



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:23 PM UTC

PDB ID : 7LYS / pdb_00007lys
EMDB ID : EMD-23600
Title : Cryo-EM structure of CasPhi-2 (Cas12j) bound to crRNA and DNA
Authors : Pausch, P.; Soczek, K.; Nogales, E.; Doudna, J.
Deposited on : 2021-03-08
Resolution : 3.05 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

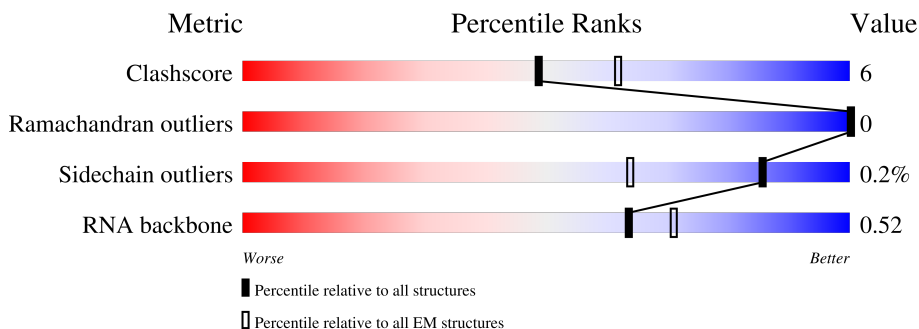
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.05 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	763	 74% 13% 12%
2	B	45	 67% 20% • 9%
3	C	39	 72% 5% 23%
4	D	39	 46% 54%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13573 atoms, of which 6374 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 CasPhi-2.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	669	Total	C	H	N	O	S	0	0
			10734	3374	5388	975	983	14		

- Molecule 2 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	41	Total	C	H	N	O	P	0	0
			1323	392	444	162	284	41		

- Molecule 3 is a DNA chain called TS-DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	30	Total	C	H	N	O	P	0	0
			948	291	338	111	178	30		

- Molecule 4 is a DNA chain called NTS-DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	18	Total	C	H	N	O	P	0	0
			568	175	204	65	107	17		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	396531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.15	0/5462	0.34	0/7394
2	B	0.16	0/983	0.21	0/1531
3	C	0.21	0/683	0.37	0/1050
4	D	0.22	0/407	0.43	0/626
All	All	0.16	0/7535	0.34	0/10601

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	5346	5388	5388	78	0
2	B	879	444	445	5	0
3	C	610	338	338	2	0
4	D	364	204	205	0	0
All	All	7199	6374	6376	78	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 6.

All (78) 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:A:313:VAL:HG13	1:A:316:LEU:HD12	1.49	0.94
1:A:24:ARG:NH2	1:A:52:GLU:OE1	2.13	0.82
1:A:263:SER:OG	1:A:266:THR:O	1.98	0.81
1:A:547:ARG:NE	2:B:16:A:OP2	2.17	0.78
1:A:236:VAL:HG21	1:A:283:MET:HG2	1.69	0.74
1:A:21:GLU:N	1:A:21:GLU:OE1	2.21	0.73
1:A:183:ASN:OD1	1:A:184:GLU:N	2.23	0.71
1:A:20:GLY:N	1:A:21:GLU:OE1	2.24	0.69
1:A:143:VAL:HG11	1:A:188:LEU:HD21	1.74	0.69
1:A:385:THR:OG1	1:A:386:GLN:OE1	2.12	0.68
1:A:240:ARG:NH2	1:A:283:MET:SD	2.68	0.67
1:A:397:GLN:OE1	1:A:397:GLN:N	2.28	0.66
1:A:511:SER:OG	1:A:514:GLN:OE1	2.14	0.66
1:A:7:GLU:N	1:A:7:GLU:OE1	2.30	0.65
1:A:147:VAL:HG21	1:A:181:ALA:HB2	1.78	0.64
1:A:313:VAL:HG12	1:A:313:VAL:O	1.99	0.62
1:A:457:GLU:N	1:A:457:GLU:OE1	2.33	0.61
1:A:325:ILE:HD11	1:A:356:TYR:CE1	2.36	0.60
1:A:78:ILE:HD13	1:A:198:PHE:CE1	2.37	0.60
1:A:386:GLN:OE1	1:A:386:GLN:N	2.33	0.60
1:A:168:GLU:N	1:A:168:GLU:OE1	2.37	0.57
1:A:204:ILE:HG22	1:A:302:VAL:HG13	1.86	0.56
1:A:489:LEU:HD12	1:A:490:PRO:HD2	1.89	0.54
1:A:204:ILE:HD12	1:A:304:ILE:HA	1.89	0.54
1:A:494:MET:O	1:A:622:GLY:N	2.41	0.53
1:A:56:PRO:HB2	1:A:358:LEU:HD12	1.90	0.53
1:A:349:ARG:NH2	2:B:4:U:OP1	2.42	0.53
1:A:144:LEU:HD23	1:A:144:LEU:O	2.08	0.53
1:A:536:LYS:NZ	3:C:-18:DG:O5'	2.41	0.52
1:A:9:GLU:OE1	1:A:35:LEU:HD21	2.10	0.52
1:A:420:LEU:HD23	1:A:596:THR:HG22	1.92	0.51
1:A:293:LYS:O	1:A:314:ARG:NH2	2.44	0.51
1:A:220:GLU:OE2	1:A:220:GLU:N	2.44	0.50
1:A:203:THR:O	1:A:204:ILE:HD13	2.12	0.50
1:A:515:VAL:HG23	1:A:516:PHE:H	1.77	0.50
1:A:189:LEU:HD23	1:A:189:LEU:H	1.76	0.49
1:A:272:VAL:O	1:A:272:VAL:HG23	2.14	0.48
1:A:564:LYS:NZ	1:A:570:TYR:OH	2.47	0.48
1:A:143:VAL:CG1	1:A:188:LEU:HD21	2.41	0.48
1:A:345:ILE:HG12	1:A:352:VAL:HG22	1.96	0.47
1:A:515:VAL:HG23	1:A:516:PHE:N	2.28	0.47
1:A:78:ILE:HD13	1:A:198:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:VAL:O	1:A:469:VAL:HG12	2.14	0.47
1:A:204:ILE:HG22	1:A:204:ILE:O	2.14	0.47
1:A:198:PHE:HB3	1:A:345:ILE:HB	1.95	0.47
1:A:489:LEU:HD11	1:A:500:PHE:HB3	1.96	0.47
1:A:478:LEU:HD21	1:A:501:ILE:HD12	1.96	0.47
1:A:204:ILE:HG23	1:A:303:ARG:O	2.16	0.46
1:A:311:ILE:HD13	1:A:352:VAL:HG21	1.98	0.46
1:A:276:SER:O	2:B:-20:G:N2	2.49	0.45
1:A:370:LEU:HD12	1:A:370:LEU:N	2.32	0.45
1:A:585:ILE:HD13	1:A:643:ALA:HB1	1.99	0.44
1:A:632:GLU:OE2	1:A:634:ARG:NE	2.51	0.44
1:A:498:THR:HG23	1:A:537:ASP:OD2	2.18	0.43
1:A:706:VAL:HG22	1:A:706:VAL:O	2.18	0.43
1:A:592:THR:CG2	1:A:601:VAL:HG21	2.48	0.43
1:A:109:HIS:NE2	1:A:130:ASN:OD1	2.47	0.43
1:A:270:VAL:O	1:A:270:VAL:HG23	2.18	0.43
1:A:340:THR:HG21	3:C:0:DT:OP2	2.19	0.43
1:A:658:VAL:O	1:A:658:VAL:HG23	2.18	0.43
1:A:407:ARG:O	1:A:407:ARG:CG	2.67	0.42
1:A:592:THR:HG21	1:A:601:VAL:HG21	2.01	0.42
1:A:307:ASP:N	1:A:307:ASP:OD1	2.52	0.42
1:A:580:LEU:HD23	1:A:580:LEU:O	2.20	0.42
1:A:422:ARG:NE	1:A:697:ASP:HA	2.34	0.42
1:A:515:VAL:HG23	1:A:516:PHE:CD1	2.55	0.42
1:A:614:HIS:CD2	2:B:10:U:H4'	2.55	0.41
1:A:282:ARG:NH1	2:B:-16:G:N7	2.67	0.41
1:A:313:VAL:O	1:A:313:VAL:CG1	2.65	0.41
1:A:505:LEU:HD22	1:A:515:VAL:HG11	2.01	0.41
1:A:450:ARG:NH2	1:A:563:LEU:HD12	2.36	0.41
1:A:285:ARG:HG3	1:A:286:TYR:N	2.36	0.41
1:A:557:ASN:OD1	1:A:558:GLU:N	2.54	0.41
1:A:68:THR:HG23	1:A:308:TRP:HZ3	1.86	0.40
1:A:313:VAL:CG1	1:A:316:LEU:HD12	2.36	0.40
1:A:699:ALA:O	1:A:703:LEU:HD13	2.21	0.40
1:A:165:ARG:HD3	1:A:169:GLY:HA3	2.04	0.40
1:A:244:GLN:OE1	1:A:244:GLN:N	2.54	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 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	663/763 (87%)	663 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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 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	573/649 (88%)	572 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	135	HIS
1	A	229	ASN
1	A	255	GLN
1	A	508	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	40/45 (88%)	8 (20%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	-20	G
2	B	-19	A
2	B	-18	U
2	B	-9	A
2	B	-8	C
2	B	-6	A
2	B	1	A
2	B	4	U

There are no RNA pucker outliers to report.

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-23600. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

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

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit

This section was not generated.