



Full wwPDB X-ray Structure Validation Report

May 23, 2020 – 08:20 pm BST


PDB ID : 4I8O
Title : Crystal structure of the toxin RnlA from Escherichia coli
Authors : Wei, Y.; Gao, Z.Q.; Zhang, H.; Dong, Y.H.
Deposited on : 2012-12-04
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

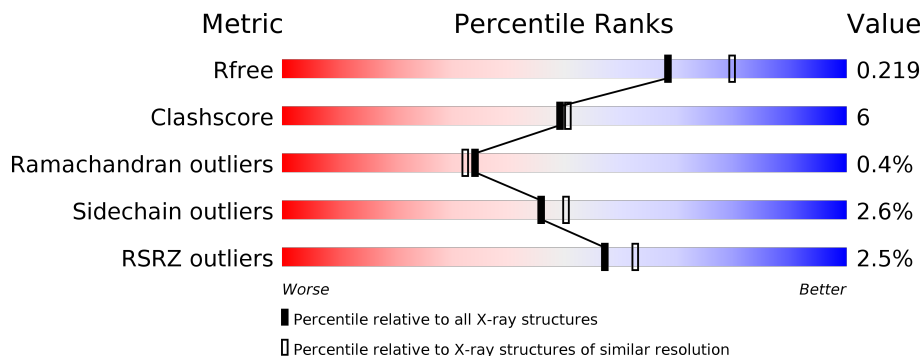
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	 2% 83% 12% . .
1	B	358	 3% 83% 13% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5762 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TOXIN RNLA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	344	2710	1730	463	505	3	9	0	2	0
1	B	344	2706	1728	463	503	3	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	EXPRESSION TAG	UNP P52129
B	1	SER	-	EXPRESSION TAG	UNP P52129

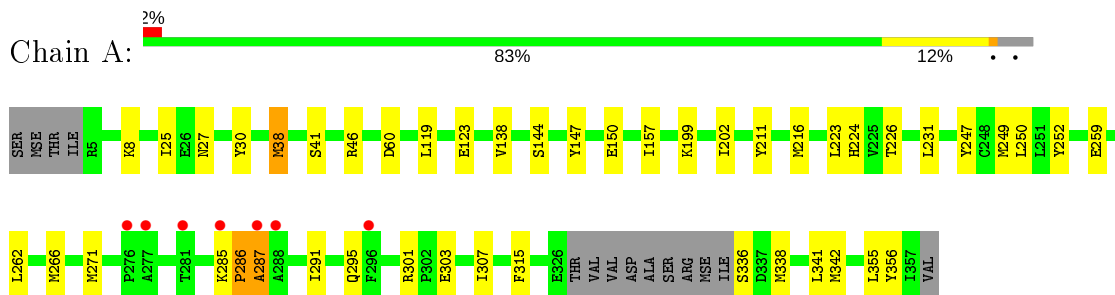
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	190	Total	O	0	0
			190	190		
2	B	156	Total	O	0	0
			156	156		

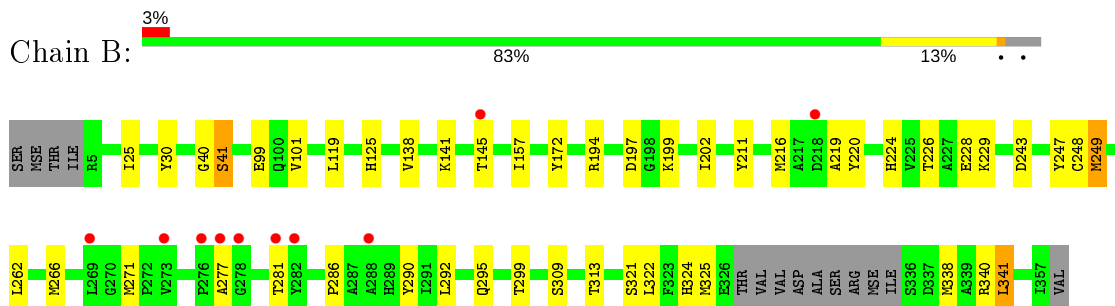
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: TOXIN RNLA



- Molecule 1: TOXIN RNLA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.21Å 64.32Å 82.62Å 69.24° 79.53° 75.03°	Depositor
Resolution (Å)	36.50 – 2.10 36.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.50-2.10) 97.6 (36.50-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.10Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.196 , 0.229 0.185 , 0.219	Depositor DCC
R_{free} test set	3056 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.444	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5762	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.45	0/2761	0.60	1/3731 (0.0%)
1	B	0.41	0/2751	0.59	2/3716 (0.1%)
All	All	0.43	0/5512	0.60	3/7447 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	LEU	CA-CB-CG	-6.36	100.67	115.30
1	B	286	PRO	N-CA-CB	6.04	110.55	103.30
1	A	286	PRO	N-CA-CB	5.75	110.20	103.30

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	2710	0	2707	27	0
1	B	2706	0	2707	37	0
2	A	190	0	0	3	0
2	B	156	0	0	6	0
All	All	5762	0	5414	64	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 (64) 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:B:40:GLY:HA3	1:B:41:SER:HB3	1.55	0.88
1:A:338:MSE:HE1	1:A:341:LEU:HD23	1.62	0.81
1:B:321:SER:O	2:B:474:HOH:O	2.00	0.80
1:B:325:MSE:N	2:B:474:HOH:O	2.23	0.72
1:A:285:LYS:NZ	1:A:287:ALA:O	2.26	0.67
1:B:290:TYR:H	1:B:313:THR:HG22	1.60	0.66
1:B:40:GLY:CA	1:B:41:SER:HB3	2.25	0.65
1:B:229:LYS:NZ	2:B:524:HOH:O	2.28	0.65
1:B:309:SER:O	1:B:313:THR:HG23	1.97	0.64
1:B:224:HIS:ND1	1:B:226:THR:HG22	2.15	0.62
1:A:262:LEU:O	1:A:266:MSE:HG2	2.03	0.59
1:B:324:HIS:N	2:B:474:HOH:O	2.36	0.59
1:B:172:TYR:HE2	1:B:249:MSE:HE1	1.69	0.57
1:A:199:LYS:O	1:A:202:ILE:HG13	2.04	0.56
1:B:271:MSE:HE1	1:B:292:LEU:HD22	1.87	0.55
1:B:247:TYR:O	1:B:341:LEU:HD13	2.08	0.54
1:A:25:ILE:HG23	1:A:30:TYR:HB2	1.90	0.52
1:B:248:CYS:HB3	1:B:322:LEU:HD21	1.92	0.52
1:A:336:SER:N	2:A:512:HOH:O	2.41	0.52
1:B:341:LEU:O	1:B:341:LEU:HG	2.10	0.52
1:B:138:VAL:HG23	1:B:157:ILE:HD11	1.92	0.52
1:B:290:TYR:H	1:B:313:THR:CG2	2.23	0.51
1:B:277:ALA:HB1	1:B:281:THR:CG2	2.41	0.51
1:B:340:ARG:NH2	2:B:437:HOH:O	2.35	0.51
1:B:194:ARG:HH21	1:B:249:MSE:HE2	1.74	0.51
1:A:38:MSE:HE1	1:A:60:ASP:CG	2.30	0.50
1:A:138:VAL:HG23	1:A:157:ILE:HD11	1.93	0.50
1:B:262:LEU:O	1:B:266:MSE:HG2	2.11	0.50
1:B:338:MSE:HE3	1:B:338:MSE:O	2.12	0.50
1:B:295:GLN:OE1	1:B:295:GLN:N	2.31	0.49
1:B:199:LYS:O	1:B:202:ILE:HG13	2.12	0.49
1:B:125:HIS:HA	1:B:145:THR:HB	1.94	0.49
1:B:338:MSE:HE1	1:B:341:LEU:CD2	2.43	0.48
1:A:223:LEU:HD23	1:A:356:TYR:CE2	2.48	0.48
1:B:99:GLU:OE2	1:B:194:ARG:NH1	2.43	0.48
1:B:266:MSE:HE3	1:B:271:MSE:HE2	1.95	0.47
1:B:194:ARG:HE	1:B:249:MSE:HE2	1.79	0.47
1:A:301:ARG:NH1	1:A:303:GLU:OE1	2.48	0.47
1:A:38:MSE:HB3	1:A:38:MSE:HE2	1.40	0.47
1:B:340:ARG:NE	2:B:418:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:MSE:HE3	1:A:252:TYR:CE1	2.50	0.46
1:A:8:LYS:HB3	1:A:8:LYS:HE2	1.69	0.46
1:B:25:ILE:HG23	1:B:30:TYR:HB2	1.96	0.46
1:A:123:GLU:O	2:A:405:HOH:O	2.21	0.46
1:B:216:MSE:HE3	1:B:219:ALA:HB3	1.98	0.45
1:A:338:MSE:HE3	1:A:338:MSE:O	2.17	0.44
1:B:271:MSE:HE1	1:B:292:LEU:CD2	2.48	0.44
1:B:40:GLY:HA3	1:B:41:SER:CB	2.38	0.43
1:A:144:SER:O	1:A:147:TYR:O	2.36	0.43
1:A:224:HIS:ND1	1:A:226:THR:HG22	2.34	0.43
1:A:307:ILE:HG22	1:A:355:LEU:HD23	2.01	0.43
1:A:27:ASN:ND2	2:A:518:HOH:O	2.41	0.43
1:A:38:MSE:HE3	1:A:46:ARG:HB2	2.01	0.42
1:B:338:MSE:HE1	1:B:341:LEU:HD23	2.01	0.42
1:B:220:TYR:OH	1:B:228:GLU:OE2	2.35	0.42
1:B:194:ARG:HE	1:B:249:MSE:CE	2.32	0.42
1:A:247:TYR:O	1:A:250:LEU:HB2	2.20	0.42
1:A:138:VAL:CG2	1:A:157:ILE:HD11	2.51	0.41
1:A:216:MSE:HE3	1:A:231:LEU:HD13	2.01	0.41
1:A:223:LEU:HA	1:A:223:LEU:HD23	1.86	0.41
1:A:259:GLU:HB2	1:A:315:PHE:CE1	2.55	0.41
1:A:266:MSE:HB2	1:A:271:MSE:HB2	2.02	0.41
1:A:338:MSE:HE2	1:A:342:MSE:SE	2.72	0.40
1:B:292:LEU:HD23	1:B:292:LEU:HA	1.85	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 X-ray entries followed by that with respect to entries of similar resolution.

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	342/358 (96%)	335 (98%)	5 (2%)	2 (1%)	25 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	340/358 (95%)	332 (98%)	7 (2%)	1 (0%)	41	41
All	All	682/716 (95%)	667 (98%)	12 (2%)	3 (0%)	34	32

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	SER
1	A	286	PRO
1	A	287	ALA

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 X-ray entries followed by that with respect to entries of similar resolution.

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	294/299 (98%)	287 (98%)	7 (2%)	49	53
1	B	293/299 (98%)	285 (97%)	8 (3%)	44	48
All	All	587/598 (98%)	572 (97%)	15 (3%)	46	50

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	MSE
1	A	41	SER
1	A	119	LEU
1	A	150	GLU
1	A	211	TYR
1	A	291	ILE
1	A	295	GLN
1	B	101	VAL
1	B	119	LEU
1	B	141	LYS
1	B	197	ASP
1	B	211	TYR
1	B	243	ASP

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Mol	Chain	Res	Type
1	B	249	MSE
1	B	299	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	ASN

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 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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/358 (93%)	-0.24	7 (2%) 63 68	20, 35, 65, 90	0
1	B	335/358 (93%)	-0.09	10 (2%) 50 56	22, 40, 71, 84	0
All	All	670/716 (93%)	-0.17	17 (2%) 57 62	20, 37, 69, 90	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	PRO	6.0
1	B	277	ALA	3.8
1	A	276	PRO	3.6
1	B	269	LEU	2.9
1	A	281	THR	2.8
1	A	296	PHE	2.7
1	B	278	GLY	2.7
1	B	218	ASP	2.4
1	B	282	TYR	2.4
1	A	287	ALA	2.2
1	B	281	THR	2.2
1	A	277	ALA	2.1
1	B	288	ALA	2.1
1	A	285	LYS	2.1
1	A	288	ALA	2.1
1	B	145	THR	2.0
1	B	273	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.