



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3FMG  
Title : Structure of rotavirus outer capsid protein VP7 trimer in complex with a neutralizing Fab  
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Deposited on : 2008-12-22  
Resolution : 3.40 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

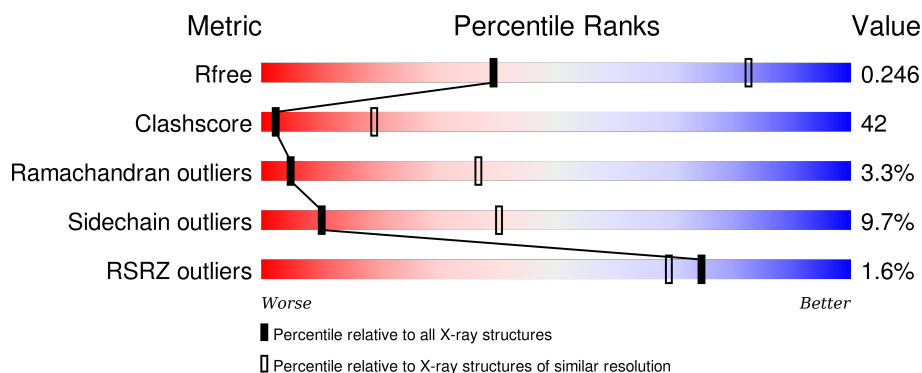
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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	L	211	<div> <div></div> <div> <div></div> <div>50%</div> <div>43%</div> <div>8%</div> </div> </div>
2	H	221	<div> <div>4%</div> <div> <div></div> <div>43%</div> <div>51%</div> <div>5%</div> </div> </div>
3	A	276	<div> <div> <div></div> <div>39%</div> <div>37%</div> <div>8%</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5166 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 of neutralizing antibody 4F8, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	211	Total	C	N	O	S	0	0	0
			1636	1025	277	328	6			

- Molecule 2 is a protein called Fab of neutralizing antibody 4F8, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1668	1055	277	328	8			

- Molecule 3 is a protein called Glycoprotein VP7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	235	Total	C	N	O	S	0	0	0
			1860	1184	292	369	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	THR	ALA	SEE REMARK 999	UNP P12476
A	324	TYR	ASN	SEE REMARK 999	UNP P12476

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		



T276	T277	A278	P279	R283	R284	R285	R286	I287	I288	H289	K290	H293	Y297	V300	D301	V302	V303	I306	I307	H310	H311	H312	ARG	SER	ARG	ARG	SER	SER	LEU	ASN	SER	ALA	ALA	PHE	TYR	TYR	ARG	ILE
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	244.18 Å   244.18 Å   244.18 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	82.8 (30.00-3.40) 97.8 (29.61-3.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 3.39 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224   ,   0.238 0.231   ,   0.246	Depositor DCC
$R_{free}$ test set	3373 reflections (9.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26   ,   54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33961 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5166	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	L	0.39	0/1677	0.71	1/2276 (0.0%)
2	H	0.40	0/1714	0.71	0/2341
3	A	0.64	4/1899 (0.2%)	0.92	8/2596 (0.3%)
All	All	0.50	4/5290 (0.1%)	0.79	9/7213 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	286	ARG	N-CA	10.31	1.67	1.46
3	A	285	MET	C-N	10.22	1.57	1.34
3	A	245	THR	CB-OG1	6.34	1.55	1.43
3	A	246	ILE	CB-CG2	6.10	1.71	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	ILE	CA-CB-CG2	-7.88	95.14	110.90
3	A	286	ARG	CB-CA-C	-7.18	96.04	110.40
3	A	223	LYS	CD-CE-NZ	6.16	125.86	111.70
3	A	286	ARG	N-CA-CB	6.05	121.49	110.60
3	A	245	THR	CA-CB-OG1	-6.01	96.38	109.00

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	L	1636	0	1582	129	0
2	H	1668	0	1625	164	0
3	A	1860	0	1819	149	1
4	A	2	0	0	0	0
All	All	5166	0	5026	431	1

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 42.

The worst 5 of 431 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:L:108:ARG:HD3	1:L:140:TYR:CD1	1.42	1.53
2:H:23:LYS:CE	2:H:79:THR:HG21	1.18	1.53
1:L:108:ARG:CD	1:L:140:TYR:CD1	1.90	1.53
2:H:23:LYS:CE	2:H:79:THR:CG2	1.82	1.52
2:H:23:LYS:HE3	2:H:79:THR:CG2	1.37	1.50

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:151:ASP:OD2	3:A:288:ASN:OD1[8_555]	2.16	0.04

## 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	L	209/211 (99%)	170 (81%)	33 (16%)	6 (3%)	<b>6</b> 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	219/221 (99%)	184 (84%)	26 (12%)	9 (4%)	3	30
3	A	233/276 (84%)	206 (88%)	20 (9%)	7 (3%)	5	39
All	All	661/708 (93%)	560 (85%)	79 (12%)	22 (3%)	5	37

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	102	HIS
2	H	145	ASN
2	H	146	SER
3	A	132	GLN
3	A	267	ASP

### 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	L	187/187 (100%)	170 (91%)	17 (9%)	12	44
2	H	188/188 (100%)	175 (93%)	13 (7%)	19	59
3	A	212/247 (86%)	185 (87%)	27 (13%)	5	26
All	All	587/622 (94%)	530 (90%)	57 (10%)	10	40

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	197	LEU
3	A	106	PHE
3	A	274	ASP
2	H	210	ARG
2	H	230	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	198	HIS
2	H	83	GLN
3	A	235	HIS
2	H	1	GLN
2	H	39	GLN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 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	L	211/211 (100%)	0.01	3 (1%) 78 73	51, 92, 128, 151	0
2	H	221/221 (100%)	0.21	8 (3%) 46 41	50, 96, 160, 183	0
3	A	235/276 (85%)	-0.16	0 100 100	43, 74, 128, 187	0
All	All	667/708 (94%)	0.02	11 (1%) 74 69	43, 85, 147, 187	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	145	ASN	3.5
2	H	144	THR	3.0
2	H	193	ASP	2.7
2	H	215	THR	2.7
2	H	140	ALA	2.5

### 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](#)

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
4	CA	A	327	1/1	0.98	0.19	0.49	89,89,89,89	0
4	CA	A	328	1/1	0.98	0.16	-0.61	75,75,75,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.