



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Aug 17, 2017 – 03:12 PM EDT

PDB ID : 5A7U
EMDB ID: : EMD-3079
Title : Single-particle cryo-EM of co-translational folded adr1 domain inside the E. coli ribosome exit tunnel.
Authors : Nilsson, O.B.; Hedman, R.; Marino, J.; Wickles, S.; Bischoff, L.; Johansson, M.; Muller-Lucks, A.; Trovato, F.; Puglisi, J.D.; O'Brien, E.; Beckmann, R.; von Heijne, G.
Deposited on : unknown
Resolution : 4.80 Å(reported)
Based on PDB ID : 2ADR

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

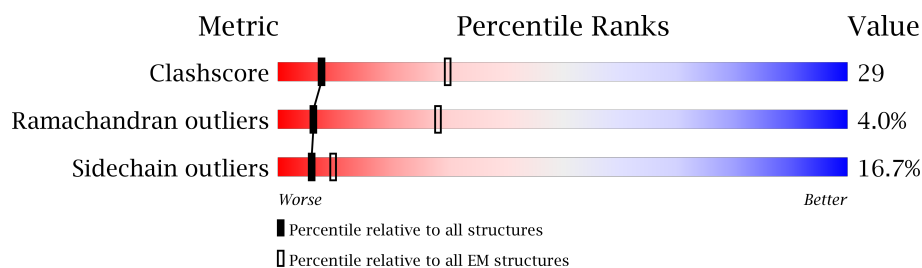
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 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

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	29	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	162	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 455 atoms, of which 231 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 REGULATORY PROTEIN ADR1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	27	Total	C	H	N	O	S	0	0
			454	140	231	47	34	2		

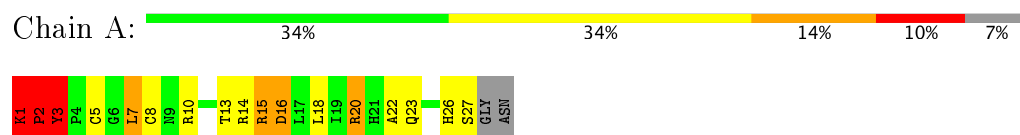
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total	Zn	0
			1	1	

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: REGULATORY PROTEIN ADR1



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	151900	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	MICROGRAPH	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.98	0/228	1.67	5/305 (1.6%)

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	13

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1	LYS	CB-CA-C	9.99	130.38	110.40
1	A	3	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	A	2	PRO	CA-N-CD	-5.78	103.41	111.50
1	A	20	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	16	ASP	CB-CG-OD2	-5.33	113.51	118.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	LYS	Peptide
1	A	10	ARG	Mainchain
1	A	14	ARG	Sidechain
1	A	15	ARG	Sidechain
1	A	16	ASP	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
1	A	2	PRO	Peptide
1	A	20	ARG	Sidechain
1	A	22	ALA	Mainchain
1	A	23	GLN	Sidechain
1	A	3	TYR	Sidechain
1	A	5	CYS	Mainchain
1	A	7	LEU	Mainchain

5.2 Too-close contacts ⓘ

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	223	231	231	13	0
2	A	1	0	0	2	0
All	All	224	231	231	13	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 29.

All (13) 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:8:CYS:HG	2:A:162:ZN:ZN	0.82	0.91
1:A:2:PRO:HG2	1:A:3:TYR:CZ	2.20	0.76
1:A:2:PRO:HG2	1:A:3:TYR:CE1	2.21	0.76
1:A:1:LYS:HB2	1:A:2:PRO:HD3	1.74	0.69
1:A:8:CYS:SG	2:A:162:ZN:ZN	1.88	0.58
1:A:1:LYS:CB	1:A:2:PRO:HD3	2.35	0.55
1:A:2:PRO:CG	1:A:3:TYR:CZ	2.90	0.55
1:A:2:PRO:HG2	1:A:3:TYR:CD1	2.44	0.51
1:A:3:TYR:CZ	1:A:15:ARG:HB2	2.46	0.50
1:A:7:LEU:HD13	1:A:26:HIS:HB3	1.95	0.48
1:A:3:TYR:CE1	1:A:15:ARG:HG3	2.49	0.47
1:A:2:PRO:HG2	1:A:3:TYR:CE2	2.50	0.45
1:A:1:LYS:HB2	1:A:2:PRO:CD	2.45	0.42

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	25/29 (86%)	18 (72%)	6 (24%)	1 (4%)	3	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO

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	24/26 (92%)	20 (83%)	4 (17%)	2	18

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

Mol	Chain	Res	Type
1	A	1	LYS
1	A	13	THR
1	A	18	LEU
1	A	27	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.