



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 22, 2017 – 03:55 AM EDT

PDB ID : 5N8O
EMDB ID: : EMD-3601
Title : Cryo EM structure of the conjugative relaxase TraI of the F/R1 plasmid system
Authors : Ilangovan, A.; Zanetti, G.; Waksman, G.
Deposited on : unknown
Resolution : 3.90 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary 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

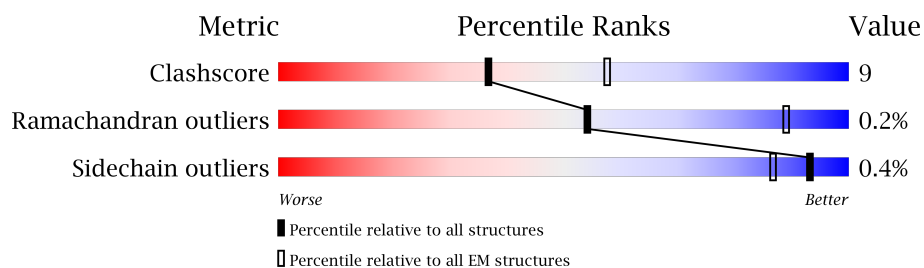
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	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	1756	
2	C	22	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 11362 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 DNA helicase I.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1432	Total	C	N	O	S	1	0
			11002	6795	2010	2152	45		

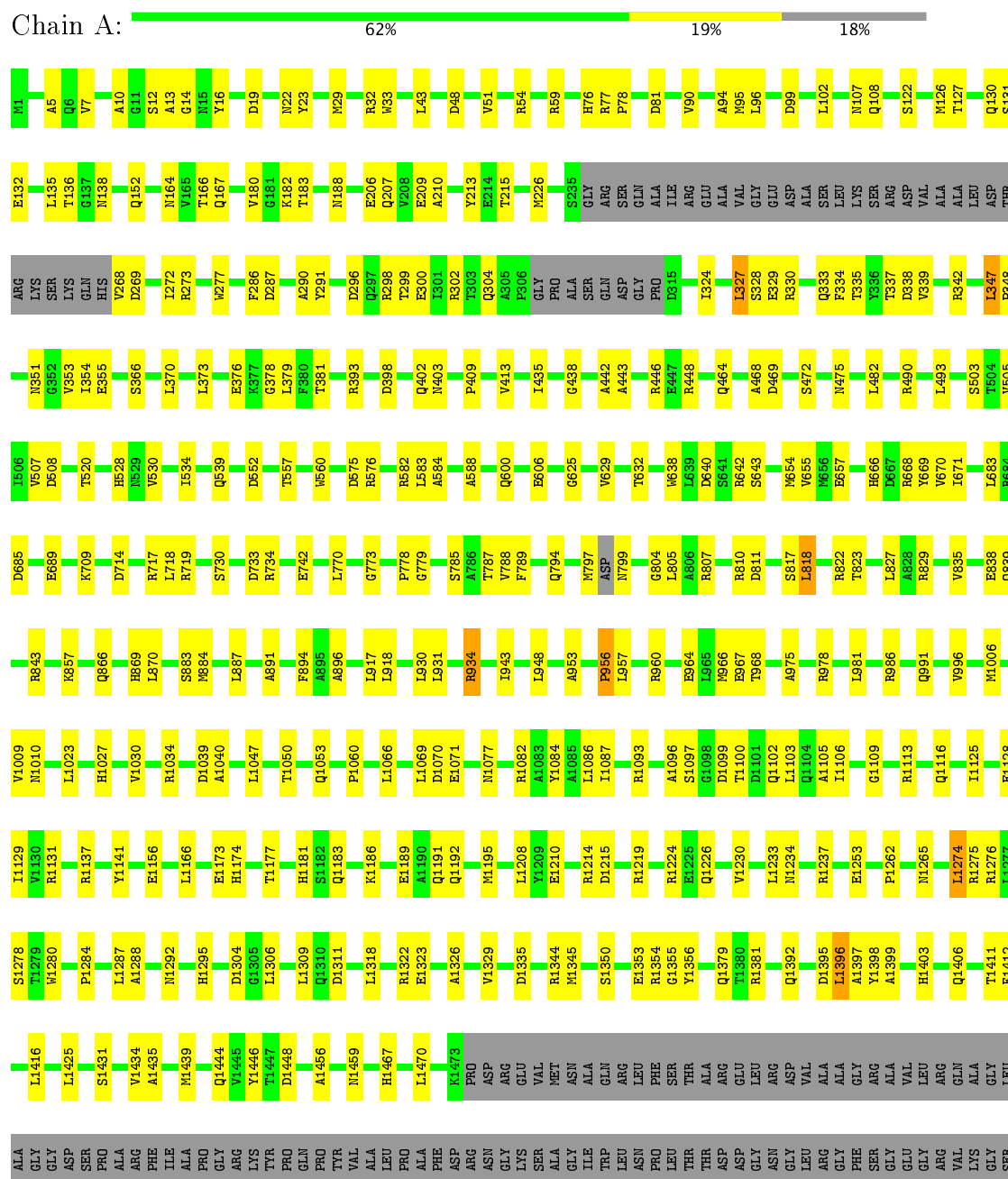
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	18	Total	C	N	O	P	0	0
			360	180	36	126	18		

3 Residue-property plots

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: DNA helicase I



GLY ASP ALA ALA GLN PHE VAL ALA LEU GLN GLY SER ARG ASN GLY GLU SER SER LEU LEU ALA ASP ASN MET GLN ASP GLY VAL ARG ILE ALA ARG ASP ASN PRO ASP GLY VAL VAL VAL ARG ILE ALA GLY GLY ARG PRO TRP THR GLY ARG VAL TRP

ASP	ILE	PRO	ASP	ASN	SER	VAL	GLN	PRO	GLY	ALA	GLY	ASN	GLY	GLY	PRO	VAL	THR	ALA	ALA	GLN	ARG	GLN	ALA	ALA	GLU	GLU	ALA	ILE	ARG	ARG	GLU	THR	GLU	GLU	ILE	VAL	ARG	LYS	MET	GLU	ALA	GLU	ASN	LYS	PRO	ASP	LEU	PRO	ASP	GLY	LYS	THR	GLU	LEU
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ALA VAL ARG ASP ILE ALA GLY GLN GLU ARG ASP ARG SER ILE ALA SER SER GLU ARG GLU THR ALA LEU ALA LEU PRO GLU SER VAL LEU ARG GLU SER GLN ARG GLU VAL ARG GLU VAL VAL ARG GLU VAL VAL ARG ARG ASN GLU LEU LEU LEU GLN ARG GLU ARG MET ASP MET VAL VAL ARG ASP

LEU
GLN
LYS
GLU
LYS
THR
LEU
GLY
GLY
ASP

- Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')

Chain C:  55% 23% 5% 18%

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	184451	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Done within relion software	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	47619	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	0.38	0/11164	0.69	14/15097 (0.1%)
2	C	0.96	0/395	1.41	1/608 (0.2%)
All	All	0.41	0/11559	0.73	15/15705 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	LEU	CA-CB-CG	8.78	135.50	115.30
1	A	1287	LEU	CB-CG-CD2	-7.98	97.44	111.00
1	A	1396	LEU	CA-CB-CG	7.20	131.86	115.30
2	C	7	DT	O4'-C1'-N1	6.71	112.69	108.00
1	A	373	LEU	CA-CB-CG	6.50	130.24	115.30

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	11002	0	10959	210	0
2	C	360	0	217	5	0
All	All	11362	0	11176	213	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 9.

The worst 5 of 213 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:576:ARG:HD3	1:A:1354:ARG:HG2	1.25	1.17
1:A:1354:ARG:HB3	1:A:1356:TYR:HE1	1.29	0.94
1:A:1354:ARG:HB3	1:A:1356:TYR:CE1	2.02	0.93
1:A:1355:GLY:O	1:A:1381:ARG:NH1	2.03	0.92
1:A:1350:SER:OG	1:A:1356:TYR:O	1.88	0.91

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	1421/1756 (81%)	1205 (85%)	213 (15%)	3 (0%)	51 84

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1284	PRO
1	A	1398	TYR
1	A	956	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	1169/1420 (82%)	1164 (100%)	5 (0%)	93 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	448	ARG
1	A	582	ARG
1	A	934	ARG
1	A	1113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	856	GLN
1	A	866	GLN
1	A	1295	HIS
1	A	794	GLN
1	A	1232	HIS

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1086:LEU	C	1087:ILE	N	4.43
1	A	354:ILE	C	355:GLU	N	3.14