Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 AM GMT

PDB ID	:	3Q9V
Title	:	Crystal structure of rra c-terminal domain(123-221) from Deinococcus radiodurans
Authors	:	Liu, Y.; Gao, Z.Q.; Dong, Y.H.; Ji, C.N.
Deposited on	:	2011-01-10
Resolution	:	1.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

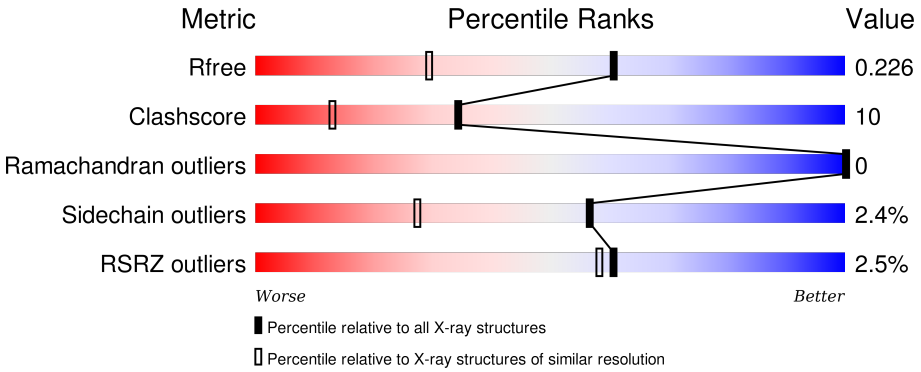
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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. 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 <=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	133	% 59% 14% · 26%
1	B	133	3% 58% 16% · 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1828 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 DNA-binding response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	1	0
			786	494	145	145	2			
1	B	99	Total	C	N	O	S	0	0	0
			786	493	146	145	2			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	EXPRESSION TAG	UNP Q9RRR8
A	90	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	91	SER	-	EXPRESSION TAG	UNP Q9RRR8
A	92	SER	-	EXPRESSION TAG	UNP Q9RRR8
A	93	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	94	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	95	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	96	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	97	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	98	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	99	SER	-	EXPRESSION TAG	UNP Q9RRR8
A	100	SER	-	EXPRESSION TAG	UNP Q9RRR8
A	101	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	102	GLU	-	EXPRESSION TAG	UNP Q9RRR8
A	103	ASN	-	EXPRESSION TAG	UNP Q9RRR8
A	104	LEU	-	EXPRESSION TAG	UNP Q9RRR8
A	105	TYR	-	EXPRESSION TAG	UNP Q9RRR8
A	106	PHE	-	EXPRESSION TAG	UNP Q9RRR8
A	107	GLU	-	EXPRESSION TAG	UNP Q9RRR8
A	108	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	109	SER	-	EXPRESSION TAG	UNP Q9RRR8
A	110	HIS	-	EXPRESSION TAG	UNP Q9RRR8
A	111	MET	-	EXPRESSION TAG	UNP Q9RRR8
A	112	ALA	-	EXPRESSION TAG	UNP Q9RRR8
A	113	SER	-	EXPRESSION TAG	UNP Q9RRR8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	114	MET	-	EXPRESSION TAG	UNP Q9RRR8
A	115	THR	-	EXPRESSION TAG	UNP Q9RRR8
A	116	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	117	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	118	GLN	-	EXPRESSION TAG	UNP Q9RRR8
A	119	GLN	-	EXPRESSION TAG	UNP Q9RRR8
A	120	MET	-	EXPRESSION TAG	UNP Q9RRR8
A	121	GLY	-	EXPRESSION TAG	UNP Q9RRR8
A	122	ARG	-	EXPRESSION TAG	UNP Q9RRR8
A	216	GLY	ALA	SEE REMARK 999	UNP Q9RRR8
A	217	TYR	THR	SEE REMARK 999	UNP Q9RRR8
A	218	ALA	PRO	SEE REMARK 999	UNP Q9RRR8
A	219	LEU	CYS	SEE REMARK 999	UNP Q9RRR8
A	220	ARG	ALA	SEE REMARK 999	UNP Q9RRR8
A	221	GLY	ALA	SEE REMARK 999	UNP Q9RRR8
B	89	MET	-	EXPRESSION TAG	UNP Q9RRR8
B	90	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	91	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	92	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	93	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	94	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	95	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	96	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	97	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	98	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	99	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	100	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	101	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	102	GLU	-	EXPRESSION TAG	UNP Q9RRR8
B	103	ASN	-	EXPRESSION TAG	UNP Q9RRR8
B	104	LEU	-	EXPRESSION TAG	UNP Q9RRR8
B	105	TYR	-	EXPRESSION TAG	UNP Q9RRR8
B	106	PHE	-	EXPRESSION TAG	UNP Q9RRR8
B	107	GLU	-	EXPRESSION TAG	UNP Q9RRR8
B	108	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	109	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	110	HIS	-	EXPRESSION TAG	UNP Q9RRR8
B	111	MET	-	EXPRESSION TAG	UNP Q9RRR8
B	112	ALA	-	EXPRESSION TAG	UNP Q9RRR8
B	113	SER	-	EXPRESSION TAG	UNP Q9RRR8
B	114	MET	-	EXPRESSION TAG	UNP Q9RRR8
B	115	THR	-	EXPRESSION TAG	UNP Q9RRR8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	116	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	117	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	118	GLN	-	EXPRESSION TAG	UNP Q9RRR8
B	119	GLN	-	EXPRESSION TAG	UNP Q9RRR8
B	120	MET	-	EXPRESSION TAG	UNP Q9RRR8
B	121	GLY	-	EXPRESSION TAG	UNP Q9RRR8
B	122	ARG	-	EXPRESSION TAG	UNP Q9RRR8
B	216	GLY	ALA	SEE REMARK 999	UNP Q9RRR8
B	217	TYR	THR	SEE REMARK 999	UNP Q9RRR8
B	218	ALA	PRO	SEE REMARK 999	UNP Q9RRR8
B	219	LEU	CYS	SEE REMARK 999	UNP Q9RRR8
B	220	ARG	ALA	SEE REMARK 999	UNP Q9RRR8
B	221	GLY	ALA	SEE REMARK 999	UNP Q9RRR8

- Molecule 2 is water.

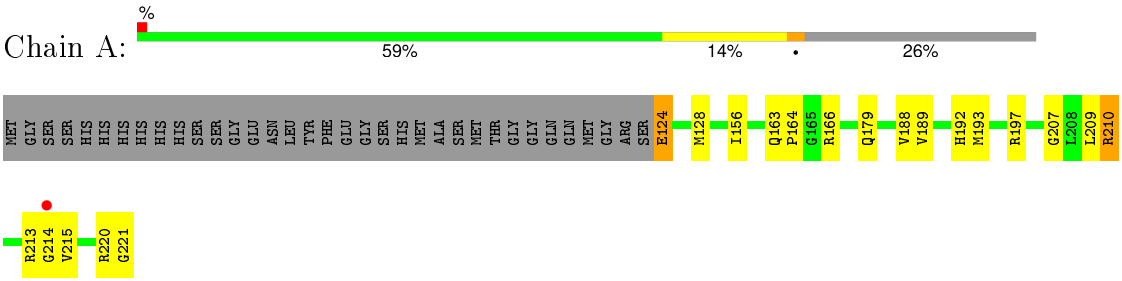
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total	O	0	0
			142	142		
2	B	114	Total	O	0	0
			114	114		

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 errors 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.

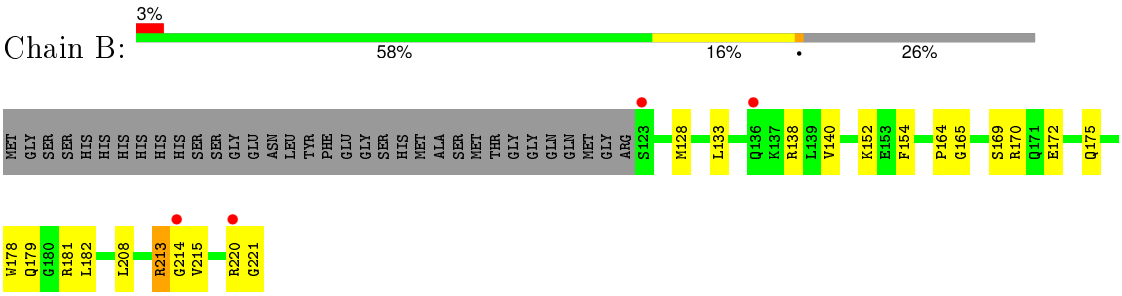
- Molecule 1: DNA-binding response regulator

Chain A:



- Molecule 1: DNA-binding response regulator

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	49.25Å 37.60Å 48.57Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	28.86 – 1.60 28.86 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.86-1.60) 96.2 (28.86-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 1.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.190 , 0.230 0.183 , 0.226	Depositor DCC
R_{free} test set	1107 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.3	EDS
Estimated twinning fraction	0.168 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 21545 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1828	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.36	0/800	0.57	0/1076
1	B	0.33	0/797	0.55	0/1072
All	All	0.35	0/1597	0.56	0/2148

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	786	0	808	16	1
1	B	786	0	807	17	0
2	A	142	0	0	5	2
2	B	114	0	0	2	0
All	All	1828	0	1615	32	3

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 10.

All (32) 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:214:GLY:HA3	2:A:227:HOH:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD22	1:B:221:GLY:HA2	1.65	0.78
1:A:188:VAL:O	1:A:192:HIS:HD2	1.72	0.71
1:B:208:LEU:CD2	1:B:221:GLY:HA2	2.28	0.63
1:B:152:LYS:HD3	1:B:178:TRP:CE2	2.36	0.59
1:A:197:ARG:NH1	2:A:244:HOH:O	2.40	0.55
1:B:128:MET:SD	1:B:164:PRO:HB3	2.47	0.55
1:A:124:GLU:OE2	1:B:221:GLY:C	2.48	0.51
1:A:197:ARG:HD2	2:A:265:HOH:O	2.09	0.51
1:B:181:ARG:HG2	2:B:225:HOH:O	2.12	0.49
1:B:152:LYS:HD3	1:B:178:TRP:CZ2	2.48	0.48
1:A:189:VAL:O	1:A:193:MET:HG2	2.14	0.48
2:A:232:HOH:O	1:B:164:PRO:HD2	2.16	0.46
1:A:214:GLY:HA2	1:A:215:VAL:HA	1.48	0.45
1:B:165:GLY:HA2	1:B:220:ARG:CD	2.47	0.45
1:B:169:SER:OG	1:B:172:GLU:HG2	2.17	0.44
1:A:188:VAL:O	1:A:192:HIS:CD2	2.62	0.44
1:B:213:ARG:HA	1:B:214:GLY:HA2	1.62	0.44
1:B:170:ARG:NH2	1:B:215:VAL:HG21	2.31	0.44
1:A:207:GLY:HA2	1:A:210:ARG:NH1	2.33	0.43
1:A:213:ARG:HA	1:A:214:GLY:HA2	1.68	0.43
1:A:156:ILE:HG21	1:A:193:MET:SD	2.58	0.43
1:B:138:ARG:HA	1:B:154:PHE:CZ	2.54	0.43
1:A:163:GLN:OE1	1:A:166:ARG:NH1	2.49	0.43
1:A:197:ARG:HB2	1:A:209:LEU:HD23	2.01	0.42
1:A:124:GLU:HG2	2:A:272:HOH:O	2.19	0.42
1:A:128:MET:HG3	1:A:164:PRO:HG3	2.03	0.41
1:A:220:ARG:HG3	1:A:221:GLY:O	2.20	0.41
1:B:133:LEU:HG	1:B:140:VAL:HG22	2.03	0.41
1:B:178:TRP:CD1	1:B:182:LEU:HD21	2.56	0.41
1:B:214:GLY:HA2	1:B:215:VAL:HA	1.60	0.40
1:B:175:GLN:HG2	2:B:241:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:265:HOH:O	2:A:265:HOH:O[2_655]	1.94	0.26
2:A:263:HOH:O	2:A:265:HOH:O[2_655]	1.96	0.24
1:A:179:GLN:NE2	1:A:179:GLN:NE2[2_656]	2.06	0.14

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	97/133 (73%)	96 (99%)	1 (1%)	0	100	100
1	B	97/133 (73%)	94 (97%)	3 (3%)	0	100	100
All	All	194/266 (73%)	190 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	84/111 (76%)	82 (98%)	2 (2%)	57	27
1	B	84/111 (76%)	82 (98%)	2 (2%)	57	27
All	All	168/222 (76%)	164 (98%)	4 (2%)	57	27

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

Mol	Chain	Res	Type
1	A	124	GLU
1	A	210	ARG
1	B	179	GLN
1	B	213	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	HIS
1	B	195	ASN

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	98/133 (73%)	-0.11	1 (1%)	84 84	10, 17, 34, 64	0
1	B	99/133 (74%)	0.17	4 (4%)	42 39	11, 21, 49, 70	0
All	All	197/266 (74%)	0.03	5 (2%)	61 58	10, 19, 42, 70	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	2.8
1	B	214	GLY	2.7
1	B	220	ARG	2.6
1	B	123	SER	2.4
1	B	136	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.