



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 7WLH / pdb_00007wlh
Title : The crystal structure of African swine fever virus I215L
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Deposited on : 2022-01-13
Resolution : 2.65 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 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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

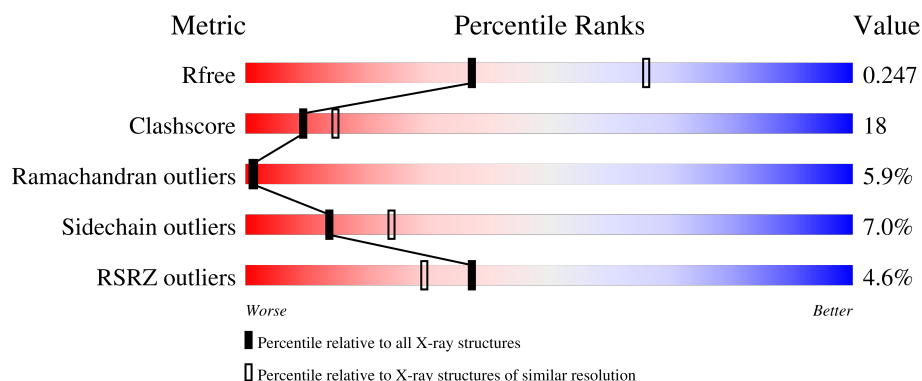
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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 of the lower 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 $\leq 5\%$. 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	B	197	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1303 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 E2 ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	156	Total	C	N	O	S	Se	0	0	0
			1265	817	200	243	2	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	HIS	-	expression tag	UNP A0A2X0TKQ7
B	191	HIS	-	expression tag	UNP A0A2X0TKQ7
B	192	HIS	-	expression tag	UNP A0A2X0TKQ7
B	193	HIS	-	expression tag	UNP A0A2X0TKQ7
B	194	HIS	-	expression tag	UNP A0A2X0TKQ7
B	195	HIS	-	expression tag	UNP A0A2X0TKQ7
B	196	HIS	-	expression tag	UNP A0A2X0TKQ7
B	197	HIS	-	expression tag	UNP A0A2X0TKQ7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	38	Total	O	0	0
			38	38		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.30Å 142.30Å 39.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.60 – 2.65 35.60 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (35.60-2.65) 94.4 (35.60-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.241 0.203 , 0.247	Depositor DCC
R_{free} test set	631 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.810	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 90.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1303	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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

5.1 Standard geometry

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	B	1.01	0/1296	1.57	7/1755 (0.4%)

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	B	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	149	MSE	CG-SE-CE	12.12	125.59	98.92
1	B	70	THR	CA-CB-OG1	-5.80	100.90	109.60
1	B	30	MSE	CG-SE-CE	5.79	111.66	98.92
1	B	26	ASN	CB-CA-C	5.43	118.93	110.67
1	B	9	GLU	N-CA-C	-5.39	105.30	111.07
1	B	139	LEU	O-C-N	5.39	128.69	122.17
1	B	66	ARG	CB-CA-C	5.32	118.30	109.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	ASN	Peptide
1	B	60	TYR	Peptide

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	B	1265	0	1243	45	0
2	B	38	0	0	17	0
All	All	1303	0	1243	45	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 18.

All (45) 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:B:4:ARG:HB3	2:B:218:HOH:O	1.39	1.23
1:B:35:VAL:HB	2:B:210:HOH:O	1.40	1.20
1:B:3:SER:HB2	2:B:207:HOH:O	1.63	0.98
1:B:133:LYS:HE3	2:B:235:HOH:O	1.68	0.93
1:B:60:TYR:O	1:B:62:TYR:N	2.04	0.89
1:B:165:GLU:O	1:B:168:GLU:HB3	1.87	0.74
1:B:89:LEU:C	1:B:113:SER:OG	2.32	0.72
1:B:59:GLU:O	1:B:60:TYR:C	2.31	0.72
1:B:83:LYS:NZ	2:B:201:HOH:O	2.23	0.71
1:B:171:LYS:HD3	2:B:206:HOH:O	1.91	0.70
1:B:174:ALA:HB2	2:B:206:HOH:O	1.97	0.64
1:B:81:ASP:OD2	1:B:83:LYS:HE3	1.98	0.64
1:B:172:ASN:C	1:B:174:ALA:H	2.09	0.61
1:B:3:SER:O	1:B:7:ILE:HG13	2.02	0.60
1:B:4:ARG:N	2:B:202:HOH:O	2.35	0.58
1:B:59:GLU:O	1:B:61:PRO:HD2	2.06	0.56
1:B:32:GLU:HB3	2:B:214:HOH:O	2.05	0.55
1:B:119:ASN:HB3	2:B:208:HOH:O	2.06	0.55
1:B:23:ILE:HG22	1:B:35:VAL:HG22	1.89	0.55
1:B:60:TYR:O	1:B:61:PRO:C	2.50	0.55
1:B:10:TYR:O	1:B:14:ILE:HG12	2.10	0.52
1:B:107:ILE:N	2:B:204:HOH:O	2.44	0.51
1:B:3:SER:CB	2:B:207:HOH:O	2.39	0.51
1:B:4:ARG:CB	2:B:218:HOH:O	2.21	0.51
1:B:128:ASN:OD1	1:B:128:ASN:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:TYR:HB3	1:B:148:PRO:HD3	1.94	0.48
1:B:81:ASP:OD2	1:B:83:LYS:CE	2.61	0.48
1:B:9:GLU:O	1:B:12:HIS:HB3	2.14	0.48
1:B:59:GLU:O	1:B:61:PRO:CD	2.62	0.47
1:B:174:ALA:CB	2:B:206:HOH:O	2.57	0.47
1:B:145:GLU:HA	1:B:145:GLU:OE1	2.14	0.47
1:B:50:PHE:CD1	1:B:73:MSE:SE	3.18	0.47
1:B:13:LEU:HD23	2:B:224:HOH:O	2.17	0.45
1:B:23:ILE:HD12	1:B:33:TRP:CE3	2.51	0.45
1:B:20:ASN:N	1:B:20:ASN:OD1	2.48	0.45
1:B:60:TYR:HB3	1:B:61:PRO:HD3	1.99	0.45
1:B:169:TYR:C	1:B:169:TYR:CD1	2.96	0.44
1:B:58:PRO:HA	2:B:232:HOH:O	2.17	0.44
1:B:13:LEU:HA	2:B:224:HOH:O	2.17	0.43
1:B:35:VAL:HG12	1:B:36:ILE:N	2.35	0.41
1:B:52:ALA:HB2	1:B:69:PHE:HA	2.02	0.41
1:B:172:ASN:C	1:B:172:ASN:OD1	2.63	0.41
1:B:120:GLU:O	1:B:121:PRO:C	2.64	0.40
1:B:10:TYR:CZ	1:B:14:ILE:HD11	2.56	0.40
1:B:23:ILE:HD12	1:B:33:TRP:CZ3	2.57	0.40

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	B	152/197 (77%)	126 (83%)	17 (11%)	9 (6%)	1 1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	TYR

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Mol	Chain	Res	Type
1	B	88	ILE
1	B	172	ASN
1	B	170	PHE
1	B	173	ALA
1	B	46	GLU
1	B	108	ASP
1	B	126	PRO
1	B	61	PRO

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	B	143/174 (82%)	133 (93%)	10 (7%)	14	24

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	SER
1	B	15	GLU
1	B	22	LYS
1	B	37	LEU
1	B	86	ILE
1	B	113	SER
1	B	122	ASN
1	B	133	LYS
1	B	136	ARG
1	B	171	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	ASN
1	B	26	ASN

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 oligosaccharides 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 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	B	153/197 (77%)	0.14	7 (4%) 37 29	75, 100, 151, 192	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	7.6
1	B	62	TYR	4.6
1	B	5	PHE	2.9
1	B	88	ILE	2.3
1	B	22	LYS	2.2
1	B	139	LEU	2.2
1	B	140	TYR	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 oligosaccharides 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.