



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 02:48 AM EST

PDB ID : 6VYV
EMDB ID : EMD-21473
Title : Human mAbs broadly protect against infection of arthritogenic alphaviruses by recognizing conserved elements of the MXR8 receptor binding domain
Authors : Miller, A.S.; Kuhn, R.J.
Deposited on : 2020-02-27
Resolution : 6.33 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

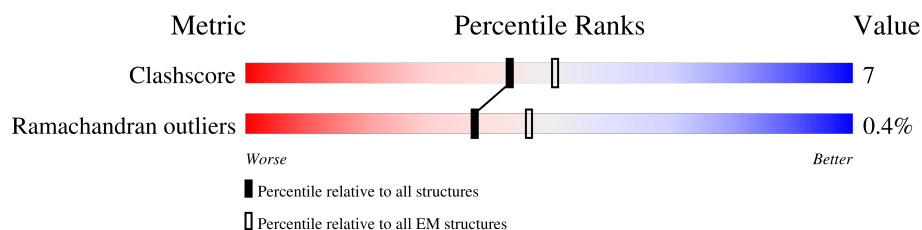
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY



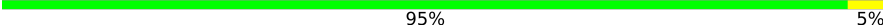
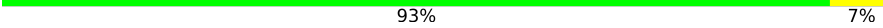


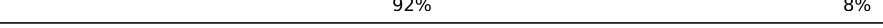



The reported resolution of this entry is 6.33 Å.

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	393	 88% 11%
1	B	393	 91% 9% .
1	C	393	 95% 5% .
1	D	393	 93% 7%
2	E	341	 90% 10%
2	F	341	 91% 9%
2	G	341	 92% 8%
2	H	341	 91% 9%
3	I	218	 90% 10%
3	J	218	 90% 9%

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Mol	Chain	Length	Quality of chain
3	K	218	 90%9%.
3	L	218	 93%7%
4	M	211	 98%.
4	N	211	 93%7%
4	O	211	 97%.
4	P	211	 91%9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18608 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 E1 glycoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	393	Total	C	N	O	0	0
			1572	786	393	393		
1	B	393	Total	C	N	O	0	0
			1572	786	393	393		
1	C	393	Total	C	N	O	0	0
			1572	786	393	393		
1	D	393	Total	C	N	O	0	0
			1572	786	393	393		

- Molecule 2 is a protein called E2 glycoprotein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	341	Total	C	N	O	0	0
			1364	682	341	341		
2	F	341	Total	C	N	O	0	0
			1364	682	341	341		
2	G	341	Total	C	N	O	0	0
			1364	682	341	341		
2	H	341	Total	C	N	O	0	0
			1364	682	341	341		

- Molecule 3 is a protein called Fab CHK-265 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	218	Total	C	N	O	0	0
			872	436	218	218		
3	J	218	Total	C	N	O	0	0
			872	436	218	218		
3	K	218	Total	C	N	O	0	0
			872	436	218	218		
3	L	218	Total	C	N	O	0	0
			872	436	218	218		

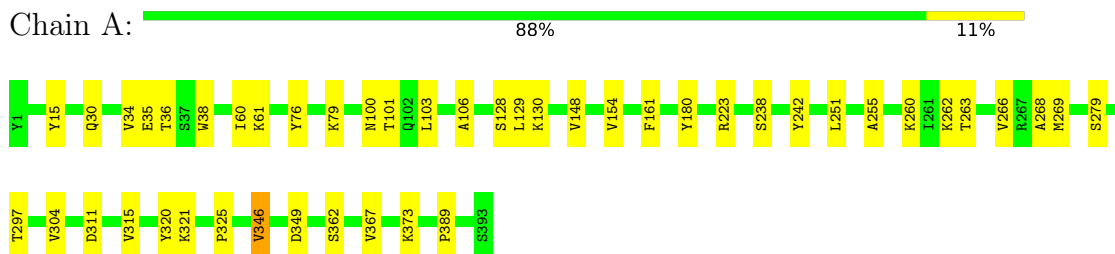
- Molecule 4 is a protein called Fab CHK-265 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	211	Total 844	C 422	N 211	O 211	0	0
4	N	211	Total 844	C 422	N 211	O 211	0	0
4	O	211	Total 844	C 422	N 211	O 211	0	0
4	P	211	Total 844	C 422	N 211	O 211	0	0

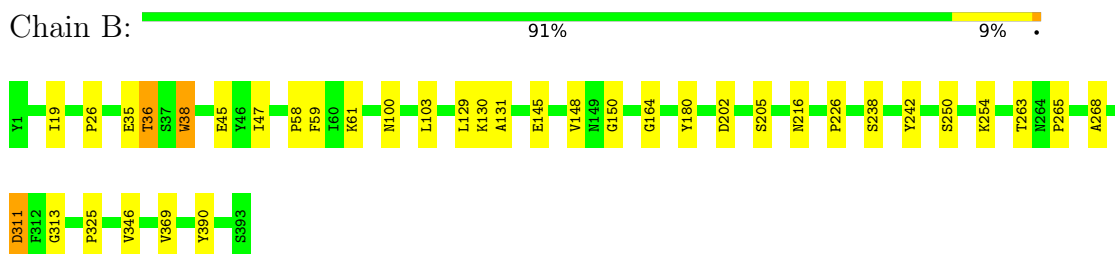
3 Residue-property plots [i](#)

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. 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. 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.

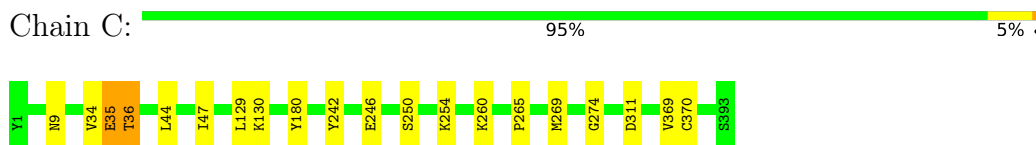
- Molecule 1: E1 glycoprotein



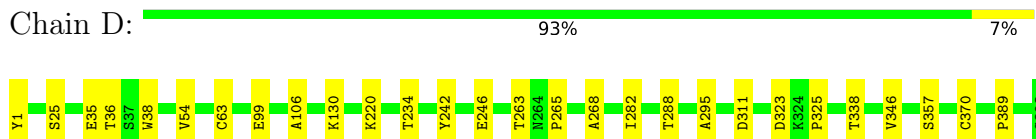
- Molecule 1: E1 glycoprotein



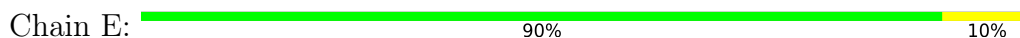
- Molecule 1: E1 glycoprotein

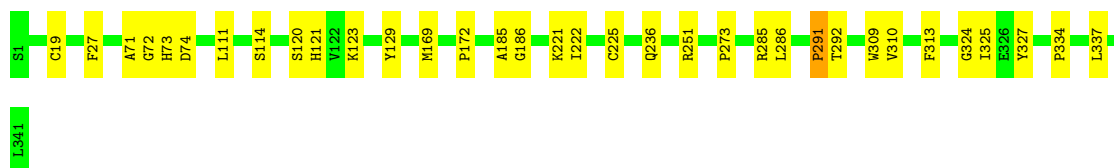


- Molecule 1: E1 glycoprotein



- Molecule 2: E2 glycoprotein





- Molecule 2: E2 glycoprotein



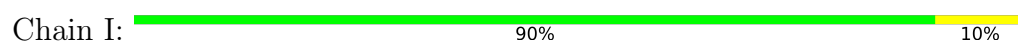
- Molecule 2: E2 glycoprotein



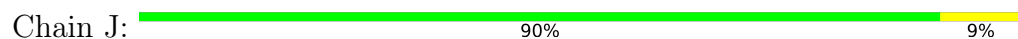
- Molecule 2: E2 glycoprotein



- Molecule 3: Fab CHK-265 heavy chain



- Molecule 3: Fab CHK-265 heavy chain

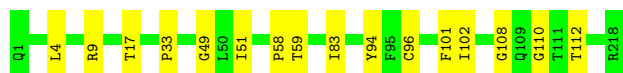


- Molecule 3: Fab CHK-265 heavy chain



- Molecule 3: Fab CHK-265 heavy chain

Chain L:  93% 7%



- Molecule 4: Fab CHK-265 light chain

Chain M:  98% .



- Molecule 4: Fab CHK-265 light chain

Chain N:  93% 7%



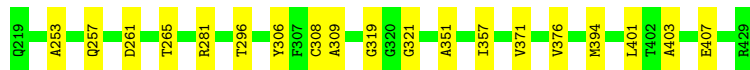
- Molecule 4: Fab CHK-265 light chain

Chain O:  97% .



- Molecule 4: Fab CHK-265 light chain

Chain P:  91% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	9559	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	18000	Depositor
Image detector	GATAN K2 BASE (4k x 4k)	Depositor

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	A	0.32	0/1571	0.70	0/1962
1	B	0.32	0/1571	0.70	0/1962
1	C	0.33	0/1571	0.72	0/1962
1	D	0.32	0/1571	0.71	0/1962
2	E	0.33	0/1363	0.71	0/1702
2	F	0.33	0/1363	0.69	0/1702
2	G	0.33	0/1363	0.66	0/1702
2	H	0.32	0/1363	0.68	0/1702
3	I	0.29	0/871	0.64	0/1087
3	J	0.29	0/871	0.68	0/1087
3	K	0.31	0/871	0.67	0/1087
3	L	0.29	0/871	0.63	0/1087
4	M	0.28	0/843	0.64	0/1052
4	N	0.28	0/843	0.65	1/1052 (0.1%)
4	O	0.28	0/843	0.64	0/1052
4	P	0.29	0/843	0.65	0/1052
All	All	0.31	0/18592	0.68	1/23212 (0.0%)

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	A	0	7
1	B	0	10
1	C	0	8
1	D	0	3
2	E	0	8
2	F	0	5
2	G	0	5
2	H	0	6
3	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	J	0	3
3	K	0	1
3	L	0	2
4	P	0	1
All	All	0	62

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	N	383	THR	C-N-CA	7.67	140.88	121.70

There are no chirality outliers.

5 of 62 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	TYR	Peptide
1	A	223	ARG	Peptide
1	A	263	THR	Peptide
1	A	311	ASP	Peptide
1	A	34	VAL	Peptide

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	A	1572	0	417	23	0
1	B	1572	0	417	15	0
1	C	1572	0	417	7	0
1	D	1572	0	417	12	0
2	E	1364	0	359	16	0
2	F	1364	0	359	12	0
2	G	1364	0	359	12	0
2	H	1364	0	359	11	0
3	I	872	0	244	10	0
3	J	872	0	244	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	872	0	244	12	0
3	L	872	0	244	7	0
4	M	844	0	232	1	0
4	N	844	0	232	7	0
4	O	844	0	232	3	0
4	P	844	0	232	10	0
All	All	18608	0	5008	165	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 7.

The worst 5 of 165 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)
2:G:324:GLY:HA3	2:G:337:LEU:O	1.65	0.95
1:C:260:LYS:CA	1:C:269:MET:O	2.23	0.86
3:I:49:GLY:HA3	3:I:59:THR:O	1.75	0.86
1:A:36:THR:CA	1:A:130:LYS:O	2.28	0.81
1:D:36:THR:CA	1:D:130:LYS:O	2.29	0.81

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 PDB entries followed by that with respect to all EM entries.

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	391/393 (100%)	305 (78%)	85 (22%)	1 (0%)	41	76
1	B	391/393 (100%)	314 (80%)	76 (19%)	1 (0%)	41	76
1	C	391/393 (100%)	301 (77%)	88 (22%)	2 (0%)	29	69
1	D	391/393 (100%)	307 (78%)	82 (21%)	2 (0%)	29	69
2	E	339/341 (99%)	245 (72%)	94 (28%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	339/341 (99%)	260 (77%)	76 (22%)	3 (1%)	17	56
2	G	339/341 (99%)	256 (76%)	81 (24%)	2 (1%)	25	66
2	H	339/341 (99%)	253 (75%)	83 (24%)	3 (1%)	17	56
3	I	216/218 (99%)	179 (83%)	36 (17%)	1 (0%)	29	69
3	J	216/218 (99%)	174 (81%)	41 (19%)	1 (0%)	29	69
3	K	216/218 (99%)	174 (81%)	41 (19%)	1 (0%)	29	69
3	L	216/218 (99%)	173 (80%)	42 (19%)	1 (0%)	29	69
4	M	209/211 (99%)	168 (80%)	39 (19%)	2 (1%)	15	54
4	N	209/211 (99%)	165 (79%)	44 (21%)	0	100	100
4	O	209/211 (99%)	169 (81%)	40 (19%)	0	100	100
4	P	209/211 (99%)	176 (84%)	33 (16%)	0	100	100
All	All	4620/4652 (99%)	3619 (78%)	981 (21%)	20 (0%)	38	72

5 of 20 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	35	GLU
2	F	74	ASP
3	I	102	ILE
3	K	102	ILE
3	L	102	ILE

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-21473. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.