



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2018 – 06:34 PM EDT

PDB ID : 5W2B
Title : Crystal structure of C-terminal domain of Ebola (Reston) nucleoprotein in complex with Fab fragment
Authors : Radwanska, M.J.; Derewenda, U.; Kossiakoff, A.A.; Derewenda, Z.S.
Deposited on : 2017-06-06
Resolution : 2.25 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 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-20031172
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-20031172

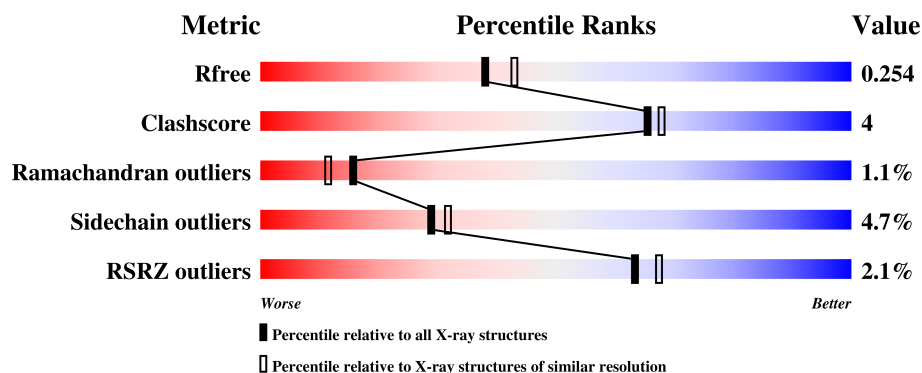
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1178 (2.26-2.26)
Clashscore	122126	1286 (2.26-2.26)
Ramachandran outliers	120053	1253 (2.26-2.26)
Sidechain outliers	120020	1254 (2.26-2.26)
RSRZ outliers	108989	1158 (2.26-2.26)

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	H	236	<div> <div>3%</div> <div>79%17%.</div> </div>
2	L	215	<div> <div>2%</div> <div>88%7%..</div> </div>
3	A	103	<div> <div></div> <div>87%7%6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4242 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	0	0
			1699	1077	282	334	6			

- Molecule 2 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1595	994	270	326	5			

- Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	97	Total	C	N	O	S	0	0	0
			837	541	137	155	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	637	GLY	-	expression tag	UNP Q8JPY1
A	638	ALA	-	expression tag	UNP Q8JPY1
A	639	MET	-	expression tag	UNP Q8JPY1
A	640	ALA	-	expression tag	UNP Q8JPY1

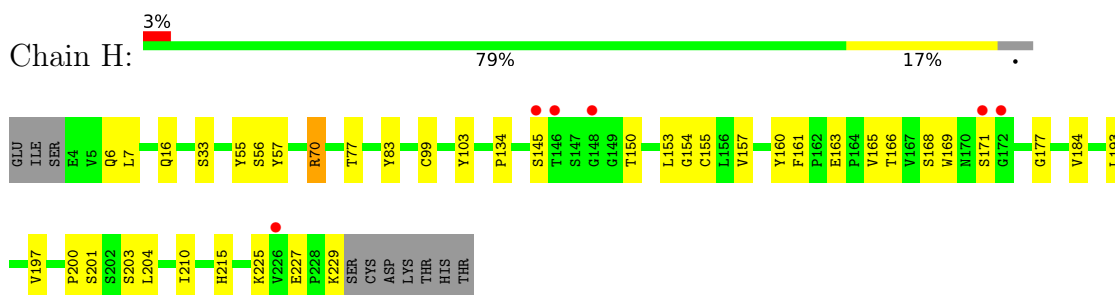
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	38	Total	O	0	0
			38	38		
4	L	51	Total	O	0	0
			51	51		
4	A	22	Total	O	0	0
			22	22		

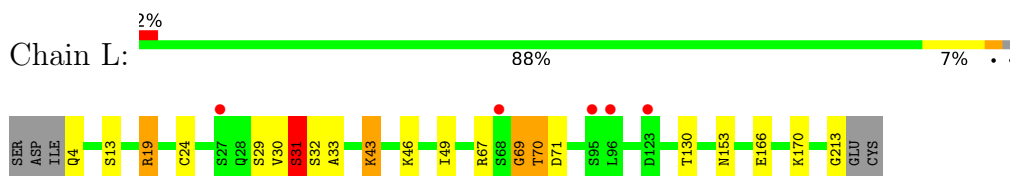
3 Residue-property plots [i](#)

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.

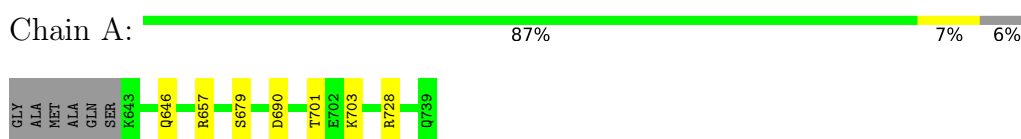
• Molecule 1: Fab Heavy Chain



• Molecule 2: Fab Light Chain



• Molecule 3: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.51Å 88.52Å 137.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.62 – 2.25 40.62 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.62-2.25) 99.8 (40.62-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.198 , 0.254 0.200 , 0.254	Depositor DCC
R_{free} test set	1417 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4242	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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	H	0.36	0/1746	0.51	0/2383
2	L	0.39	0/1627	0.54	0/2207
3	A	0.38	0/865	0.50	0/1172
All	All	0.37	0/4238	0.52	0/5762

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 [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	H	1699	0	1637	21	0
2	L	1595	0	1562	12	0
3	A	837	0	786	4	0
4	A	22	0	0	2	0
4	H	38	0	0	5	0
4	L	51	0	0	3	0
All	All	4242	0	3985	36	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 4.

All (36) 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:A:728:ARG:NH2	4:A:803:HOH:O	2.11	0.78
2:L:31:SER:HA	2:L:67:ARG:HH12	1.49	0.77
1:H:163:GLU:OE1	4:H:301:HOH:O	2.01	0.76
1:H:83:TYR:OH	4:H:302:HOH:O	2.01	0.76
3:A:679:SER:OG	4:A:802:HOH:O	2.07	0.72
1:H:6:GLN:NE2	4:H:304:HOH:O	2.20	0.70
1:H:201:SER:HA	1:H:204:LEU:HD23	1.75	0.67
2:L:213:GLY:O	4:L:301:HOH:O	2.14	0.66
2:L:19:ARG:HH11	2:L:19:ARG:HB2	1.61	0.66
2:L:31:SER:HA	2:L:67:ARG:NH1	2.10	0.65
1:H:70:ARG:HH11	1:H:70:ARG:HG2	1.67	0.58
2:L:43:LYS:NZ	2:L:43:LYS:HB3	2.19	0.58
3:A:701:THR:HG22	3:A:703:LYS:H	1.69	0.58
1:H:225:LYS:HE3	1:H:227:GLU:OE2	2.05	0.56
1:H:134:PRO:HB3	1:H:160:TYR:HB3	1.89	0.55
1:H:157:VAL:HB	1:H:193:LEU:HD23	1.89	0.55
1:H:33:SER:HA	1:H:56:SER:HB2	1.89	0.53
1:H:150:THR:HA	1:H:200:PRO:HA	1.92	0.52
1:H:56:SER:OG	4:H:303:HOH:O	2.18	0.51
2:L:43:LYS:HZ3	2:L:43:LYS:HB3	1.77	0.48
2:L:69:GLY:C	2:L:71:ASP:H	2.16	0.48
1:H:103:TYR:CZ	3:A:657:ARG:HG2	2.48	0.48
2:L:46:LYS:HE2	4:L:304:HOH:O	2.16	0.46
1:H:229:LYS:HB3	1:H:229:LYS:HE2	1.80	0.46
2:L:29:SER:HB3	2:L:70:THR:HG22	1.98	0.45
2:L:4:GLN:NE2	4:L:311:HOH:O	2.50	0.45
2:L:69:GLY:O	2:L:71:ASP:N	2.51	0.43
2:L:166:GLU:OE2	2:L:166:GLU:HA	2.19	0.43
1:H:200:PRO:O	1:H:203:SER:OG	2.31	0.42
1:H:201:SER:O	1:H:204:LEU:HB2	2.21	0.41
1:H:7:LEU:HB3	1:H:99:CYS:SG	2.61	0.41
1:H:154:GLY:HA2	1:H:169:TRP:CZ2	2.56	0.41
1:H:177:GLY:O	1:H:197:VAL:HA	2.21	0.41
1:H:161:PHE:O	1:H:215:HIS:HE1	2.04	0.40
1:H:55:TYR:CE2	1:H:57:TYR:HB3	2.56	0.40
1:H:145:SER:CB	4:H:306:HOH:O	2.70	0.40

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	H	224/236 (95%)	213 (95%)	11 (5%)	0	100	100
2	L	208/215 (97%)	195 (94%)	7 (3%)	6 (3%)	5	2
3	A	95/103 (92%)	95 (100%)	0	0	100	100
All	All	527/554 (95%)	503 (95%)	18 (3%)	6 (1%)	16	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	31	SER
2	L	33	ALA
2	L	70	THR
2	L	69	GLY
2	L	170	LYS
2	L	32	SER

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	H	188/198 (95%)	177 (94%)	11 (6%)	21	21
2	L	185/190 (97%)	176 (95%)	9 (5%)	27	30
3	A	91/95 (96%)	89 (98%)	2 (2%)	55	64
All	All	464/483 (96%)	442 (95%)	22 (5%)	29	32

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	16	GLN
1	H	70	ARG
1	H	77	THR
1	H	153	LEU
1	H	155	CYS
1	H	165	VAL
1	H	166	THR
1	H	168	SER
1	H	171	SER
1	H	184	VAL
1	H	210	ILE
2	L	13	SER
2	L	19	ARG
2	L	24	CYS
2	L	30	VAL
2	L	31	SER
2	L	43	LYS
2	L	49	ILE
2	L	130	THR
2	L	153	ASN
3	A	646	GLN
3	A	690	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	H	226/236 (95%)	0.03	6 (2%) 54 59	40, 62, 88, 111	0
2	L	210/215 (97%)	-0.08	5 (2%) 59 63	35, 55, 85, 97	0
3	A	97/103 (94%)	0.04	0 100 100	38, 51, 81, 95	0
All	All	533/554 (96%)	-0.01	11 (2%) 63 67	35, 57, 87, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	146	THR	6.2
1	H	171	SER	4.3
1	H	148	GLY	3.8
1	H	172	GLY	3.6
2	L	95	SER	3.6
2	L	123	ASP	3.3
2	L	68	SER	2.8
1	H	145	SER	2.5
2	L	27	SER	2.3
1	H	226	VAL	2.1
2	L	96	LEU	2.1

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.