



Full wwPDB EM Validation Report ⓘ

Sep 28, 2025 – 12:10 AM JST

PDB ID : 9JO8 / pdb_00009jo8
EMDB ID : EMD-61646
Title : Cryo-EM structure of the mono-DdCBE bound to a dsDNA substrate.
Authors : Jiangchao, X.; Wenchao, X.; Jia, C.; Bei, Y.
Deposited on : 2024-09-24
Resolution : 3.00 Å(reported)
Based on initial models : 3UGM, 8e5e

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 : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

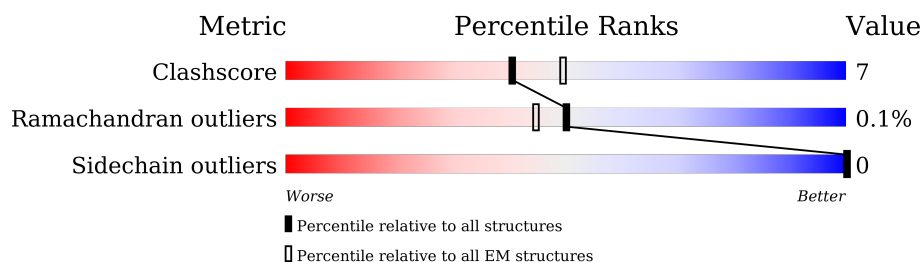
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	679	
2	B	33	
3	C	33	
4	D	133	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7001 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 TALE repeat protein targeting mitochondrial ND1-L gene..

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	638	Total	C	N	O	S	0	0
			4664	2916	860	873	15		

- Molecule 2 is a DNA chain called TALE repeat protein recognized single-strand DNA sequence and mitochondrial ND4 gene sequence..

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	33	Total	C	N	O	P	0	0
			670	321	117	199	33		

- Molecule 3 is a DNA chain called a complementary strand of TALE repeat protein recognized single-strand DNA sequence and a complementary strand of mitochondrial ND4 gene sequence..

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	33	Total	C	N	O	P	0	0
			683	325	128	197	33		

- Molecule 4 is a protein called Double-stranded DNA deaminase toxin A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	133	Total	C	N	O	S	0	0
			982	625	163	189	5		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1326	GLY	SER	engineered mutation	UNP P0DUH5
D	1330	ILE	SER	engineered mutation	UNP P0DUH5
D	1341	VAL	ALA	engineered mutation	UNP P0DUH5
D	1342	SER	ASN	engineered mutation	UNP P0DUH5
D	1348	SER	GLY	engineered mutation	UNP P0DUH5
D	1370	LYS	GLU	engineered mutation	UNP P0DUH5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1380	ILE	THR	engineered mutation	UNP P0DUH5
D	1398	VAL	ALA	engineered mutation	UNP P0DUH5
D	1413	ILE	THR	engineered mutation	UNP P0DUH5
D	1418	GLY	SER	engineered mutation	UNP P0DUH5

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
5	D	1	Total Zn 1 1	0

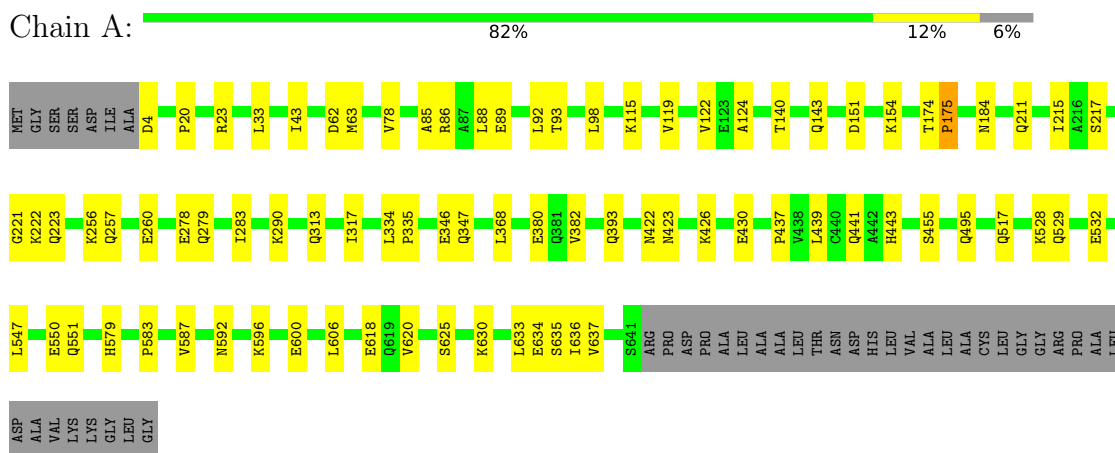
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total O 1 1	0

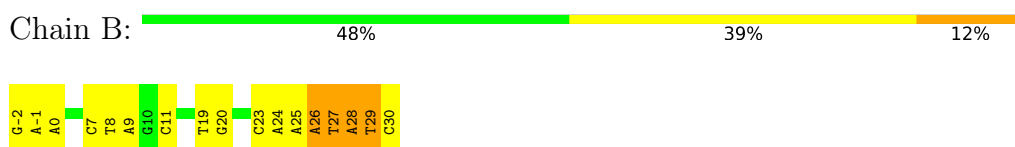
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

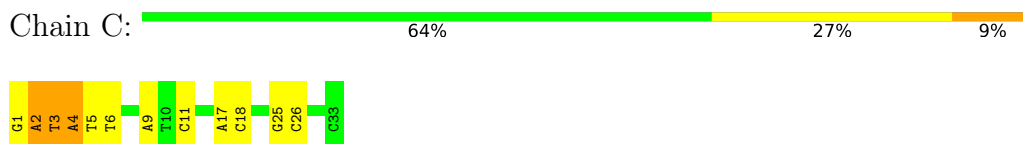
- Molecule 1: TALE repeat protein targeting mitochondrial ND1-L gene.



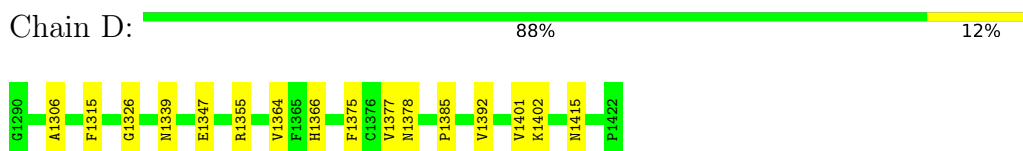
- Molecule 2: TALE repeat protein recognized single-strand DNA sequence and mitochondrial ND4 gene sequence.



- Molecule 3: a complementary strand of TALE repeat protein recognized single-strand DNA sequence and a complementary strand of mitochondrial ND4 gene sequence.



- Molecule 4: Double-stranded DNA deaminase toxin A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	248533	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor

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: 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	0.17	0/4732	0.36	4/6456 (0.1%)
2	B	0.34	0/749	0.69	4/1152 (0.3%)
3	C	0.34	0/767	0.62	3/1183 (0.3%)
4	D	0.11	0/1009	0.26	0/1375
All	All	0.21	0/7257	0.44	11/10166 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	29	DT	P-O3'-C3'	-7.01	109.68	120.20
3	C	3	DT	P-O3'-C3'	-6.50	110.46	120.20
1	A	151	ASP	CB-CA-C	6.37	119.84	109.90
2	B	26	DA	P-O3'-C3'	-6.32	110.73	120.20
3	C	2	DA	P-O3'-C3'	-6.02	111.17	120.20
1	A	151	ASP	N-CA-C	-6.02	101.13	110.10
2	B	28	DA	P-O3'-C3'	-5.82	111.47	120.20
3	C	4	DA	P-O3'-C3'	-5.81	111.49	120.20
2	B	27	DT	P-O3'-C3'	-5.77	111.55	120.20
1	A	175	PRO	CA-N-CD	5.69	119.97	112.00
1	A	423	ASN	N-CA-C	-5.13	101.33	109.59

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	4664	0	4834	52	0
2	B	670	0	374	18	0
3	C	683	0	373	15	0
4	D	982	0	951	17	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
All	All	7001	0	6532	92	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 7.

All (92) 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)
4:D:1347:GLU:OE2	4:D:1366:HIS:CD2	2.15	0.99
3:C:9:DA:H2''	4:D:1375:PHE:CE2	1.98	0.99
2:B:24:DA:H2'	2:B:25:DA:C8	2.16	0.80
3:C:9:DA:C2'	4:D:1375:PHE:CE2	2.65	0.77
3:C:9:DA:H2''	4:D:1375:PHE:HE2	1.48	0.73
1:A:278:GLU:N	1:A:278:GLU:OE1	2.24	0.71
1:A:346:GLU:OE1	1:A:346:GLU:N	2.26	0.67
1:A:174:THR:CG2	1:A:175:PRO:HD2	2.25	0.66
3:C:2:DA:H2''	3:C:3:DT:O2	1.98	0.63
1:A:124:ALA:HB2	1:A:154:LYS:HG3	1.83	0.60
1:A:174:THR:HG22	1:A:175:PRO:HD2	1.84	0.60
2:B:8:DT:H2''	2:B:9:DA:H5''	1.84	0.59
4:D:1347:GLU:OE2	4:D:1366:HIS:HD2	1.84	0.59
2:B:26:DA:H2''	2:B:27:DT:H73	1.84	0.59
3:C:3:DT:H2''	3:C:4:DA:H5'	1.85	0.58
2:B:29:DT:H2''	2:B:30:DC:C6	2.39	0.58
2:B:26:DA:H2''	2:B:27:DT:C7	2.35	0.57
2:B:28:DA:H1'	2:B:29:DT:H5'	1.86	0.57
1:A:426:LYS:O	1:A:430:GLU:HG3	2.05	0.56
2:B:27:DT:H3	3:C:4:DA:H2	1.53	0.55
1:A:4:ASP:N	1:A:4:ASP:OD1	2.41	0.54
1:A:528:LYS:O	1:A:532:GLU:HG3	2.07	0.54
1:A:63:MET:HE2	1:A:88:LEU:HB3	1.90	0.54
1:A:86:ARG:NH2	2:B:0:DA:OP2	2.41	0.54
1:A:592:ASN:ND2	1:A:625:SER:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:DT:H2''	2:B:28:DA:C8	2.42	0.54
3:C:9:DA:H2'	4:D:1375:PHE:CZ	2.44	0.53
4:D:1315:PHE:HD1	4:D:1364:VAL:HG22	1.73	0.53
3:C:17:DA:H2'	3:C:18:DC:C6	2.43	0.53
2:B:23:DC:H2''	2:B:24:DA:C8	2.44	0.52
3:C:25:DG:H2'	3:C:26:DC:C6	2.45	0.52
1:A:620:VAL:HG23	1:A:633:LEU:HD21	1.91	0.52
2:B:7:DC:H2''	2:B:8:DT:H5''	1.93	0.51
1:A:279:GLN:O	1:A:283:ILE:HG13	2.10	0.51
1:A:635:SER:O	1:A:637:VAL:N	2.40	0.51
1:A:495:GLN:NE2	2:B:11:DC:OP1	2.44	0.50
2:B:25:DA:H2''	2:B:26:DA:O5'	2.12	0.50
1:A:437:PRO:O	1:A:441:GLN:HG3	2.12	0.49
1:A:439:LEU:HD23	1:A:443:HIS:CD2	2.47	0.49
2:B:28:DA:C2	3:C:4:DA:C2	3.00	0.49
1:A:20:PRO:HA	1:A:23:ARG:HG3	1.95	0.48
1:A:256:LYS:O	1:A:260:GLU:HG3	2.13	0.48
4:D:1401:VAL:HG13	4:D:1402:LYS:HG3	1.94	0.48
1:A:455:SER:O	1:A:455:SER:OG	2.27	0.47
4:D:1355:ARG:HB2	4:D:1385:PRO:HD3	1.95	0.47
2:B:25:DA:H2'	2:B:26:DA:C8	2.50	0.46
1:A:257:GLN:HB3	1:A:290:LYS:HD2	1.97	0.46
4:D:1347:GLU:HG2	4:D:1392:VAL:HG21	1.97	0.46
1:A:211:GLN:O	1:A:215:ILE:HG23	2.16	0.46
2:B:19:DT:H2'	2:B:20:DG:C4	2.51	0.46
1:A:119:VAL:HA	1:A:122:VAL:HG22	1.98	0.45
3:C:9:DA:C2'	4:D:1375:PHE:CZ	2.98	0.45
4:D:1339:ASN:OD1	4:D:1339:ASN:N	2.47	0.45
4:D:1315:PHE:CD1	4:D:1364:VAL:HG22	2.52	0.45
1:A:313:GLN:O	1:A:317:ILE:HG13	2.16	0.45
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.79	0.44
1:A:174:THR:HG23	1:A:175:PRO:HD2	1.98	0.44
1:A:347:GLN:NE2	1:A:380:GLU:OE1	2.51	0.43
1:A:579:HIS:CD2	1:A:606:LEU:HD23	2.52	0.43
4:D:1377:VAL:HG23	4:D:1378:ASN:OD1	2.17	0.43
1:A:630:LYS:NZ	1:A:634:GLU:OE1	2.29	0.43
1:A:63:MET:HG3	1:A:92:LEU:HD11	2.01	0.43
1:A:583:PRO:O	1:A:587:VAL:HG13	2.18	0.43
1:A:184:ASN:ND2	1:A:217:SER:O	2.51	0.43
1:A:89:GLU:O	1:A:93:THR:HG23	2.19	0.42
1:A:368:LEU:HD13	1:A:382:VAL:HG11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.81	0.42
1:A:221:GLY:O	1:A:222:LYS:HB3	2.19	0.42
1:A:517:GLN:NE2	1:A:550:GLU:OE1	2.52	0.42
2:B:25:DA:C6	2:B:26:DA:C6	3.07	0.42
4:D:1315:PHE:O	4:D:1326:GLY:HA2	2.19	0.42
3:C:1:DG:H2''	3:C:2:DA:C8	2.54	0.42
1:A:85:ALA:O	1:A:89:GLU:HG3	2.19	0.42
1:A:551:GLN:OE1	1:A:587:VAL:HG21	2.19	0.42
1:A:635:SER:OG	1:A:636:ILE:N	2.52	0.42
4:D:1415:ASN:OD1	4:D:1415:ASN:C	2.62	0.41
3:C:11:DC:H5'	3:C:11:DC:H6	1.84	0.41
2:B:-2:DG:H2''	2:B:-1:DA:C8	2.55	0.41
1:A:174:THR:HA	1:A:175:PRO:HD3	1.89	0.41
1:A:221:GLY:C	1:A:223:GLN:H	2.27	0.41
1:A:618:GLU:OE1	4:D:1306:ALA:HB1	2.20	0.41
3:C:5:DT:H2''	3:C:6:DT:H71	2.03	0.41
1:A:140:THR:HB	1:A:143:GLN:HG3	2.02	0.41
3:C:4:DA:H2''	3:C:5:DT:C6	2.56	0.41
1:A:550:GLU:OE1	1:A:550:GLU:HA	2.21	0.41
1:A:334:LEU:HB3	1:A:335:PRO:HD3	2.03	0.41
1:A:393:GLN:H	1:A:393:GLN:HG2	1.63	0.41
1:A:78:VAL:HG22	1:A:115:LYS:HB2	2.04	0.40
1:A:33:LEU:HD13	1:A:43:ILE:HG12	2.03	0.40
1:A:62:ASP:N	1:A:62:ASP:OD1	2.53	0.40
1:A:528:LYS:HG3	1:A:529:GLN:N	2.37	0.40
1:A:596:LYS:HG2	1:A:600:GLU:OE2	2.21	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	636/679 (94%)	614 (96%)	21 (3%)	1 (0%)	44	77
4	D	131/133 (98%)	125 (95%)	6 (5%)	0	100	100
All	All	767/812 (94%)	739 (96%)	27 (4%)	1 (0%)	50	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	ASN

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 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	495/523 (95%)	495 (100%)	0	100	100
4	D	106/106 (100%)	106 (100%)	0	100	100
All	All	601/629 (96%)	601 (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. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	GLN
1	A	245	GLN
1	A	341	HIS
1	A	354	ASN
1	A	443	HIS
1	A	511	HIS
1	A	529	GLN
1	A	545	HIS
1	A	558	ASN
1	A	585	GLN
4	D	1308	ASN
4	D	1349	GLN
4	D	1366	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.