



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:43 PM GMT

PDB ID : 4U2X
Title : Ebola virus VP24 in complex with Karyopherin alpha 5 C-terminus
Authors : Xu, W.; Leung, D.; Borek, D.; Amarasinghe, G.
Deposited on : 2014-07-18
Resolution : 3.15 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
<http://wwpdb.org/validation/2016/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
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

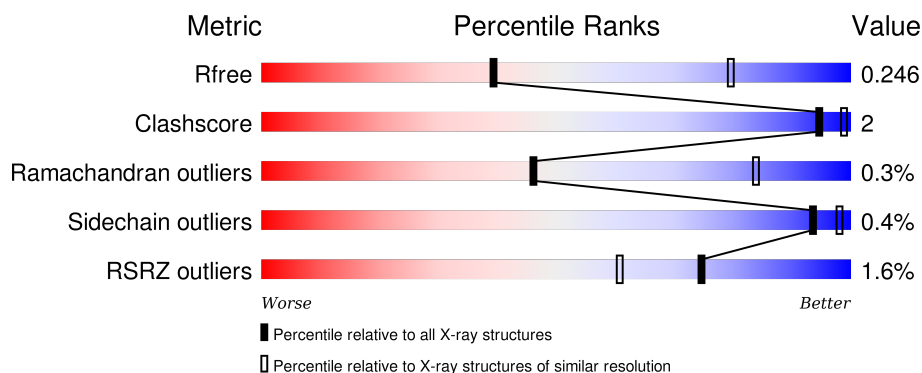
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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	216	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>6%</div> </div> </div>
1	B	216	<div> <div></div> <div>94%</div> <div>5%</div> </div>
1	C	216	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	D	175	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>
2	E	175	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	175	<div><div></div><div>6%</div><div>95%</div><div>5%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9199 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 Membrane-associated protein VP24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	1	0
			1727	1110	299	310	8			
1	B	215	Total	C	N	O	S	0	0	0
			1710	1100	295	307	8			
1	C	213	Total	C	N	O	S	0	0	0
			1693	1088	293	304	8			

- Molecule 2 is a protein called Importin subunit alpha-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	170	Total	C	N	O	S	0	0	0
			1327	846	224	250	7			
2	E	173	Total	C	N	O	S	0	0	0
			1350	861	228	254	7			
2	F	175	Total	C	N	O	S	0	0	0
			1366	870	231	258	7			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		
4	B	7	Total	O	0	0
			7	7		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	E	6	Total 6	O 6	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 errors 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: Membrane-associated protein VP24



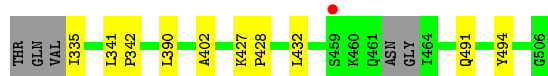
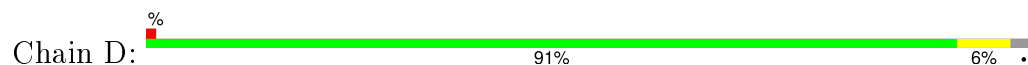
- Molecule 1: Membrane-associated protein VP24



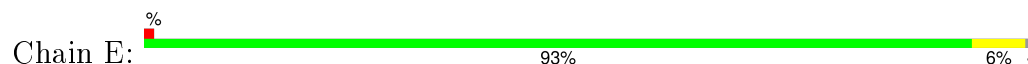
- Molecule 1: Membrane-associated protein VP24



- Molecule 2: Importin subunit alpha-6

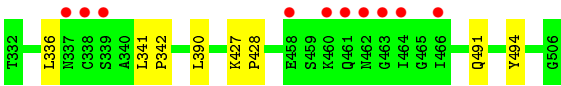


- Molecule 2: Importin subunit alpha-6



- Molecule 2: Importin subunit alpha-6





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.92Å 103.92Å 333.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.12 – 3.15 35.12 – 3.15	Depositor EDS
% Data completeness (in resolution range)	83.2 (35.12-3.15) 83.3 (35.12-3.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.215 , 0.249 0.210 , 0.246	Depositor DCC
R_{free} test set	1555 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 48.3	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30849 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9199	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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:
CL

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	0.27	0/1764	0.47	0/2393
1	B	0.27	0/1746	0.45	0/2368
1	C	0.26	0/1727	0.45	0/2340
2	D	0.28	0/1348	0.44	0/1825
2	E	0.27	0/1372	0.46	0/1860
2	F	0.28	0/1388	0.45	0/1882
All	All	0.27	0/9345	0.46	0/12668

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	A	1727	0	1763	6	0
1	B	1710	0	1750	5	0
1	C	1693	0	1739	6	0
2	D	1327	0	1343	5	0
2	E	1350	0	1370	6	0
2	F	1366	0	1387	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	9	0	0	0	0
4	B	7	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
All	All	9199	0	9352	32	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 2.

All (32) 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)
2:F:491:GLN:HA	2:F:494:TYR:CE2	2.37	0.59
2:E:491:GLN:HA	2:E:494:TYR:CE2	2.38	0.59
2:D:491:GLN:HA	2:D:494:TYR:CE2	2.37	0.58
1:B:106:LEU:HD21	1:B:152:LEU:HG	1.88	0.56
1:B:112:ILE:HG12	1:B:114:PRO:HD2	1.89	0.55
1:C:106:LEU:HD21	1:C:152:LEU:HG	1.89	0.55
1:A:106:LEU:HD21	1:A:152:LEU:HG	1.88	0.54
1:C:63:ASN:OD1	1:C:73:ARG:NH1	2.43	0.52
1:A:176:LEU:O	1:A:176:LEU:HD12	2.12	0.49
2:E:419:TYR:O	2:E:423:LEU:HD13	2.14	0.47
1:B:103:GLN:HG2	1:B:183:THR:HG22	1.97	0.47
2:F:427:LYS:HB3	2:F:428:PRO:HD3	1.97	0.47
1:C:161:ILE:HG23	1:C:227:LEU:HD12	1.96	0.47
2:D:427:LYS:HB3	2:D:428:PRO:HD3	1.97	0.47
2:E:427:LYS:HB3	2:E:428:PRO:HD3	1.97	0.46
2:F:341:LEU:N	2:F:342:PRO:HD2	2.32	0.45
1:A:103:GLN:HG2	1:A:183:THR:HG22	1.99	0.44
1:C:222:LEU:HD23	1:C:227:LEU:HD21	2.01	0.43
1:A:170:VAL:HG23	1:A:192:ARG:O	2.19	0.43
2:E:341:LEU:N	2:E:342:PRO:HD2	2.32	0.43
2:D:402:ALA:HB2	2:D:432:LEU:HD21	2.00	0.43
1:C:170:VAL:HG23	1:C:192:ARG:O	2.19	0.43
2:D:341:LEU:N	2:D:342:PRO:HD2	2.32	0.43
1:C:103:GLN:HG2	1:C:183:THR:HG22	2.00	0.43
1:A:121:LEU:HD12	1:A:141:VAL:HG21	2.02	0.42
2:E:457:GLN:N	2:E:457:GLN:OE1	2.52	0.42
2:F:390:LEU:HD23	2:F:428:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:VAL:HG23	1:B:192:ARG:O	2.19	0.41
2:D:390:LEU:HD23	2:D:428:PRO:HB2	2.02	0.41
2:E:390:LEU:HD23	2:E:428:PRO:HB2	2.02	0.41
1:B:125:TRP:CE2	1:B:134:PHE:HB2	2.56	0.41
1:A:125:TRP:CE2	1:A:134:PHE:HB2	2.55	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	A	215/216 (100%)	204 (95%)	10 (5%)	1 (0%)	34	76
1	B	213/216 (99%)	202 (95%)	10 (5%)	1 (0%)	34	76
1	C	209/216 (97%)	199 (95%)	9 (4%)	1 (0%)	34	76
2	D	166/175 (95%)	162 (98%)	4 (2%)	0	100	100
2	E	171/175 (98%)	168 (98%)	3 (2%)	0	100	100
2	F	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
All	All	1147/1173 (98%)	1104 (96%)	40 (4%)	3 (0%)	46	84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	GLY
1	B	37	GLY
1	C	37	GLY

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	193/192 (100%)	193 (100%)	0	100	100
1	B	191/192 (100%)	191 (100%)	0	100	100
1	C	190/192 (99%)	189 (100%)	1 (0%)	92	97
2	D	144/149 (97%)	143 (99%)	1 (1%)	88	97
2	E	147/149 (99%)	146 (99%)	1 (1%)	88	97
2	F	149/149 (100%)	148 (99%)	1 (1%)	88	97
All	All	1014/1023 (99%)	1010 (100%)	4 (0%)	93	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	112	ILE
2	D	335	ILE
2	E	335	ILE
2	F	336	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	337	ASN

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

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

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	216/216 (100%)	-0.43	2 (0%) 85 77	31, 57, 115, 148	0
1	B	215/216 (99%)	-0.41	0 100 100	32, 58, 116, 207	0
1	C	213/216 (98%)	-0.20	4 (1%) 70 54	45, 74, 128, 168	0
2	D	170/175 (97%)	-0.02	1 (0%) 90 84	52, 98, 135, 150	0
2	E	173/175 (98%)	-0.25	2 (1%) 81 69	33, 64, 125, 200	0
2	F	175/175 (100%)	0.13	10 (5%) 27 14	59, 94, 137, 191	0
All	All	1162/1173 (99%)	-0.21	19 (1%) 74 61	31, 73, 133, 207	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	462	ASN	5.0
1	C	69	TRP	4.8
2	F	338	CYS	3.6
2	F	463	GLY	3.6
2	F	464	ILE	3.4
2	F	461	GLN	2.9
1	A	108	ASP	2.7
1	C	174	GLY	2.6
2	F	337	ASN	2.5
2	D	459	SER	2.4
2	F	339	SER	2.4
2	F	466	ILE	2.3
2	F	458	GLU	2.2
2	E	337	ASN	2.2
1	C	211	ARG	2.1
1	A	174	GLY	2.1
1	C	68	ALA	2.1
2	E	463	GLY	2.0
2	F	460	LYS	2.0

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, 95th 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(Å ²)	Q<0.9
3	CL	A	301	1/1	0.92	0.21	-	60,60,60,60	1
3	CL	B	301	1/1	0.78	0.22	-	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.