



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Sep 6, 2017 – 04:29 PM EDT

PDB ID : 5XWY
EMDB ID: : EMD-6777
Title : Electron cryo-microscopy structure of LbuCas13a-crRNA binary complex
Authors : Zhang, X.; Wang, Y.; Ma, J.; Liu, L.; Li, X.; Li, Z.; You, L.; Wang, J.; Wang, M.
Deposited on : unknown
Resolution : 3.20 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

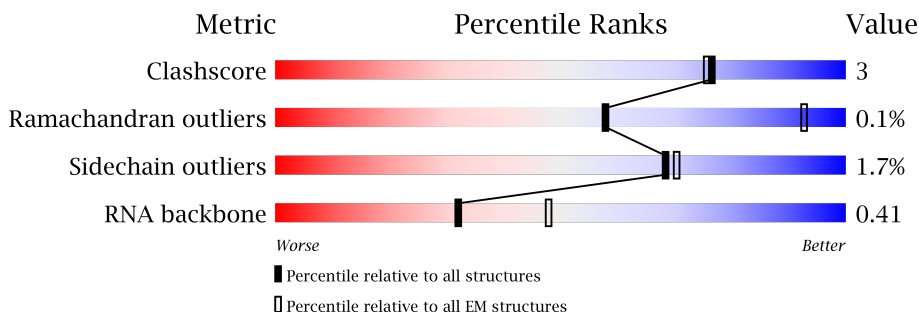
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

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 3.20 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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

Mol	Chain	Length	Quality of chain
1	A	1159	
2	B	59	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10493 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 A type VI-A CRISPR-Cas RNA-guided RNA ribonuclease, Cas13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1117	9407	6040	1582	1761	24	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1048	ALA	ARG	engineered mutation	UNP C7NBY4
A	1053	ALA	HIS	engineered mutation	UNP C7NBY4

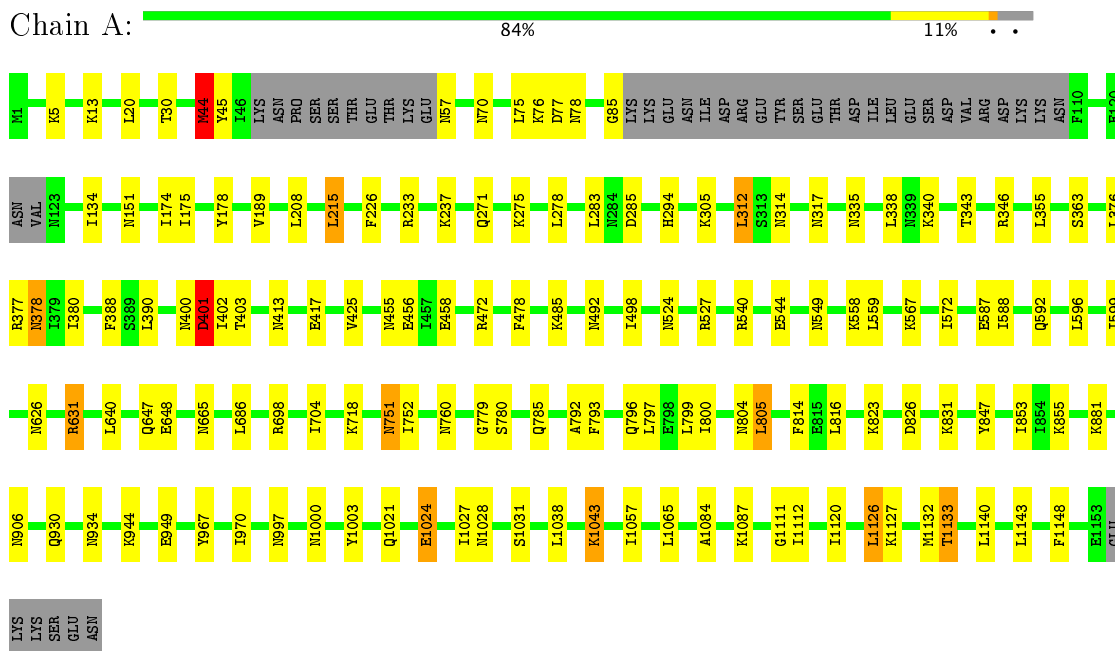
- Molecule 2 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	51	1086	488	202	345	51	0	0

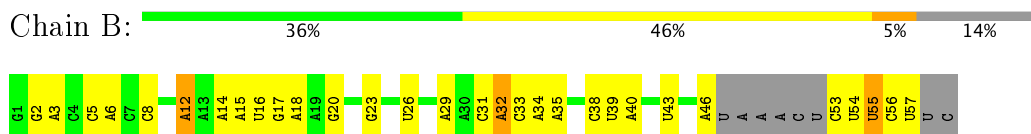
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: A type VI-A CRISPR-Cas RNA-guided RNA ribonuclease, Cas13a



- Molecule 2: RNA (59-MER)



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	238758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k 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 >2	RMSZ	# Z >2
1	A	0.41	0/9562	0.65	13/12783 (0.1%)
2	B	0.73	0/1215	0.95	0/1887
All	All	0.46	0/10777	0.69	13/14670 (0.1%)

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	A	0	9

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1126	LEU	CA-CB-CG	9.13	136.30	115.30
1	A	312	LEU	CA-CB-CG	7.96	133.62	115.30
1	A	215	LEU	CA-CB-CG	7.86	133.38	115.30
1	A	544	GLU	C-N-CA	6.78	138.66	121.70
1	A	1143	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	805	LEU	CA-CB-CG	5.80	128.64	115.30
1	A	401	ASP	C-N-CA	5.53	135.52	121.70
1	A	215	LEU	CB-CG-CD1	5.49	120.34	111.00
1	A	44	MET	C-N-CA	5.45	135.33	121.70
1	A	390	LEU	CA-CB-CG	5.29	127.45	115.30
1	A	704	ILE	C-N-CA	5.22	133.27	122.30
1	A	355	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	799	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1024	GLU	Peptide
1	A	1043	LYS	Peptide
1	A	1132	MET	Peptide
1	A	312	LEU	Peptide
1	A	401	ASP	Peptide
1	A	403	THR	Peptide
1	A	44	MET	Peptide
1	A	814	PHE	Peptide
1	A	847	TYR	Peptide

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	9407	0	9554	69	0
2	B	1086	0	554	12	0
All	All	10493	0	10108	70	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 3.

All (70) 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:233:ARG:NH2	2:B:18:A:O2'	2.31	0.64
1:A:997:ASN:HD21	1:A:1000:ASN:HB2	1.61	0.64
1:A:5:LYS:NZ	2:B:23:G:OP2	2.31	0.62
1:A:1021:GLN:HA	1:A:1027:ILE:HD11	1.85	0.58
1:A:275:LYS:HD2	2:B:12:A:H5'	1.86	0.57
1:A:816:LEU:HD23	1:A:855:LYS:HG2	1.86	0.57
1:A:44:MET:H	1:A:45:TYR:HB2	1.69	0.56
1:A:631:ARG:NH1	2:B:55:U:O2	2.37	0.56
1:A:527:ARG:NH2	1:A:587:GLU:OE1	2.38	0.56
1:A:1000:ASN:ND2	1:A:1003:TYR:O	2.39	0.55
1:A:596:LEU:HA	1:A:599:ILE:HD12	1.89	0.55
1:A:189:VAL:HG22	1:A:338:LEU:HD21	1.88	0.54
1:A:343:THR:HG22	1:A:346:ARG:HH12	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ASN:OD1	1:A:718:LYS:NZ	2.36	0.54
1:A:853:ILE:HG22	1:A:855:LYS:H	1.71	0.54
2:B:2:G:H5'	2:B:3:A:H5'	1.89	0.54
1:A:413:ASN:H	1:A:417:GLU:HA	1.71	0.53
1:A:20:LEU:HD12	1:A:30:THR:HA	1.91	0.52
1:A:1120:ILE:O	1:A:1133:THR:OG1	2.26	0.52
1:A:1087:LYS:NZ	2:B:5:C:OP2	2.43	0.51
1:A:237:LYS:NZ	2:B:14:A:OP1	2.43	0.51
1:A:626:ASN:HD22	1:A:640:LEU:HG	1.75	0.51
1:A:271:GLN:HG2	1:A:294:HIS:HD2	1.75	0.51
1:A:13:LYS:HG2	1:A:363:SER:HB3	1.93	0.51
1:A:823:LYS:O	1:A:831:LYS:NZ	2.43	0.51
1:A:401:ASP:HA	1:A:402:ILE:HG12	1.92	0.50
1:A:567:LYS:HA	1:A:572:ILE:HD12	1.93	0.50
1:A:881:LYS:O	1:A:944:LYS:NZ	2.42	0.49
1:A:558:LYS:NZ	2:B:31:C:OP1	2.45	0.49
1:A:1028:ASN:HA	1:A:1031:SER:HB2	1.94	0.49
1:A:1065:LEU:HG	1:A:1148:PHE:HB3	1.95	0.49
1:A:949:GLU:HB3	1:A:1140:LEU:HD13	1.95	0.49
1:A:1065:LEU:HD11	1:A:1112:ILE:HG13	1.96	0.48
1:A:485:LYS:HB3	1:A:792:ALA:HB1	1.95	0.48
1:A:5:LYS:HB3	1:A:665:ASN:HD21	1.79	0.47
1:A:305:LYS:NZ	2:B:20:G:N7	2.54	0.47
1:A:1127:LYS:NZ	2:B:53:C:OP1	2.48	0.47
1:A:797:LEU:HD13	1:A:800:ILE:HD12	1.97	0.47
1:A:1038:LEU:HD12	1:A:1043:LYS:HB2	1.98	0.46
1:A:930:GLN:O	1:A:934:ASN:ND2	2.49	0.46
1:A:1065:LEU:HD13	1:A:1111:GLY:HA2	1.98	0.46
1:A:785:GLN:HE21	1:A:793:PHE:H	1.64	0.45
1:A:1024:GLU:HG2	1:A:1027:ILE:HB	1.98	0.45
1:A:388:PHE:HE1	1:A:1057:ILE:HG21	1.81	0.45
1:A:402:ILE:HA	1:A:402:ILE:HD13	1.93	0.45
1:A:178:TYR:OH	1:A:285:ASP:OD1	2.28	0.44
1:A:456:GLU:HG2	1:A:498:ILE:HG13	2.00	0.44
1:A:380:ILE:HG23	1:A:472:ARG:HH22	1.82	0.44
1:A:425:VAL:HG21	1:A:458:GLU:HA	1.99	0.44
1:A:751:ASN:HD22	1:A:752:ILE:H	1.66	0.43
1:A:174:ILE:HG22	1:A:283:LEU:HD11	2.01	0.43
1:A:175:ILE:HD11	1:A:278:LEU:HD11	1.99	0.43
1:A:826:ASP:HB3	1:A:881:LYS:HD3	2.00	0.43
1:A:779:GLY:HA3	2:B:32:A:H2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LEU:HD23	1:A:134:ILE:HG21	2.01	0.43
1:A:793:PHE:HB3	1:A:796:GLN:HB2	2.01	0.43
1:A:378:ASN:OD1	1:A:780:SER:OG	2.31	0.43
1:A:340:LYS:HG2	2:B:8:C:H5"	2.01	0.43
1:A:208:LEU:HD23	1:A:226:PHE:HD2	1.84	0.42
1:A:376:LEU:HD11	1:A:478:PHE:HD2	1.83	0.42
1:A:540:ARG:HB3	1:A:698:ARG:HH11	1.84	0.42
1:A:967:TYR:OH	1:A:1084:ALA:O	2.33	0.42
1:A:377:ARG:HD2	1:A:970:ILE:HG12	2.02	0.42
1:A:75:LEU:HD12	1:A:78:ASN:HA	2.02	0.42
1:A:855:LYS:HZ3	1:A:855:LYS:HB3	1.85	0.42
1:A:76:LYS:HA	1:A:77:ASP:HA	1.69	0.41
1:A:70:ASN:OD1	1:A:85:GLY:N	2.40	0.41
1:A:559:LEU:HD11	1:A:686:LEU:HB2	2.02	0.41
1:A:647:GLN:HG2	1:A:648:GLU:H	1.85	0.41
1:A:588:ILE:O	1:A:592:GLN:N	2.50	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	1109/1159 (96%)	1024 (92%)	84 (8%)	1 (0%)	55 89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1133	THR

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	1037/1081 (96%)	1019 (98%)	18 (2%)	66 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	151	ASN
1	A	215	LEU
1	A	314	ASN
1	A	317	ASN
1	A	335	ASN
1	A	378	ASN
1	A	400	ASN
1	A	455	ASN
1	A	492	ASN
1	A	549	ASN
1	A	631	ARG
1	A	751	ASN
1	A	760	ASN
1	A	804	ASN
1	A	805	LEU
1	A	906	ASN
1	A	1126	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	151	ASN
1	A	173	ASN
1	A	191	ASN
1	A	294	HIS
1	A	335	ASN
1	A	400	ASN

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Mol	Chain	Res	Type
1	A	455	ASN
1	A	492	ASN
1	A	547	ASN
1	A	549	ASN
1	A	665	ASN
1	A	751	ASN
1	A	776	ASN
1	A	785	GLN
1	A	788	ASN
1	A	906	ASN
1	A	908	HIS
1	A	934	ASN
1	A	994	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	49/59 (83%)	19 (38%)	1 (2%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	6	A
2	B	12	A
2	B	15	A
2	B	16	U
2	B	17	G
2	B	26	U
2	B	29	A
2	B	32	A
2	B	33	C
2	B	34	A
2	B	35	A
2	B	38	C
2	B	39	U
2	B	40	A
2	B	43	U
2	B	46	A
2	B	54	U
2	B	55	U
2	B	57	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	56	C

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](#)

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.