wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 04:33 AM EDT

PDB ID	:	6NIU
Title	:	Crystal structure of a human anti-ZIKV-DENV neutralizing antibody MZ4 in complex with ZIKV E glycoprotein
Authors	:	Sankhala, R.S.; Dussupt, V.; Donofrio, G.; Choe, M.; Modjarrad, K.; Michael, N.L.; Krebs, S.J.; Joyce, M.G.
Deposited on	:	2018-12-31
Resolution	:	4.30 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

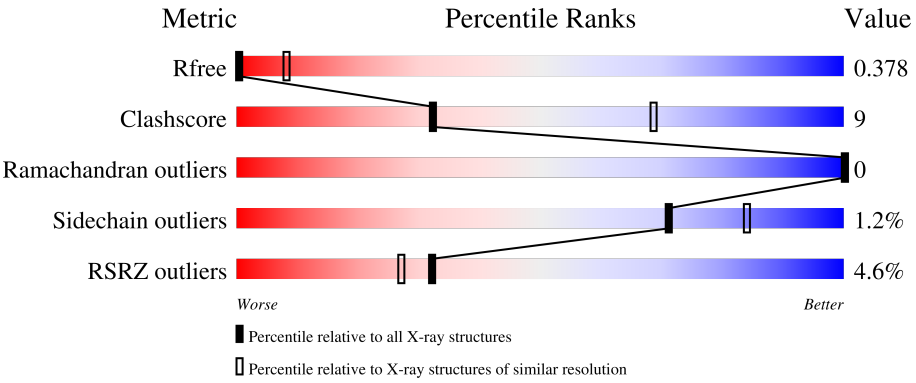
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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 <=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	F	120	6% 72% 28%
1	H	120	5% 74% 25%
1	I	120	3% 68% 31%
1	M	120	5% 69% 29%
2	G	111	5% 79% 21%

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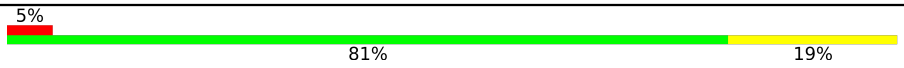
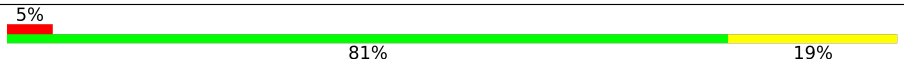
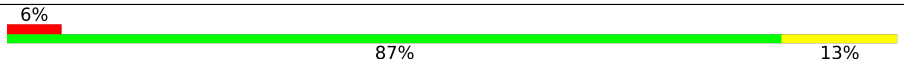
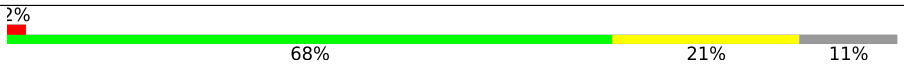
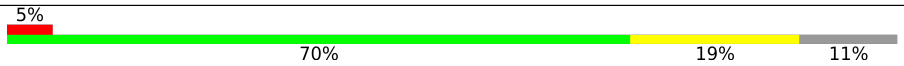
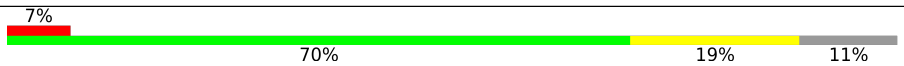
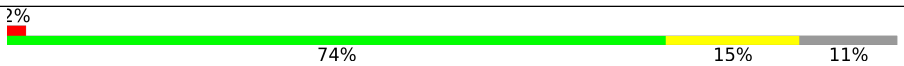
Mol	Chain	Length	Quality of chain
2	J	111	
2	L	111	
2	N	111	
3	A	447	
3	B	447	
3	E	447	
3	Z	447	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 19232 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 Human MZ4 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	F	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	I	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			
1	M	120	Total	C	N	O	S	0	0	0
			930	584	157	185	4			

- Molecule 2 is a protein called Human MZ4 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	G	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	J	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			
2	N	111	Total	C	N	O	S	0	0	0
			825	513	145	165	2			

- Molecule 3 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			
3	A	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			
3	Z	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			
3	E	399	Total	C	N	O	S	0	0	0
			3053	1907	534	586	26			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	406	GLY	-	expression tag	UNP A0A024B7W1
B	407	PRO	-	expression tag	UNP A0A024B7W1
B	408	LEU	-	expression tag	UNP A0A024B7W1
B	409	GLU	-	expression tag	UNP A0A024B7W1
B	410	VAL	-	expression tag	UNP A0A024B7W1
B	411	LEU	-	expression tag	UNP A0A024B7W1
B	412	PHE	-	expression tag	UNP A0A024B7W1
B	413	GLN	-	expression tag	UNP A0A024B7W1
B	414	GLY	-	expression tag	UNP A0A024B7W1
B	415	PRO	-	expression tag	UNP A0A024B7W1
B	416	GLY	-	expression tag	UNP A0A024B7W1
B	417	SER	-	expression tag	UNP A0A024B7W1
B	418	ALA	-	expression tag	UNP A0A024B7W1
B	419	TRP	-	expression tag	UNP A0A024B7W1
B	420	SER	-	expression tag	UNP A0A024B7W1
B	421	HIS	-	expression tag	UNP A0A024B7W1
B	422	PRO	-	expression tag	UNP A0A024B7W1
B	423	GLN	-	expression tag	UNP A0A024B7W1
B	424	PHE	-	expression tag	UNP A0A024B7W1
B	425	GLU	-	expression tag	UNP A0A024B7W1
B	426	LYS	-	expression tag	UNP A0A024B7W1
B	427	GLY	-	expression tag	UNP A0A024B7W1
B	428	GLY	-	expression tag	UNP A0A024B7W1
B	429	GLY	-	expression tag	UNP A0A024B7W1
B	430	SER	-	expression tag	UNP A0A024B7W1
B	431	GLY	-	expression tag	UNP A0A024B7W1
B	432	GLY	-	expression tag	UNP A0A024B7W1
B	433	GLY	-	expression tag	UNP A0A024B7W1
B	434	SER	-	expression tag	UNP A0A024B7W1
B	435	GLY	-	expression tag	UNP A0A024B7W1
B	436	GLY	-	expression tag	UNP A0A024B7W1
B	437	GLY	-	expression tag	UNP A0A024B7W1
B	438	SER	-	expression tag	UNP A0A024B7W1
B	439	ALA	-	expression tag	UNP A0A024B7W1
B	440	TRP	-	expression tag	UNP A0A024B7W1
B	441	SER	-	expression tag	UNP A0A024B7W1
B	442	HIS	-	expression tag	UNP A0A024B7W1
B	443	PRO	-	expression tag	UNP A0A024B7W1
B	444	GLN	-	expression tag	UNP A0A024B7W1
B	445	PHE	-	expression tag	UNP A0A024B7W1
B	446	GLU	-	expression tag	UNP A0A024B7W1
B	447	LYS	-	expression tag	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLY	-	expression tag	UNP A0A024B7W1
A	407	PRO	-	expression tag	UNP A0A024B7W1
A	408	LEU	-	expression tag	UNP A0A024B7W1
A	409	GLU	-	expression tag	UNP A0A024B7W1
A	410	VAL	-	expression tag	UNP A0A024B7W1
A	411	LEU	-	expression tag	UNP A0A024B7W1
A	412	PHE	-	expression tag	UNP A0A024B7W1
A	413	GLN	-	expression tag	UNP A0A024B7W1
A	414	GLY	-	expression tag	UNP A0A024B7W1
A	415	PRO	-	expression tag	UNP A0A024B7W1
A	416	GLY	-	expression tag	UNP A0A024B7W1
A	417	SER	-	expression tag	UNP A0A024B7W1
A	418	ALA	-	expression tag	UNP A0A024B7W1
A	419	TRP	-	expression tag	UNP A0A024B7W1
A	420	SER	-	expression tag	UNP A0A024B7W1
A	421	HIS	-	expression tag	UNP A0A024B7W1
A	422	PRO	-	expression tag	UNP A0A024B7W1
A	423	GLN	-	expression tag	UNP A0A024B7W1
A	424	PHE	-	expression tag	UNP A0A024B7W1
A	425	GLU	-	expression tag	UNP A0A024B7W1
A	426	LYS	-	expression tag	UNP A0A024B7W1
A	427	GLY	-	expression tag	UNP A0A024B7W1
A	428	GLY	-	expression tag	UNP A0A024B7W1
A	429	GLY	-	expression tag	UNP A0A024B7W1
A	430	SER	-	expression tag	UNP A0A024B7W1
A	431	GLY	-	expression tag	UNP A0A024B7W1
A	432	GLY	-	expression tag	UNP A0A024B7W1
A	433	GLY	-	expression tag	UNP A0A024B7W1
A	434	SER	-	expression tag	UNP A0A024B7W1
A	435	GLY	-	expression tag	UNP A0A024B7W1
A	436	GLY	-	expression tag	UNP A0A024B7W1
A	437	GLY	-	expression tag	UNP A0A024B7W1
A	438	SER	-	expression tag	UNP A0A024B7W1
A	439	ALA	-	expression tag	UNP A0A024B7W1
A	440	TRP	-	expression tag	UNP A0A024B7W1
A	441	SER	-	expression tag	UNP A0A024B7W1
A	442	HIS	-	expression tag	UNP A0A024B7W1
A	443	PRO	-	expression tag	UNP A0A024B7W1
A	444	GLN	-	expression tag	UNP A0A024B7W1
A	445	PHE	-	expression tag	UNP A0A024B7W1
A	446	GLU	-	expression tag	UNP A0A024B7W1
A	447	LYS	-	expression tag	UNP A0A024B7W1

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Chain	Residue	Modelled	Actual	Comment	Reference
Z	406	GLY	-	expression tag	UNP A0A024B7W1
Z	407	PRO	-	expression tag	UNP A0A024B7W1
Z	408	LEU	-	expression tag	UNP A0A024B7W1
Z	409	GLU	-	expression tag	UNP A0A024B7W1
Z	410	VAL	-	expression tag	UNP A0A024B7W1
Z	411	LEU	-	expression tag	UNP A0A024B7W1
Z	412	PHE	-	expression tag	UNP A0A024B7W1
Z	413	GLN	-	expression tag	UNP A0A024B7W1
Z	414	GLY	-	expression tag	UNP A0A024B7W1
Z	415	PRO	-	expression tag	UNP A0A024B7W1
Z	416	GLY	-	expression tag	UNP A0A024B7W1
Z	417	SER	-	expression tag	UNP A0A024B7W1
Z	418	ALA	-	expression tag	UNP A0A024B7W1
Z	419	TRP	-	expression tag	UNP A0A024B7W1
Z	420	SER	-	expression tag	UNP A0A024B7W1
Z	421	HIS	-	expression tag	UNP A0A024B7W1
Z	422	PRO	-	expression tag	UNP A0A024B7W1
Z	423	GLN	-	expression tag	UNP A0A024B7W1
Z	424	PHE	-	expression tag	UNP A0A024B7W1
Z	425	GLU	-	expression tag	UNP A0A024B7W1
Z	426	LYS	-	expression tag	UNP A0A024B7W1
Z	427	GLY	-	expression tag	UNP A0A024B7W1
Z	428	GLY	-	expression tag	UNP A0A024B7W1
Z	429	GLY	-	expression tag	UNP A0A024B7W1
Z	430	SER	-	expression tag	UNP A0A024B7W1
Z	431	GLY	-	expression tag	UNP A0A024B7W1
Z	432	GLY	-	expression tag	UNP A0A024B7W1
Z	433	GLY	-	expression tag	UNP A0A024B7W1
Z	434	SER	-	expression tag	UNP A0A024B7W1
Z	435	GLY	-	expression tag	UNP A0A024B7W1
Z	436	GLY	-	expression tag	UNP A0A024B7W1
Z	437	GLY	-	expression tag	UNP A0A024B7W1
Z	438	SER	-	expression tag	UNP A0A024B7W1
Z	439	ALA	-	expression tag	UNP A0A024B7W1
Z	440	TRP	-	expression tag	UNP A0A024B7W1
Z	441	SER	-	expression tag	UNP A0A024B7W1
Z	442	HIS	-	expression tag	UNP A0A024B7W1
Z	443	PRO	-	expression tag	UNP A0A024B7W1
Z	444	GLN	-	expression tag	UNP A0A024B7W1
Z	445	PHE	-	expression tag	UNP A0A024B7W1
Z	446	GLU	-	expression tag	UNP A0A024B7W1
Z	447	LYS	-	expression tag	UNP A0A024B7W1

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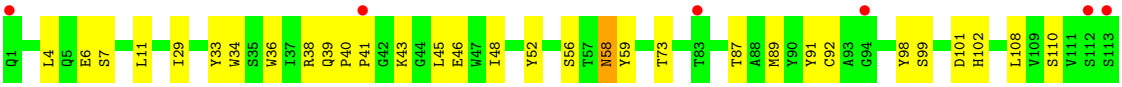
Chain	Residue	Modelled	Actual	Comment	Reference
E	406	GLY	-	expression tag	UNP A0A024B7W1
E	407	PRO	-	expression tag	UNP A0A024B7W1
E	408	LEU	-	expression tag	UNP A0A024B7W1
E	409	GLU	-	expression tag	UNP A0A024B7W1
E	410	VAL	-	expression tag	UNP A0A024B7W1
E	411	LEU	-	expression tag	UNP A0A024B7W1
E	412	PHE	-	expression tag	UNP A0A024B7W1
E	413	GLN	-	expression tag	UNP A0A024B7W1
E	414	GLY	-	expression tag	UNP A0A024B7W1
E	415	PRO	-	expression tag	UNP A0A024B7W1
E	416	GLY	-	expression tag	UNP A0A024B7W1
E	417	SER	-	expression tag	UNP A0A024B7W1
E	418	ALA	-	expression tag	UNP A0A024B7W1
E	419	TRP	-	expression tag	UNP A0A024B7W1
E	420	SER	-	expression tag	UNP A0A024B7W1
E	421	HIS	-	expression tag	UNP A0A024B7W1
E	422	PRO	-	expression tag	UNP A0A024B7W1
E	423	GLN	-	expression tag	UNP A0A024B7W1
E	424	PHE	-	expression tag	UNP A0A024B7W1
E	425	GLU	-	expression tag	UNP A0A024B7W1
E	426	LYS	-	expression tag	UNP A0A024B7W1
E	427	GLY	-	expression tag	UNP A0A024B7W1
E	428	GLY	-	expression tag	UNP A0A024B7W1
E	429	GLY	-	expression tag	UNP A0A024B7W1
E	430	SER	-	expression tag	UNP A0A024B7W1
E	431	GLY	-	expression tag	UNP A0A024B7W1
E	432	GLY	-	expression tag	UNP A0A024B7W1
E	433	GLY	-	expression tag	UNP A0A024B7W1
E	434	SER	-	expression tag	UNP A0A024B7W1
E	435	GLY	-	expression tag	UNP A0A024B7W1
E	436	GLY	-	expression tag	UNP A0A024B7W1
E	437	GLY	-	expression tag	UNP A0A024B7W1
E	438	SER	-	expression tag	UNP A0A024B7W1
E	439	ALA	-	expression tag	UNP A0A024B7W1
E	440	TRP	-	expression tag	UNP A0A024B7W1
E	441	SER	-	expression tag	UNP A0A024B7W1
E	442	HIS	-	expression tag	UNP A0A024B7W1
E	443	PRO	-	expression tag	UNP A0A024B7W1
E	444	GLN	-	expression tag	UNP A0A024B7W1
E	445	PHE	-	expression tag	UNP A0A024B7W1
E	446	GLU	-	expression tag	UNP A0A024B7W1
E	447	LYS	-	expression tag	UNP A0A024B7W1

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.

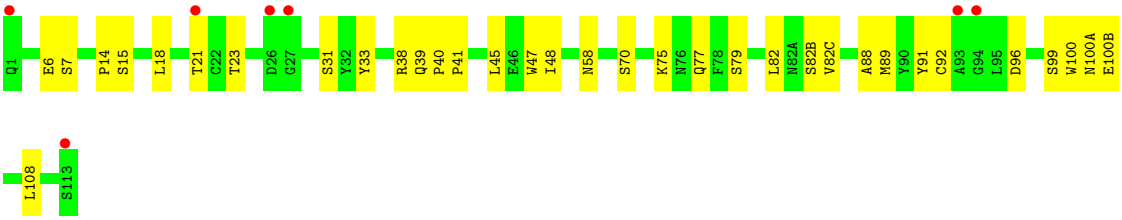
• Molecule 1: Human MZ4 Fab heavy chain

Chain H:



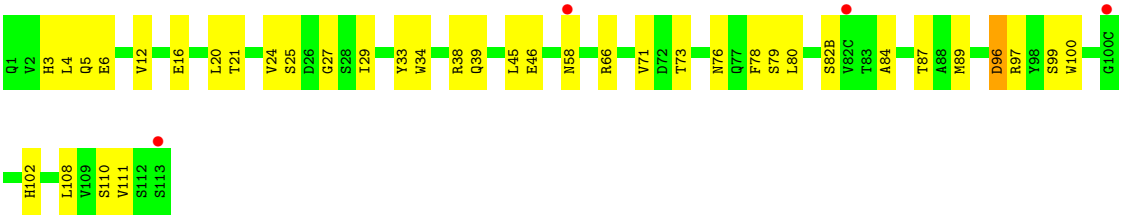
• Molecule 1: Human MZ4 Fab heavy chain

Chain F:



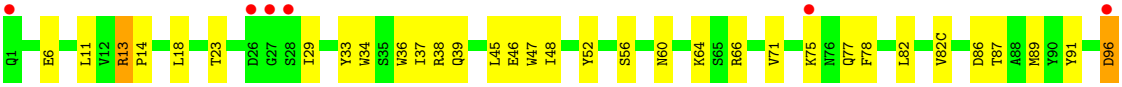
• Molecule 1: Human MZ4 Fab heavy chain

Chain I:



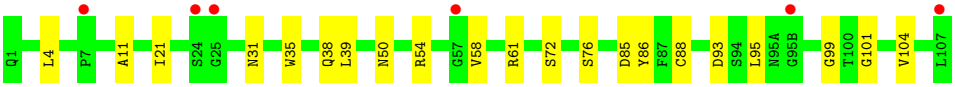
• Molecule 1: Human MZ4 Fab heavy chain

Chain M:



• Molecule 2: Human MZ4 Fab light chain

Chain L:

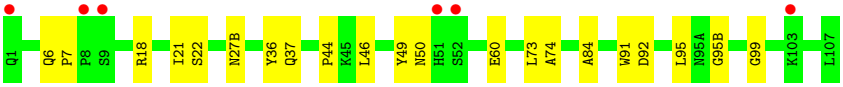


• Molecule 2: Human MZ4 Fab light chain

Chain G:

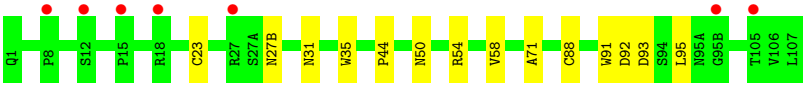
• Molecule 2: Human MZ4 Fab light chain

Chain J:



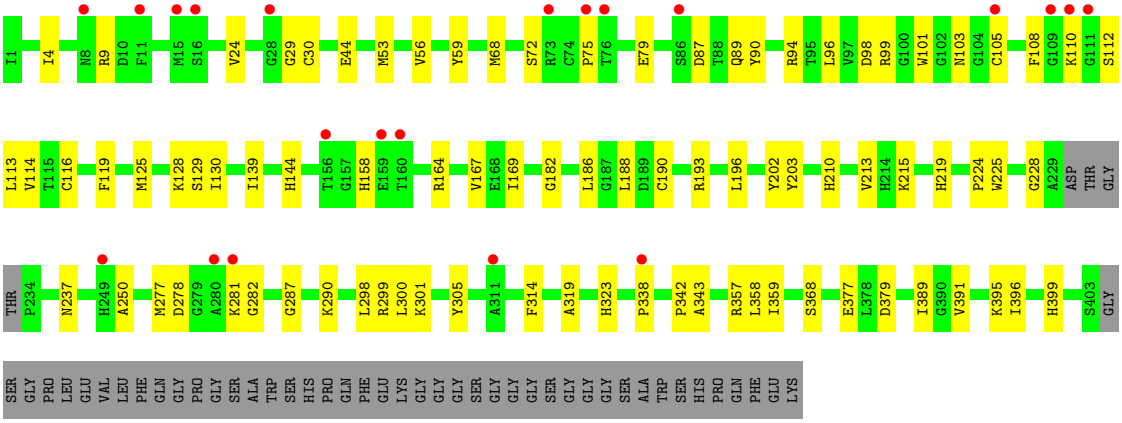
• Molecule 2: Human MZ4 Fab light chain

Chain N:



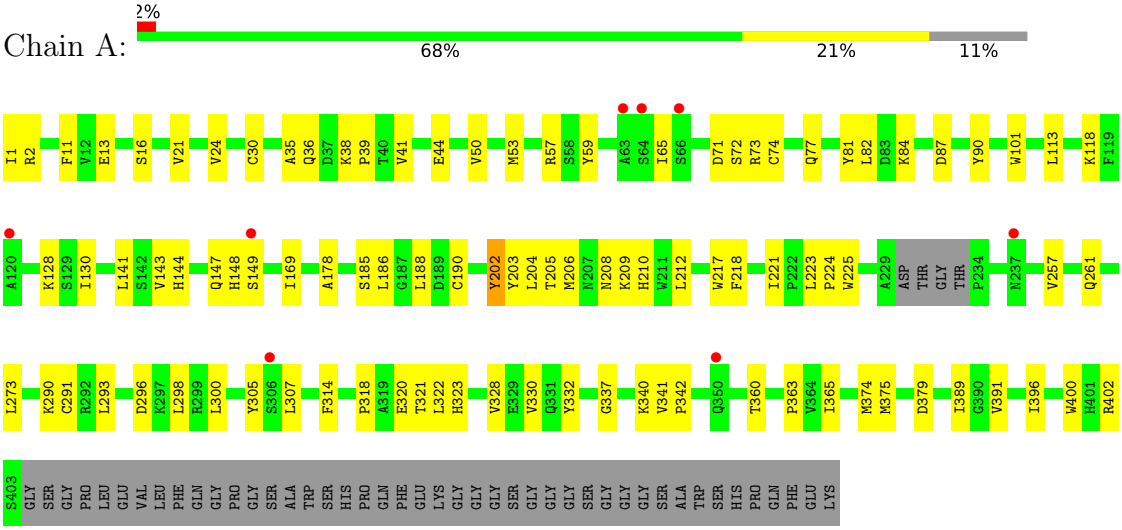
• Molecule 3: Envelope protein E

Chain B:



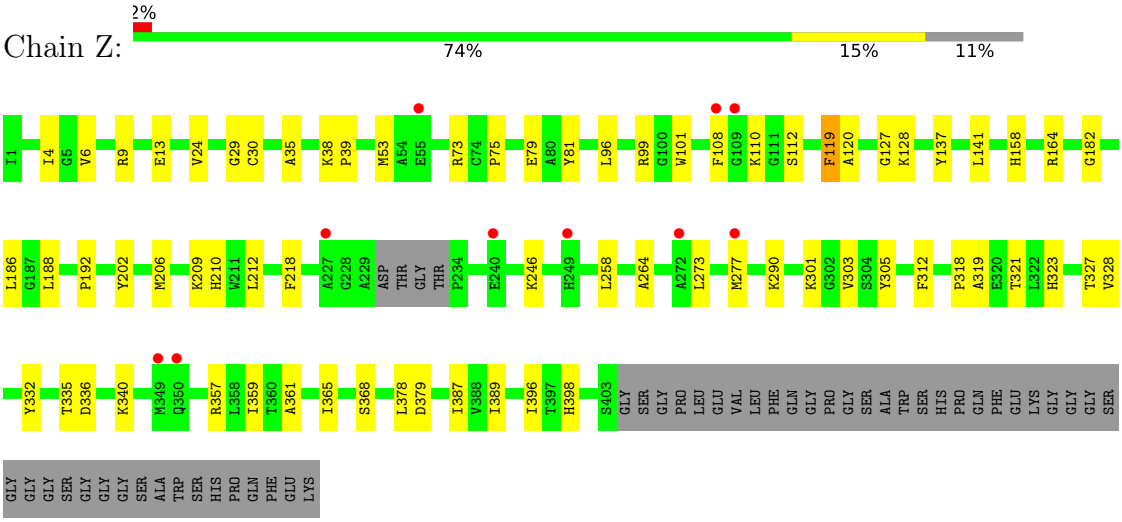
• Molecule 3: Envelope protein E

Chain A:



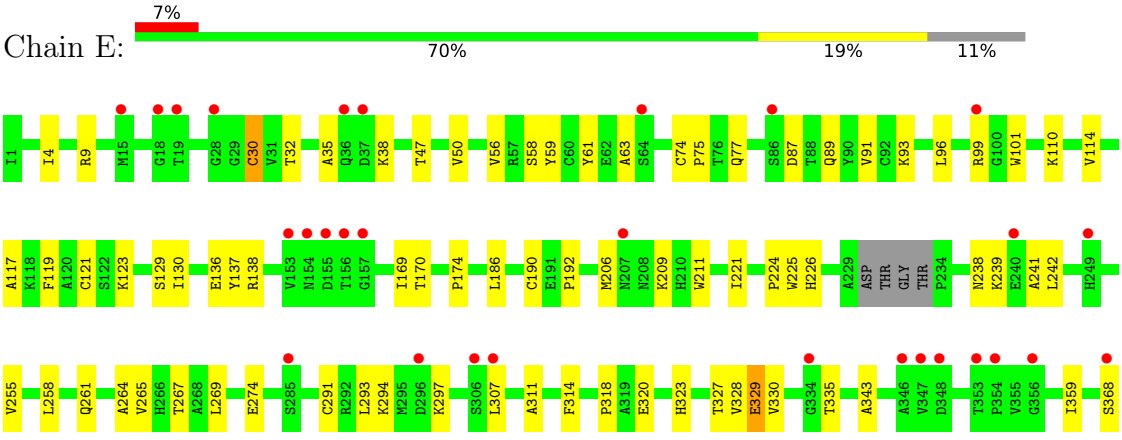
• Molecule 3: Envelope protein E

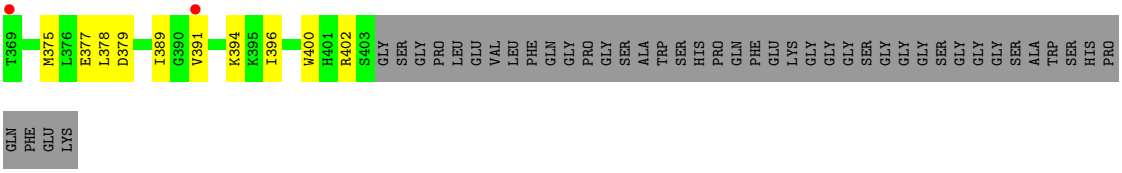
Chain Z:



• Molecule 3: Envelope protein E

Chain E:




T369
M375
L376
E377
L378
D379
I389
G390
V391
K394
K395
I396
W400
H401
R402
S403
GLY SER GLY PRO LEU GLU VAL LEU PHE GLN GLY PRO GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER GLY GLY GLY GLY SER ALA TRP SER HIS PRO
GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	113.53Å 137.26Å 136.79Å 80.12° 65.74° 65.75°	Depositor
Resolution (Å)	10.00 – 4.30 47.75 – 4.28	Depositor EDS
% Data completeness (in resolution range)	29.6 (10.00-4.30) 30.7 (47.75-4.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.264 , 0.359 0.281 , 0.378	Depositor DCC
R_{free} test set	734 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.045 for h,h-l,k 0.045 for h,l,h-k 0.358 for h,h-k,h-l 0.048 for -h,-k,-h+l 0.053 for -h,-h+k,-l 0.350 for -h,-l,-k 0.356 for -h,-h+l,-h+k	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	19232	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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	F	0.25	0/955	0.47	0/1302
1	H	0.26	0/955	0.48	0/1302
1	I	0.26	0/955	0.47	0/1302
1	M	0.25	0/955	0.48	0/1302
2	G	0.26	0/844	0.47	0/1149
2	J	0.26	0/844	0.49	0/1149
2	L	0.26	0/844	0.46	0/1149
2	N	0.26	0/844	0.48	0/1149
3	A	0.25	0/3117	0.48	0/4220
3	B	0.25	0/3117	0.48	0/4220
3	E	0.25	0/3117	0.48	0/4220
3	Z	0.25	0/3117	0.49	0/4220
All	All	0.25	0/19664	0.48	0/26684

There are no bond length outliers.

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	F	930	0	882	22	0
1	H	930	0	882	24	0
1	I	930	0	882	25	0
1	M	930	0	882	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	825	0	803	17	0
2	J	825	0	803	15	0
2	L	825	0	803	15	0
2	N	825	0	803	10	0
3	A	3053	0	2987	62	0
3	B	3053	0	2987	52	0
3	E	3053	0	2987	59	0
3	Z	3053	0	2987	48	0
All	All	19232	0	18688	333	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 9.

The worst 5 of 333 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:I:66:ARG:HD3	1:I:82(B):SER:HB3	1.60	0.81
1:F:18:LEU:HB3	1:F:82:LEU:HB3	1.63	0.80
3:A:337:GLY:HA3	3:A:365:ILE:HD11	1.65	0.78
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.66	0.76
3:B:139:ILE:HB	3:B:167:VAL:HB	1.68	0.75

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	F	118/120 (98%)	118 (100%)	0	0	100	100
1	H	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
1	I	118/120 (98%)	116 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
2	G	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
2	J	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
2	L	109/111 (98%)	100 (92%)	9 (8%)	0	100	100
2	N	109/111 (98%)	103 (94%)	6 (6%)	0	100	100
3	A	395/447 (88%)	384 (97%)	11 (3%)	0	100	100
3	B	395/447 (88%)	380 (96%)	15 (4%)	0	100	100
3	E	395/447 (88%)	378 (96%)	17 (4%)	0	100	100
3	Z	395/447 (88%)	379 (96%)	16 (4%)	0	100	100
All	All	2488/2712 (92%)	2395 (96%)	93 (4%)	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	F	104/104 (100%)	101 (97%)	3 (3%)	42	64
1	H	104/104 (100%)	102 (98%)	2 (2%)	57	75
1	I	104/104 (100%)	101 (97%)	3 (3%)	42	64
1	M	104/104 (100%)	101 (97%)	3 (3%)	42	64
2	G	92/92 (100%)	92 (100%)	0	100	100
2	J	92/92 (100%)	92 (100%)	0	100	100
2	L	92/92 (100%)	92 (100%)	0	100	100
2	N	92/92 (100%)	91 (99%)	1 (1%)	73	85
3	A	334/366 (91%)	331 (99%)	3 (1%)	78	88
3	B	334/366 (91%)	330 (99%)	4 (1%)	71	84
3	E	334/366 (91%)	329 (98%)	5 (2%)	65	80
3	Z	334/366 (91%)	332 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2120/2248 (94%)	2094 (99%)	26 (1%)	71 84

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	329	GLU
1	F	91	TYR
1	M	96	ASP
1	F	33	TYR
1	F	96	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	50	ASN
3	B	226	HIS
3	A	226	HIS
2	G	50	ASN
2	J	37	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

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, 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	F	120/120 (100%)	0.11	7 (5%)	23	19	82, 139, 210, 287	0
1	H	120/120 (100%)	0.04	6 (5%)	28	25	55, 141, 203, 244	0
1	I	120/120 (100%)	0.13	4 (3%)	46	37	62, 148, 216, 259	0
1	M	120/120 (100%)	0.14	6 (5%)	28	25	53, 141, 214, 272	0
2	G	111/111 (100%)	0.07	5 (4%)	33	28	60, 138, 203, 225	0
2	J	111/111 (100%)	0.06	6 (5%)	25	22	51, 133, 200, 250	0
2	L	111/111 (100%)	0.08	6 (5%)	25	22	66, 133, 202, 272	0
2	N	111/111 (100%)	0.20	7 (6%)	20	16	66, 132, 208, 248	0
3	A	399/447 (89%)	0.13	8 (2%)	65	56	72, 149, 210, 272	0
3	B	399/447 (89%)	0.21	21 (5%)	26	23	65, 142, 223, 320	0
3	E	399/447 (89%)	0.34	31 (7%)	13	11	33, 149, 249, 306	0
3	Z	399/447 (89%)	0.08	10 (2%)	57	48	58, 130, 207, 274	0
All	All	2520/2712 (92%)	0.16	117 (4%)	32	27	33, 141, 221, 320	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	347	VAL	10.0
1	M	27	GLY	6.9
3	B	280	ALA	5.4
2	L	107	LEU	5.1
3	E	153	VAL	5.0

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 (i)

There are no monosaccharides 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.