T116
K117
G118
P122
V121
P123
L124
A125
P126
S130
T131
T135
A136
A137
L138
G139
D140
L141
V142
K143
D144
F145
F146
P147
E148
G149
V150
T151
V152
S153
W154
M155
A158
L159
T160
V163
H164
P167
A168
Q171
S172
L175
Y176
S177
L178
S179
S180
V181
T183

V184
P185
S188
L189
G190
T193
C196
N197
V198
H200
K201
P202
T205
K210
V211
E212
P213
K214

• Molecule 2: Fab 47e heavy chain

Chain H: 

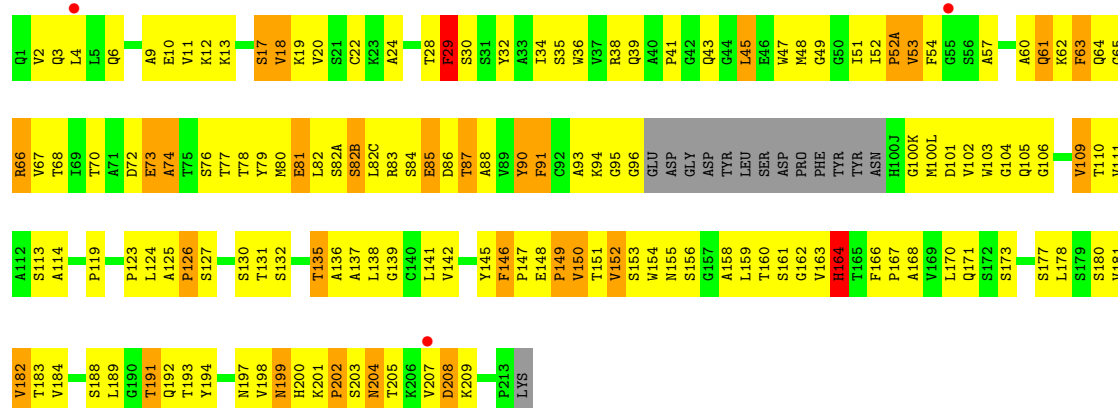
Q1
V2
Q3
L4
L5
Q6
S7
E10
V11
K12
K13
G15
S16
S17
V18
K19
V20
S21
C22
A24
S25
G26
G27
F29
V89
Y90
S91
Y92
A93
I94
S95
W96
Q99
Q43
V47
M48
P51
I52
P52A
V53
F54
G55
S56
A57
N58
Y59
Q61
K62
F63
Q64

G55
R66
V67
T68
I69
T70
A71
D72
E73
A74
T75
S76
T77
T78
M80
E81
L82
S82A
S82B
L82C
R83
S84
E85
D86
T87
A88
V89
F91
S91
Y92
A93
I94
S95
W96
Q99
GLU
ASP
GLY
ASP
TYR
LEU
SER
ASN
H100J
I51
M100L
D101
V102
V103
G104
Q105
T107
T108
V109
T110
V111

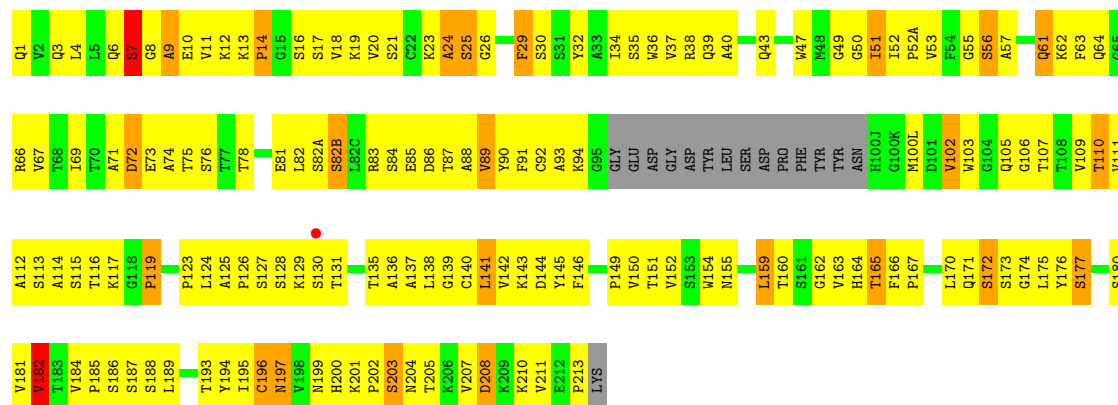
A112
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A114
S115
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K117
G118
P119
S120
V121
P122
P123
L124
S127
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S130
T131
G134
T135
A136
A137
L138
G139
D140
L141
V142
K143
D144
Y145
F146
P147
E148
G149
V150
T151
V152
S153
W154
M155
S156
L159
T160
S161
G162
V163
H164
T165
P166
P167
A168
V169
Q171
S172
S173
T174



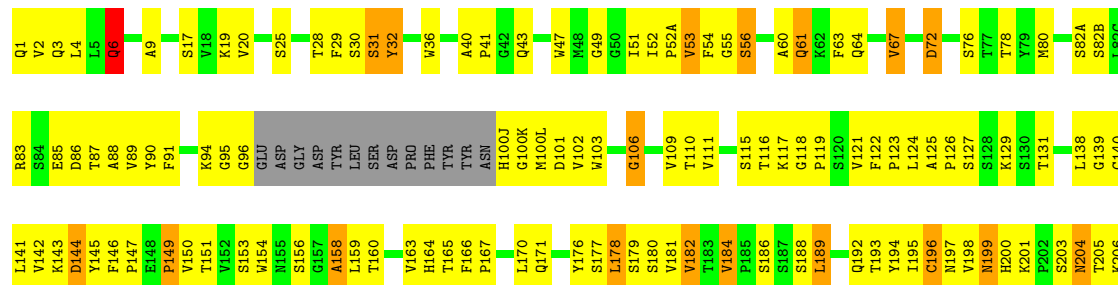
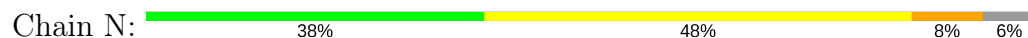
• Molecule 2: Fab 47e heavy chain



• Molecule 2: Fab 47e heavy chain



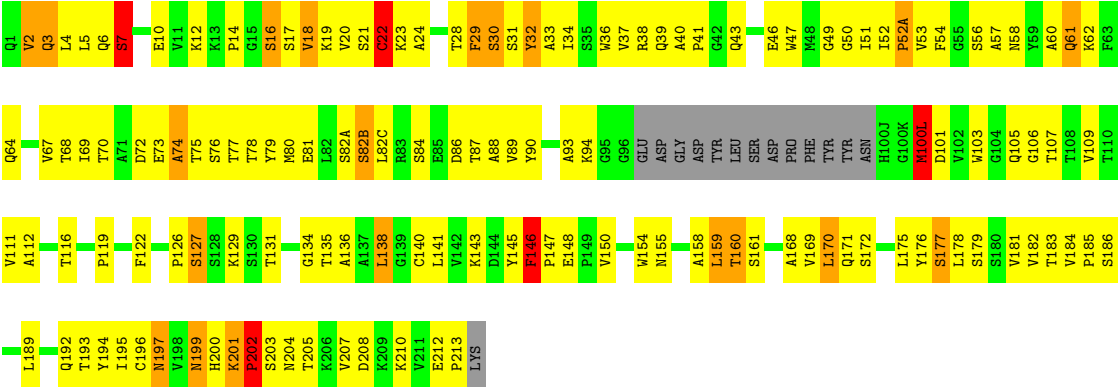
• Molecule 2: Fab 47e heavy chain





● Molecule 2: Fab 47e heavy chain

Chain P: 32% 51% 9% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.43Å 111.64Å 133.31Å 85.48° 90.00° 89.71°	Depositor
Resolution (Å)	20.00 – 2.90 19.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.90) 68.9 (19.88-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.321 0.232 , 0.319	Depositor DCC
R_{free} test set	7671 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.299 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25973	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% 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	0.62	1/1654 (0.1%)	1.01	5/2244 (0.2%)
1	C	0.54	2/1662 (0.1%)	0.97	7/2255 (0.3%)
1	E	0.52	1/1654 (0.1%)	0.94	8/2244 (0.4%)
1	G	0.51	1/1654 (0.1%)	0.93	4/2244 (0.2%)
1	I	0.60	3/1654 (0.2%)	0.90	8/2244 (0.4%)
1	K	0.56	2/1654 (0.1%)	0.93	4/2244 (0.2%)
1	M	0.55	0/1654	0.97	3/2244 (0.1%)
1	O	0.58	0/1654	0.99	10/2244 (0.4%)
2	B	0.45	0/1611	0.73	0/2192
2	D	0.47	0/1611	0.72	0/2192
2	F	0.44	0/1621	0.73	0/2203
2	H	0.42	0/1611	0.70	0/2192
2	J	0.44	0/1611	0.70	0/2192
2	L	0.45	0/1607	0.71	0/2187
2	N	0.46	0/1611	0.74	0/2192
2	P	0.46	0/1611	0.72	0/2192
All	All	0.51	10/26134 (0.0%)	0.85	49/35505 (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	C	0	1
1	K	0	1
All	All	0	2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	7	SER	C-N	8.01	1.49	1.34
1	K	7	SER	C-N	6.78	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	SER	C-N	6.56	1.46	1.34
1	K	10	SER	N-CA	6.17	1.58	1.46
1	I	7	SER	CA-C	5.69	1.67	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	7	SER	C-N-CD	-21.67	72.93	120.60
1	G	7	SER	C-N-CD	-19.01	78.78	120.60
1	O	7	SER	C-N-CD	-18.75	79.34	120.60
1	C	7	SER	C-N-CD	-18.65	79.58	120.60
1	K	7	SER	C-N-CD	-18.12	80.74	120.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	TYR	Sidechain
1	K	49	TYR	Sidechain

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	1620	0	1575	198	0
1	C	1628	0	1582	169	0
1	E	1620	0	1575	167	0
1	G	1620	0	1575	202	0
1	I	1620	0	1575	186	0
1	K	1620	0	1575	205	0
1	M	1620	0	1575	165	0
1	O	1620	0	1575	165	0
2	B	1576	0	1554	203	0
2	D	1576	0	1554	167	0
2	F	1586	0	1567	209	0
2	H	1576	0	1554	239	0
2	J	1576	0	1554	206	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1572	0	1551	209	0
2	N	1576	0	1554	139	0
2	P	1576	0	1554	172	0
3	A	34	0	0	4	0
3	B	29	0	0	3	0
3	C	25	0	0	6	0
3	D	27	0	0	0	0
3	E	26	0	0	2	0
3	F	18	0	0	2	0
3	G	23	0	0	3	0
3	H	31	0	0	2	0
3	I	21	0	0	2	0
3	J	17	0	0	2	0
3	K	21	0	0	3	0
3	L	20	0	0	3	0
3	M	23	0	0	4	0
3	N	31	0	0	2	0
3	O	22	0	0	1	0
3	P	23	0	0	0	0
All	All	25973	0	25049	2857	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 56.

The worst 5 of 2857 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:11:LEU:CD2	1:A:104:LEU:HD22	1.56	1.32
1:A:11:LEU:CD2	1:A:104:LEU:CD2	2.20	1.18
2:J:2:VAL:HG21	2:J:94:LYS:HZ3	1.09	1.15
1:E:199:GLN:HA	1:I:199:GLN:HE22	1.12	1.15
2:H:150:VAL:HG22	2:H:151:THR:H	1.11	1.14

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	209/212 (99%)	170 (81%)	29 (14%)	10 (5%)	2	10
1	C	210/212 (99%)	171 (81%)	24 (11%)	15 (7%)	1	3
1	E	209/212 (99%)	168 (80%)	32 (15%)	9 (4%)	3	12
1	G	209/212 (99%)	167 (80%)	28 (13%)	14 (7%)	1	4
1	I	209/212 (99%)	160 (77%)	39 (19%)	10 (5%)	2	10
1	K	209/212 (99%)	160 (77%)	37 (18%)	12 (6%)	2	6
1	M	209/212 (99%)	166 (79%)	32 (15%)	11 (5%)	2	7
1	O	209/212 (99%)	164 (78%)	34 (16%)	11 (5%)	2	7
2	B	212/230 (92%)	153 (72%)	40 (19%)	19 (9%)	1	2
2	D	212/230 (92%)	152 (72%)	44 (21%)	16 (8%)	1	3
2	F	213/230 (93%)	153 (72%)	42 (20%)	18 (8%)	1	2
2	H	212/230 (92%)	146 (69%)	42 (20%)	24 (11%)	0	1
2	J	212/230 (92%)	151 (71%)	40 (19%)	21 (10%)	1	1
2	L	211/230 (92%)	152 (72%)	39 (18%)	20 (10%)	1	1
2	N	212/230 (92%)	164 (77%)	30 (14%)	18 (8%)	1	2
2	P	212/230 (92%)	152 (72%)	37 (18%)	23 (11%)	0	1
All	All	3369/3536 (95%)	2549 (76%)	569 (17%)	251 (8%)	1	3

5 of 251 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	211	ARG
2	B	22	CYS
2	B	30	SER
2	B	61	GLN

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	187/188 (100%)	159 (85%)	28 (15%)	3	10
1	C	188/188 (100%)	162 (86%)	26 (14%)	4	12
1	E	187/188 (100%)	161 (86%)	26 (14%)	4	12
1	G	187/188 (100%)	168 (90%)	19 (10%)	8	26
1	I	187/188 (100%)	166 (89%)	21 (11%)	7	21
1	K	187/188 (100%)	165 (88%)	22 (12%)	6	18
1	M	187/188 (100%)	163 (87%)	24 (13%)	5	15
1	O	187/188 (100%)	157 (84%)	30 (16%)	3	8
2	B	176/189 (93%)	153 (87%)	23 (13%)	5	14
2	D	176/189 (93%)	164 (93%)	12 (7%)	18	47
2	F	177/189 (94%)	160 (90%)	17 (10%)	10	29
2	H	176/189 (93%)	158 (90%)	18 (10%)	8	26
2	J	176/189 (93%)	158 (90%)	18 (10%)	8	26
2	L	176/189 (93%)	158 (90%)	18 (10%)	8	26
2	N	176/189 (93%)	160 (91%)	16 (9%)	11	32
2	P	176/189 (93%)	153 (87%)	23 (13%)	5	14
All	All	2906/3016 (96%)	2565 (88%)	341 (12%)	6	18

5 of 341 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	54	PHE
2	J	17	SER
1	O	199	GLN
2	H	70	THR
1	I	43	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	210	ASN
1	I	89	GLN
1	O	137	ASN
2	H	1	GLN
2	H	164	HIS

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](#)

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, 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	211/212 (99%)	-0.45	0 100 100	27, 49, 72, 79	0
1	C	212/212 (100%)	-0.51	1 (0%) 90 90	24, 45, 68, 75	0
1	E	211/212 (99%)	-0.52	0 100 100	30, 49, 65, 76	0
1	G	211/212 (99%)	-0.40	0 100 100	33, 53, 86, 100	0
1	I	211/212 (99%)	-0.49	0 100 100	31, 50, 71, 82	0
1	K	211/212 (99%)	-0.51	0 100 100	36, 52, 66, 76	0
1	M	211/212 (99%)	-0.55	0 100 100	24, 45, 59, 75	0
1	O	211/212 (99%)	-0.53	0 100 100	25, 44, 61, 67	0
2	B	216/230 (93%)	-0.40	0 100 100	32, 58, 81, 89	0
2	D	216/230 (93%)	-0.28	3 (1%) 75 74	27, 58, 87, 99	0
2	F	217/230 (94%)	-0.31	1 (0%) 90 90	28, 64, 93, 105	0
2	H	216/230 (93%)	-0.17	1 (0%) 90 90	39, 71, 96, 99	0
2	J	216/230 (93%)	-0.36	3 (1%) 75 74	39, 65, 91, 96	0
2	L	215/230 (93%)	-0.32	1 (0%) 90 90	37, 63, 82, 100	0
2	N	216/230 (93%)	-0.43	0 100 100	29, 54, 75, 87	0
2	P	216/230 (93%)	-0.41	0 100 100	28, 52, 86, 92	0
All	All	3417/3536 (96%)	-0.41	10 (0%) 93 93	24, 53, 84, 105	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	130	SER	3.7
2	D	128	SER	2.9
2	J	55	GLY	2.8
2	D	24	ALA	2.5
2	H	203	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 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.