



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 23, 2019 – 11:50 AM EDT

PDB ID : 6C6X
Title : Crystal structure of Middle-East Respiratory Syndrome (MERS) coronavirus neutralizing antibody JC57-14 isolated from a vaccinated rhesus macaque.
Authors : Joyce, M.G.; Mascola, J.R.; Graham, B.S.; Kwong, P.D.
Deposited on : 2018-01-19
Resolution : 1.99 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

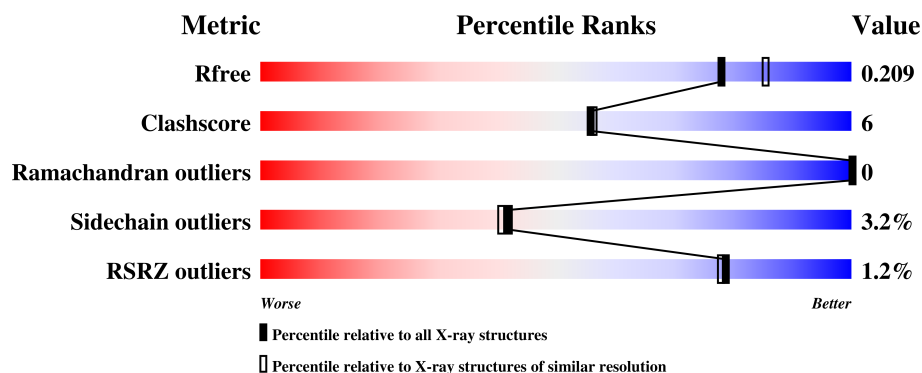
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (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 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	225	
1	C	225	
1	E	225	
1	H	225	
2	B	214	

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Mol	Chain	Length	Quality of chain
2	D	214	<div><div></div><div>86%</div><div>12%</div><div></div></div>
2	F	214	<div><div></div><div>86%</div><div>14%</div><div></div></div>
2	L	214	<div><div></div><div>%</div><div>90%</div><div>10%</div><div></div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13929 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 JC57-14 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1582	998	262	318	4			
1	C	213	Total	C	N	O	S	0	0	0
			1588	1001	263	320	4			
1	E	215	Total	C	N	O	S	0	0	0
			1601	1008	265	324	4			
1	H	215	Total	C	N	O	S	0	0	0
			1600	1007	265	324	4			

- Molecule 2 is a protein called JC57-14 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1650	1030	275	340	5			
2	D	214	Total	C	N	O	S	0	0	0
			1656	1033	276	341	6			
2	F	214	Total	C	N	O	S	0	0	0
			1656	1033	276	341	6			
2	L	214	Total	C	N	O	S	0	0	0
			1656	1033	276	341	6			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	86	Total	O	0	0
			86	86		
3	C	180	Total	O	0	0
			180	180		
3	D	129	Total	O	0	0
			129	129		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	108	Total 108	O 108	0	0
3	F	92	Total 92	O 92	0	0
3	H	98	Total 98	O 98	0	0
3	L	116	Total 116	O 116	0	0

3 Residue-property plots [i](#)

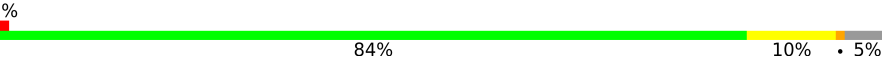
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

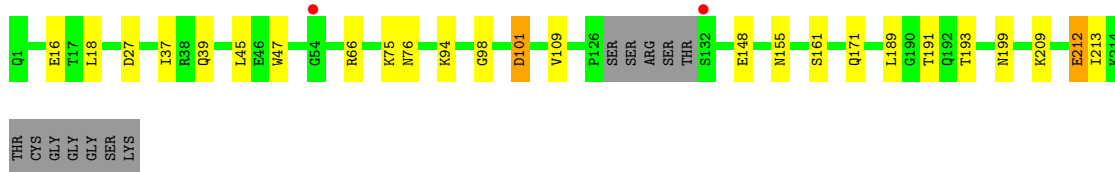
- Molecule 1: JC57-14 Heavy chain

Chain A: 




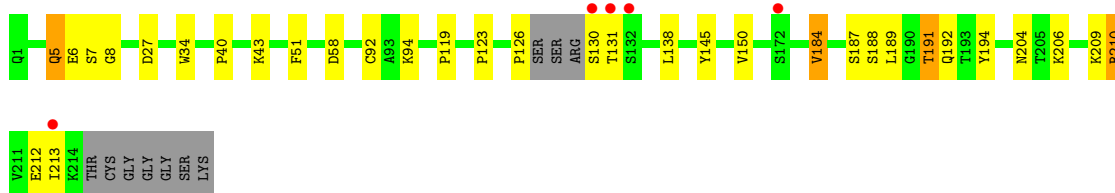
- Molecule 1: JC57-14 Heavy chain

Chain C: 




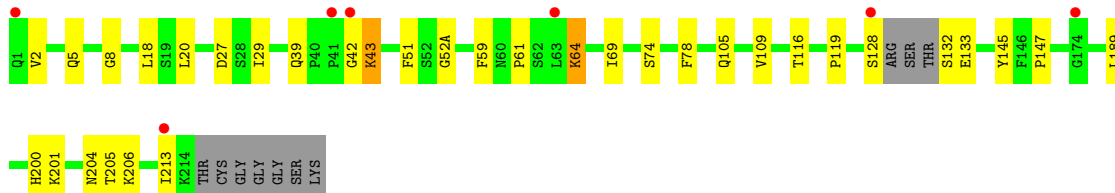
- Molecule 1: JC57-14 Heavy chain

Chain E: 

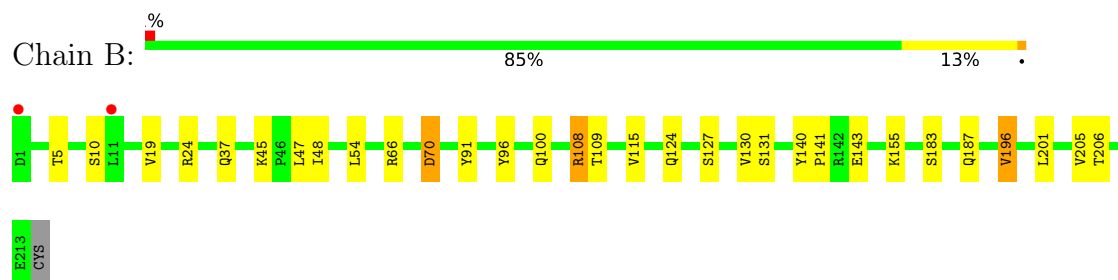


- Molecule 1: JC57-14 Heavy chain

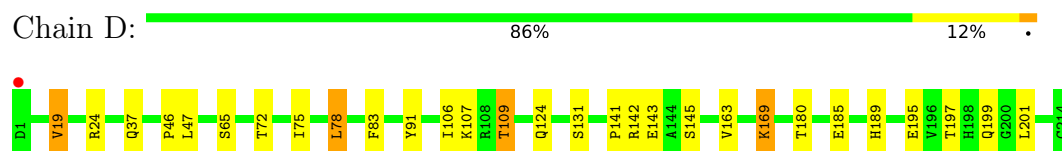
Chain H: 



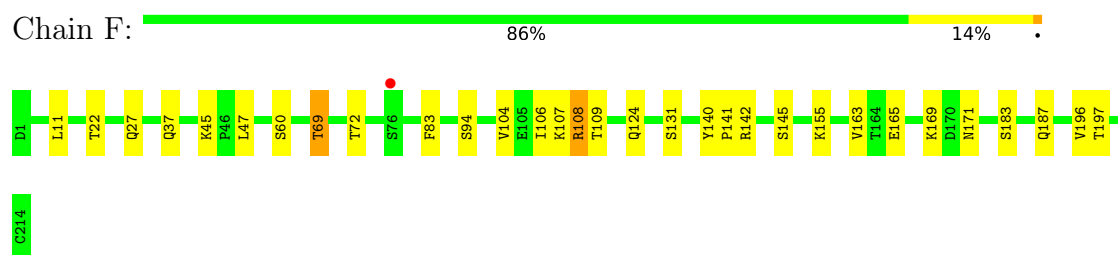
• Molecule 2: JC57-14 Light chain



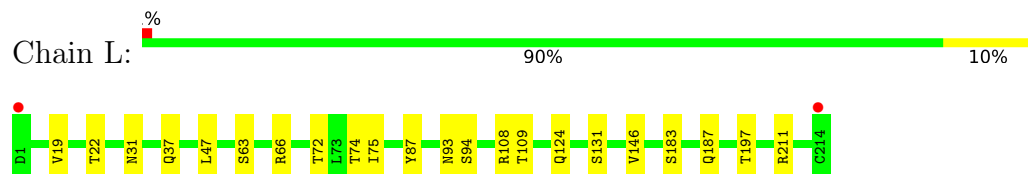
• Molecule 2: JC57-14 Light chain



• Molecule 2: JC57-14 Light chain



• Molecule 2: JC57-14 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.70Å 129.80Å 84.00Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	41.28 – 1.99 41.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	89.8 (41.28-1.99) 89.8 (41.28-1.99)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.176 , 0.208 0.177 , 0.209	Depositor DCC
R_{free} test set	5059 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.066 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13929	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.05% 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	A	0.33	0/1620	0.50	0/2213
1	C	0.32	0/1626	0.52	0/2221
1	E	0.46	0/1639	0.57	2/2239 (0.1%)
1	H	0.28	0/1638	0.51	0/2237
2	B	0.33	0/1686	0.52	0/2292
2	D	0.29	0/1692	0.52	0/2300
2	F	0.43	0/1692	0.54	0/2300
2	L	0.36	0/1692	0.53	0/2300
All	All	0.36	0/13285	0.53	2/18102 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	184	VAL	C-N-CD	5.81	140.60	128.40
1	E	8	GLY	C-N-CD	5.48	139.91	128.40

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	A	1582	0	1544	11	0
1	C	1588	0	1549	21	0
1	E	1601	0	1561	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	1600	0	1559	21	0
2	B	1650	0	1591	17	0
2	D	1656	0	1596	21	0
2	F	1656	0	1596	18	0
2	L	1656	0	1596	12	0
3	A	131	0	0	4	0
3	B	86	0	0	3	0
3	C	180	0	0	9	0
3	D	129	0	0	8	0
3	E	108	0	0	8	0
3	F	92	0	0	4	0
3	H	98	0	0	4	0
3	L	116	0	0	4	0
All	All	13929	0	12592	141	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 6.

The worst 5 of 141 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:H:42:GLY:O	1:H:43:LYS:NZ	1.99	0.96
1:C:161:SER:OG	3:C:301:HOH:O	1.88	0.89
1:E:27:ASP:OD2	1:E:94:LYS:NZ	2.09	0.85
2:D:180:THR:OG1	3:D:301:HOH:O	1.93	0.84
1:A:1:GLN:N	3:A:301:HOH:O	2.09	0.84

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	208/225 (92%)	204 (98%)	4 (2%)	0	100	100
1	C	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
1	E	211/225 (94%)	201 (95%)	10 (5%)	0	100	100
1	H	211/225 (94%)	208 (99%)	3 (1%)	0	100	100
2	B	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
2	D	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
2	F	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
2	L	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
All	All	1686/1756 (96%)	1645 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	183/194 (94%)	179 (98%)	4 (2%)	55	58
1	C	184/194 (95%)	179 (97%)	5 (3%)	48	49
1	E	186/194 (96%)	180 (97%)	6 (3%)	42	41
1	H	186/194 (96%)	179 (96%)	7 (4%)	36	33
2	B	191/192 (100%)	180 (94%)	11 (6%)	22	17
2	D	192/192 (100%)	186 (97%)	6 (3%)	43	42
2	F	192/192 (100%)	186 (97%)	6 (3%)	43	42
2	L	192/192 (100%)	189 (98%)	3 (2%)	65	70
All	All	1506/1544 (98%)	1458 (97%)	48 (3%)	42	41

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	78	LEU
1	E	5	GLN

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Mol	Chain	Res	Type
1	H	206	LYS
2	D	109	THR
2	D	185	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	199	GLN
2	F	171	ASN
1	H	171	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	212/225 (94%)	-0.21	1 (0%) 90 90	21, 33, 57, 78	0
1	C	213/225 (94%)	-0.13	2 (0%) 84 83	19, 30, 53, 121	0
1	E	215/225 (95%)	0.07	5 (2%) 60 59	18, 39, 78, 97	0
1	H	215/225 (95%)	-0.00	7 (3%) 46 46	24, 38, 66, 121	0
2	B	213/214 (99%)	-0.06	2 (0%) 84 83	26, 46, 69, 95	0
2	D	214/214 (100%)	-0.23	1 (0%) 90 90	23, 39, 56, 71	0
2	F	214/214 (100%)	-0.11	1 (0%) 90 90	23, 44, 67, 82	0
2	L	214/214 (100%)	-0.24	2 (0%) 84 83	24, 36, 59, 93	0
All	All	1710/1756 (97%)	-0.11	21 (1%) 79 78	18, 38, 65, 121	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	SER	18.2
1	H	1	GLN	7.8
1	E	130	SER	4.8
1	H	42	GLY	4.1
1	E	131	THR	3.9

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.