wwPDB EM Validation Summary Report

May 16, 2024 – 09:50 am BST

PDB ID	:	6Z0U
EMDB ID	:	EMD-11023
Title	:	CryoEM structure of the Chikungunya virus nsP1 complex
Authors	:	Reguera, J.; Jones, R.; Arranz-Avila, R.
Deposited on	:	2020-05-11
Resolution	:	2.90 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

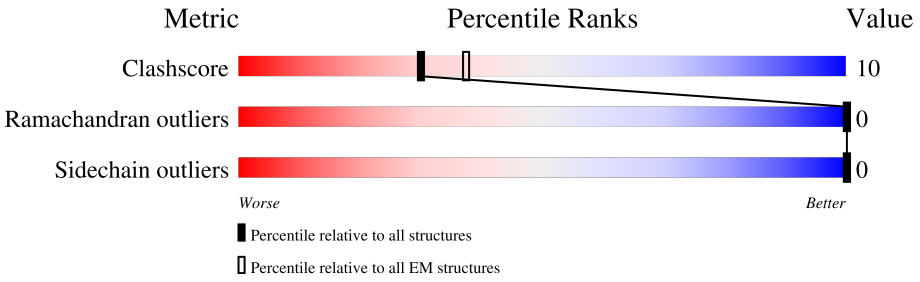
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 87288 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Polyprotein P1234.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	C	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	E	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	G	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	I	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	K	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	M	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	O	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	Q	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	S	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	V	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	X	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	Z	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	BA	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	DA	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	FA	454	Total 3578	C 2263	N 621	O 664	S 30	7	0
1	HA	454	Total 3578	C 2263	N 621	O 664	S 30	7	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	JA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	LA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	NA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	PA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	RA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	TA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		
1	VA	454	Total	C	N	O	S	7	0
			3578	2263	621	664	30		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	
2	E	1	Total	Zn	0
			1	1	
2	G	1	Total	Zn	0
			1	1	
2	I	1	Total	Zn	0
			1	1	
2	K	1	Total	Zn	0
			1	1	
2	M	1	Total	Zn	0
			1	1	
2	O	1	Total	Zn	0
			1	1	
2	Q	1	Total	Zn	0
			1	1	
2	S	1	Total	Zn	0
			1	1	
2	V	1	Total	Zn	0
			1	1	
2	X	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
2	Z	1	Total Zn 1 1	0
2	BA	1	Total Zn 1 1	0
2	DA	1	Total Zn 1 1	0
2	FA	1	Total Zn 1 1	0
2	HA	1	Total Zn 1 1	0
2	JA	1	Total Zn 1 1	0
2	LA	1	Total Zn 1 1	0
2	NA	1	Total Zn 1 1	0
2	PA	1	Total Zn 1 1	0
2	RA	1	Total Zn 1 1	0
2	TA	1	Total Zn 1 1	0
2	VA	1	Total Zn 1 1	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	AltConf
3	A	59	Total O 59 59	0
3	C	58	Total O 58 58	0
3	E	57	Total O 57 57	0
3	G	59	Total O 59 59	0
3	I	58	Total O 58 58	0
3	K	57	Total O 57 57	0
3	M	59	Total O 59 59	0

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Mol	Chain	Residues	Atoms	AltConf
3	O	58	Total O 58 58	0
3	Q	57	Total O 57 57	0
3	S	58	Total O 58 58	0
3	V	59	Total O 59 59	0
3	X	57	Total O 57 57	0
3	Z	59	Total O 59 59	0
3	BA	58	Total O 58 58	0
3	DA	57	Total O 57 57	0
3	FA	59	Total O 59 59	0
3	HA	58	Total O 58 58	0
3	JA	57	Total O 57 57	0
3	LA	59	Total O 59 59	0
3	NA	58	Total O 58 58	0
3	PA	57	Total O 57 57	0
3	RA	59	Total O 59 59	0
3	TA	58	Total O 58 58	0
3	VA	57	Total O 57 57	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D12	Depositor
Number of particles used	47338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF was estimated from movie frames aligned without dose-weighting. Per particle CTF correction was also performed with polished particles.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

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

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	0.38	0/3669	0.49	1/4975 (0.0%)
1	BA	0.38	0/3669	0.49	1/4975 (0.0%)
1	C	0.38	0/3669	0.49	1/4975 (0.0%)
1	DA	0.38	0/3669	0.49	1/4975 (0.0%)
1	E	0.38	0/3669	0.49	1/4975 (0.0%)
1	FA	0.38	0/3669	0.50	1/4975 (0.0%)
1	G	0.38	0/3669	0.49	1/4975 (0.0%)
1	HA	0.38	0/3669	0.49	1/4975 (0.0%)
1	I	0.38	0/3669	0.49	1/4975 (0.0%)
1	JA	0.38	0/3669	0.49	1/4975 (0.0%)
1	K	0.38	0/3669	0.49	1/4975 (0.0%)
1	LA	0.38	0/3669	0.49	1/4975 (0.0%)
1	M	0.38	0/3669	0.49	1/4975 (0.0%)
1	NA	0.38	0/3669	0.49	1/4975 (0.0%)
1	O	0.38	0/3669	0.49	1/4975 (0.0%)
1	PA	0.38	0/3669	0.49	1/4975 (0.0%)
1	Q	0.38	0/3669	0.49	1/4975 (0.0%)
1	RA	0.38	0/3669	0.49	1/4975 (0.0%)
1	S	0.38	0/3669	0.49	1/4975 (0.0%)
1	TA	0.38	0/3669	0.49	1/4975 (0.0%)
1	V	0.38	0/3669	0.49	1/4975 (0.0%)
1	VA	0.38	0/3669	0.49	1/4975 (0.0%)
1	X	0.38	0/3669	0.49	1/4975 (0.0%)
1	Z	0.38	0/3669	0.49	1/4975 (0.0%)
All	All	0.38	0/88056	0.49	24/119400 (0.0%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	108	LEU	CA-CB-CG	5.19	127.23	115.30
1	E	108	LEU	CA-CB-CG	5.19	127.23	115.30
1	JA	108	LEU	CA-CB-CG	5.19	127.23	115.30
1	PA	108	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	108	LEU	CA-CB-CG	5.18	127.20	115.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	3578	0	3536	87	0
1	BA	3578	0	3536	87	0
1	C	3578	0	3536	87	0
1	DA	3578	0	3536	74	0
1	E	3578	0	3536	71	0
1	FA	3578	0	3536	86	0
1	G	3578	0	3536	80	0
1	HA	3578	0	3536	84	0
1	I	3578	0	3536	86	0
1	JA	3578	0	3536	73	0
1	K	3578	0	3536	75	0
1	LA	3578	0	3536	87	0
1	M	3578	0	3536	87	0
1	NA	3578	0	3536	86	0
1	O	3578	0	3536	87	0
1	PA	3578	0	3536	72	0
1	Q	3578	0	3536	77	0
1	RA	3578	0	3536	80	0
1	S	3578	0	3536	88	0
1	TA	3578	0	3536	88	0
1	V	3578	0	3536	86	0
1	VA	3578	0	3536	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	3578	0	3536	71	0
1	Z	3578	0	3536	85	0
2	A	1	0	0	0	0
2	BA	1	0	0	0	0
2	C	1	0	0	0	0
2	DA	1	0	0	0	0
2	E	1	0	0	0	0
2	FA	1	0	0	0	0
2	G	1	0	0	0	0
2	HA	1	0	0	0	0
2	I	1	0	0	0	0
2	JA	1	0	0	0	0
2	K	1	0	0	0	0
2	LA	1	0	0	0	0
2	M	1	0	0	0	0
2	NA	1	0	0	0	0
2	O	1	0	0	0	0
2	PA	1	0	0	0	0
2	Q	1	0	0	0	0
2	RA	1	0	0	0	0
2	S	1	0	0	0	0
2	TA	1	0	0	0	0
2	V	1	0	0	0	0
2	VA	1	0	0	0	0
2	X	1	0	0	0	0
2	Z	1	0	0	0	0
3	A	59	0	0	4	0
3	BA	58	0	0	4	0
3	C	58	0	0	2	0
3	DA	57	0	0	2	0
3	E	57	0	0	2	0
3	FA	59	0	0	4	0
3	G	59	0	0	3	0
3	HA	58	0	0	3	0
3	I	58	0	0	3	0
3	JA	57	0	0	2	0
3	K	57	0	0	2	0
3	LA	59	0	0	4	0
3	M	59	0	0	4	0
3	NA	58	0	0	3	0
3	O	58	0	0	3	0
3	PA	57	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	57	0	0	2	0
3	RA	59	0	0	3	0
3	S	58	0	0	4	0
3	TA	58	0	0	3	0
3	V	59	0	0	4	0
3	VA	57	0	0	2	0
3	X	57	0	0	2	0
3	Z	59	0	0	4	0
All	All	87288	0	84864	1704	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 10.

The worst 5 of 1704 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:PA:52:GLU:O	1:PA:76:ARG:NH2	2.21	0.74
1:E:52:GLU:O	1:E:76:ARG:NH2	2.21	0.74
1:HA:232:LYS:HD3	1:HA:234:GLU:HG2	1.70	0.73
1:V:232:LYS:HD3	1:V:234:GLU:HG2	1.70	0.73
1:LA:52:GLU:O	1:LA:76:ARG:NH2	2.21	0.73

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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 PDB entries followed by that with respect to all EM entries.

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	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	BA	455/472 (96%)	427 (94%)	28 (6%)	0	100	100
1	C	455/472 (96%)	425 (93%)	30 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	DA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	E	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	FA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	G	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	HA	455/472 (96%)	423 (93%)	32 (7%)	0	100	100
1	I	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	JA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	K	455/472 (96%)	426 (94%)	29 (6%)	0	100	100
1	LA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	M	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	NA	455/472 (96%)	424 (93%)	31 (7%)	0	100	100
1	O	455/472 (96%)	424 (93%)	31 (7%)	0	100	100
1	PA	455/472 (96%)	426 (94%)	29 (6%)	0	100	100
1	Q	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	RA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	S	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	TA	455/472 (96%)	424 (93%)	31 (7%)	0	100	100
1	V	455/472 (96%)	424 (93%)	31 (7%)	0	100	100
1	VA	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
1	X	455/472 (96%)	426 (94%)	29 (6%)	0	100	100
1	Z	455/472 (96%)	425 (93%)	30 (7%)	0	100	100
All	All	10920/11328 (96%)	10199 (93%)	721 (7%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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 PDB entries followed by that with respect to all EM entries.

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	386/409 (94%)	386 (100%)	0	100	100
1	BA	386/409 (94%)	386 (100%)	0	100	100
1	C	386/409 (94%)	386 (100%)	0	100	100
1	DA	386/409 (94%)	386 (100%)	0	100	100
1	E	386/409 (94%)	386 (100%)	0	100	100
1	FA	386/409 (94%)	386 (100%)	0	100	100
1	G	386/409 (94%)	386 (100%)	0	100	100
1	HA	386/409 (94%)	386 (100%)	0	100	100
1	I	386/409 (94%)	386 (100%)	0	100	100
1	JA	386/409 (94%)	386 (100%)	0	100	100
1	K	386/409 (94%)	386 (100%)	0	100	100
1	LA	386/409 (94%)	386 (100%)	0	100	100
1	M	386/409 (94%)	386 (100%)	0	100	100
1	NA	386/409 (94%)	386 (100%)	0	100	100
1	O	386/409 (94%)	386 (100%)	0	100	100
1	PA	386/409 (94%)	386 (100%)	0	100	100
1	Q	386/409 (94%)	386 (100%)	0	100	100
1	RA	386/409 (94%)	386 (100%)	0	100	100
1	S	386/409 (94%)	386 (100%)	0	100	100
1	TA	386/409 (94%)	386 (100%)	0	100	100
1	V	386/409 (94%)	386 (100%)	0	100	100
1	VA	386/409 (94%)	386 (100%)	0	100	100
1	X	386/409 (94%)	386 (100%)	0	100	100
1	Z	386/409 (94%)	386 (100%)	0	100	100
All	All	9264/9816 (94%)	9264 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 181 such sidechains are listed below:

Mol	Chain	Res	Type
1	FA	95	ASN
1	LA	259	HIS
1	FA	203	GLN

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Mol	Chain	Res	Type
1	JA	39	ASN
1	NA	441	GLN

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 24 ligands modelled in this entry, 24 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.

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Map visualisation

This section contains visualisations of the EMDB entry EMD-11023. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections

This section was not generated.

5.2 Central slices

This section was not generated.

5.3 Largest variance slices

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

5.5 Orthogonal surface views

This section was not generated.

5.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

6 Map analysis

This section contains the results of statistical analysis of the map.

6.1 Map-value distribution

This section was not generated.

6.2 Volume estimate versus contour level

This section was not generated.

6.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

7 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

8 Map-model fit

This section was not generated.