



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:46 am GMT

PDB ID : 3S88  
Title : Crystal structure of Sudan Ebolavirus Glycoprotein (strain Gulu) bound to 16F6  
Authors : Sapphire, E.O.; Dias, J.M.; Bale, S.  
Deposited on : 2011-05-27  
Resolution : 3.35 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
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

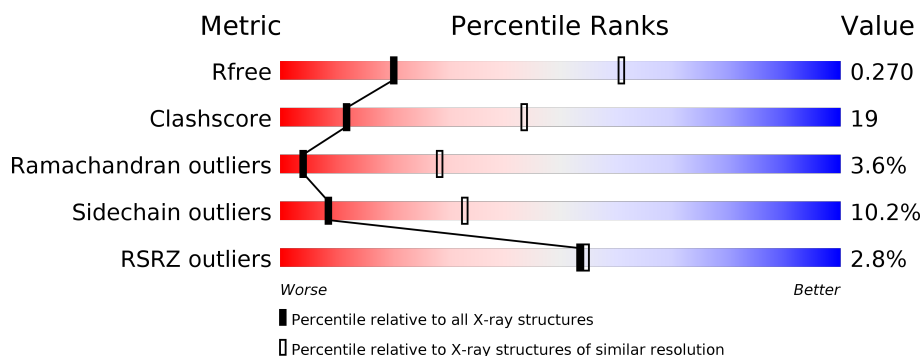
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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  $\geq 3$ , 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	220	
2	I	298	
3	J	167	
4	L	212	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6040 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 16F6 - Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	0	0	0
			1660	1055	273	324	8			

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	249	Total	C	N	O	S	0	0	0
			1859	1180	318	355	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	16	TYR	-	EXPRESSION TAG	UNP Q7T9D9
I	17	PRO	-	EXPRESSION TAG	UNP Q7T9D9
I	18	TYR	-	EXPRESSION TAG	UNP Q7T9D9
I	19	ASP	-	EXPRESSION TAG	UNP Q7T9D9
I	20	VAL	-	EXPRESSION TAG	UNP Q7T9D9
I	21	PRO	-	EXPRESSION TAG	UNP Q7T9D9
I	22	ASP	-	EXPRESSION TAG	UNP Q7T9D9
I	23	TYR	-	EXPRESSION TAG	UNP Q7T9D9
I	24	ALA	-	EXPRESSION TAG	UNP Q7T9D9
I	25	ILE	-	EXPRESSION TAG	UNP Q7T9D9
I	26	GLU	-	EXPRESSION TAG	UNP Q7T9D9
I	27	GLY	-	EXPRESSION TAG	UNP Q7T9D9
I	28	ARG	-	EXPRESSION TAG	UNP Q7T9D9
I	29	GLY	-	EXPRESSION TAG	UNP Q7T9D9
I	30	ALA	-	EXPRESSION TAG	UNP Q7T9D9
I	31	ARG	-	EXPRESSION TAG	UNP Q7T9D9

- Molecule 3 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	106	Total	C	N	O	S	0	0	0
			817	514	149	148	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	631	VAL	ILE	ENGINEERED MUTATION	UNP Q7T9D9
J	638	VAL	GLN	ENGINEERED MUTATION	UNP Q7T9D9

- Molecule 4 is a protein called 16F6 - Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	212	Total	C	N	O	S	0	0	0
			1648	1030	281	330	7			

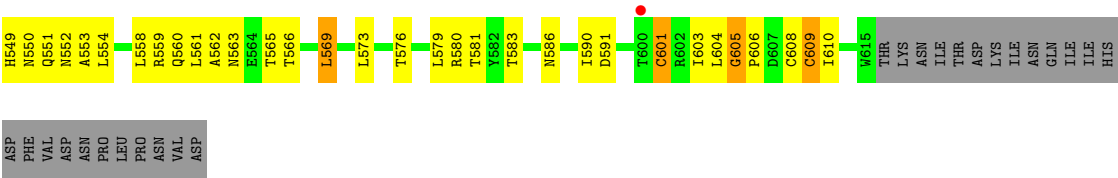
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	2	Total	C	N	O	0	0
			28	16	2	10		
5	J	2	Total	C	N	O	0	0
			28	16	2	10		

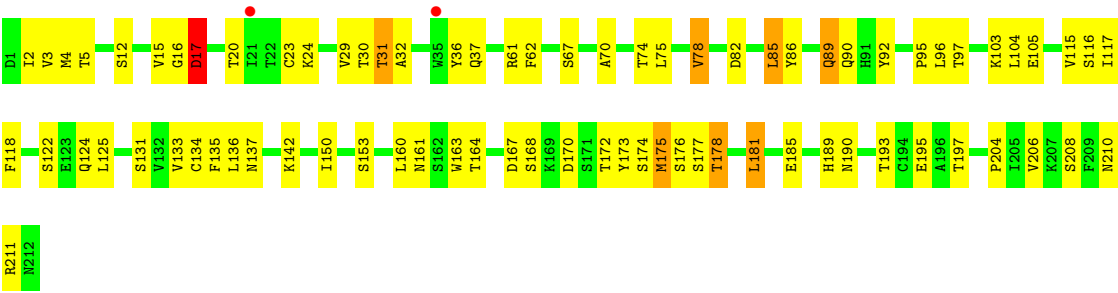


- Molecule 1: 16F6 - Heavy chain





● Molecule 4: 16F6 - Light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.59Å 193.59Å 193.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.63 – 3.35 45.63 – 3.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.63-3.35) 97.2 (45.63-3.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.222 , 0.278 0.216 , 0.270	Depositor DCC
$R_{free}$ test set	864 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	104.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6040	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.72	0/1704	0.74	0/2326
2	I	0.56	0/1904	0.68	0/2593
3	J	0.62	0/838	0.70	0/1144
4	L	0.64	0/1687	0.74	0/2295
All	All	0.64	0/6133	0.72	0/8358

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	1660	0	1615	64	0
2	I	1859	0	1709	70	0
3	J	817	0	756	40	0
4	L	1648	0	1588	68	0
5	I	28	0	25	0	0
5	J	28	0	25	2	0
All	All	6040	0	5718	227	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 19.



The worst 5 of 227 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:88:SER:O	1:H:91:THR:HG22	1.47	1.13
3:J:521:GLN:HA	3:J:522:GLU:HB3	1.20	1.13
3:J:521:GLN:HA	3:J:522:GLU:CB	1.89	1.01
4:L:193:THR:HG22	4:L:208:SER:HB2	1.53	0.89
4:L:20:THR:CG2	4:L:74:THR:HG23	2.09	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 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	218/220 (99%)	200 (92%)	11 (5%)	7 (3%)	5	31
2	I	243/298 (82%)	196 (81%)	37 (15%)	10 (4%)	3	25
3	J	104/167 (62%)	88 (85%)	7 (7%)	9 (9%)	1	7
4	L	210/212 (99%)	191 (91%)	17 (8%)	2 (1%)	18	56
All	All	775/897 (86%)	675 (87%)	72 (9%)	28 (4%)	4	28

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	194	ARG
2	I	225	PHE
2	I	274	ILE
3	J	522	GLU
3	J	604	LEU

### 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	H	183/183 (100%)	166 (91%)	17 (9%)	10	37
2	I	186/256 (73%)	164 (88%)	22 (12%)	6	25
3	J	80/142 (56%)	72 (90%)	8 (10%)	9	33
4	L	187/187 (100%)	169 (90%)	18 (10%)	10	35
All	All	636/768 (83%)	571 (90%)	65 (10%)	8	33

5 of 65 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	139	HIS
2	I	246	ARG
4	L	168	SER
2	I	155	LYS
2	I	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
4	L	6	GLN
4	L	89	GLN
4	L	190	ASN
3	J	586	ASN
4	L	189	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](#)

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	I	750	2,5	14,14,15	0.50	0	15,19,21	0.87	0
5	NAG	I	751	5	14,14,15	0.56	0	15,19,21	0.88	0
5	NAG	J	801	3,5	14,14,15	0.55	0	15,19,21	2.01	4 (26%)
5	NAG	J	802	5	14,14,15	0.47	0	15,19,21	1.97	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	750	2,5	-	0/6/23/26	0/1/1/1
5	NAG	I	751	5	-	0/6/23/26	0/1/1/1
5	NAG	J	801	3,5	-	0/6/23/26	0/1/1/1
5	NAG	J	802	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	801	NAG	O5-C1-C2	-5.31	104.09	111.47
5	J	802	NAG	O5-C1-C2	-4.02	105.88	111.47
5	J	802	NAG	C4-C3-C2	-3.58	105.77	111.02
5	J	801	NAG	C3-C4-C5	-3.31	104.39	110.22
5	J	801	NAG	O6-C6-C5	-2.75	102.07	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	801	NAG	2	0
5	J	802	NAG	1	0

## 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	H	220/220 (100%)	-0.21	1 (0%) 90 92	62, 93, 130, 162	0
2	I	249/298 (83%)	0.21	16 (6%) 20 21	81, 144, 248, 271	0
3	J	106/167 (63%)	0.24	3 (2%) 53 54	78, 121, 229, 260	0
4	L	212/212 (100%)	-0.16	2 (0%) 84 86	67, 104, 145, 165	0
All	All	787/897 (87%)	-0.00	22 (2%) 53 54	62, 111, 229, 271	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	287	GLU	5.1
2	I	87	GLY	4.0
1	H	134	SER	3.4
2	I	222	ILE	3.2
2	I	86	TRP	3.2

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	I	750	14/15	0.82	0.32	0.63	190,198,203,203	0
5	NAG	J	801	14/15	0.94	0.20	-1.24	129,136,143,150	0
5	NAG	I	751	14/15	0.77	0.39	-	202,206,212,213	0
5	NAG	J	802	14/15	0.92	0.21	-	156,162,165,165	0

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.