



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:12 PM GMT

PDB ID : 3RV0  
Title : Crystal structure of K. polysporus Dcr1 without the C-terminal dsRBD  
Authors : Nakanishi, K.; Weinberg, D.E.; Bartel, D.P.; Patel, D.J.  
Deposited on : 2011-05-05  
Resolution : 2.29 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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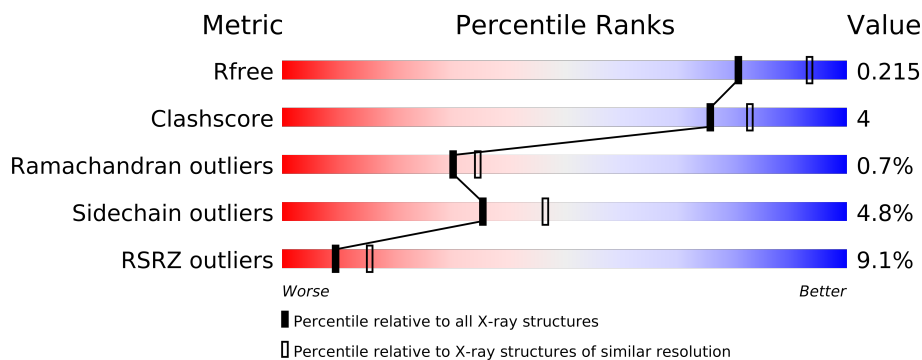
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.29 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))
$R_{free}$	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	341	
1	B	341	
1	C	341	
1	D	341	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8628 atoms, of which 0 are hydrogen and 0 are deuterium.

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 K. polysporus Dcr1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	0	0
			1939	1236	321	374	8			
1	B	304	Total	C	N	O	S	0	0	0
			2477	1577	417	474	9			
1	C	228	Total	C	N	O	S	0	0	0
			1856	1186	307	356	7			
1	D	232	Total	C	N	O	S	0	0	0
			1885	1204	311	363	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

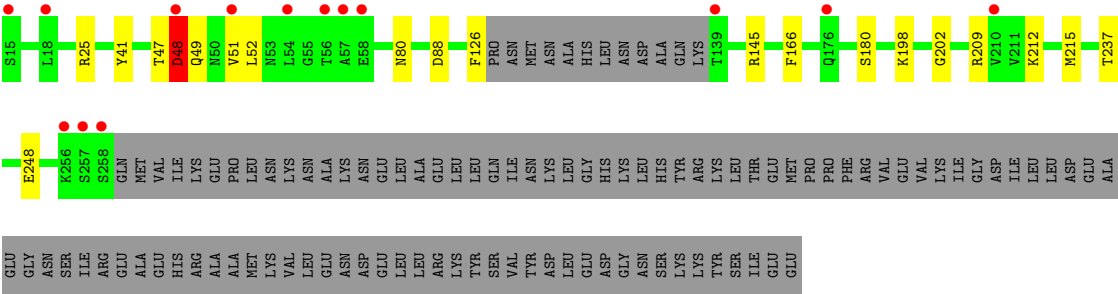
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	141	Total	O	0	0
			141	141		
3	C	98	Total	O	0	0
			98	98		
3	D	98	Total	O	0	0
			98	98		



Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.04Å 112.97Å 135.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.41 – 2.29 43.41 – 2.29	Depositor EDS
% Data completeness (in resolution range)	92.4 (43.41-2.29) 92.4 (43.41-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.64 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_538)	Depositor
R, $R_{free}$	0.175 , 0.220 0.172 , 0.215	Depositor DCC
$R_{free}$ test set	3302 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 64887 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8628	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.38	0/1974	0.52	0/2666
1	B	0.38	0/2517	0.50	0/3392
1	C	0.38	0/1889	0.51	0/2554
1	D	0.37	0/1919	0.52	0/2594
All	All	0.38	0/8299	0.51	0/11206

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1939	0	0	10	0
1	B	2477	0	0	10	0
1	C	1856	0	0	7	0
1	D	1885	0	0	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	130	0	0	1	0
3	B	141	0	0	5	0
3	C	98	0	0	0	0
3	D	98	0	0	2	0
All	All	8628	0	0	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (32) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:PHE:O	1:D:145:ARG:NH2	2.27	0.67
1:A:145:ARG:NH2	1:B:166:PHE:O	2.30	0.65
1:D:80:ASN:ND2	3:D:380:HOH:O	2.30	0.64
1:C:145:ARG:NH2	1:D:166:PHE:O	2.34	0.61
1:D:47:THR:O	1:D:49:GLN:N	2.37	0.57
1:A:32:LYS:NZ	3:B:449:HOH:O	2.36	0.57
1:B:25:ARG:NH1	3:B:438:HOH:O	2.39	0.56
1:A:117:GLU:OE2	1:A:199:ARG:NH2	2.40	0.55
1:C:184:ASN:ND2	1:C:217:LYS:NZ	2.56	0.54
1:B:315:ASN:N	1:B:315:ASN:OD1	2.41	0.54
1:A:165:ARG:NH2	1:B:251:GLU:OE2	2.41	0.53
1:A:213:ASP:OD1	1:A:213:ASP:N	2.44	0.51
1:B:145:ARG:NH1	3:B:366:HOH:O	2.45	0.50
1:D:47:THR:O	1:D:48:ASP:C	2.50	0.49
1:D:126:PHE:CZ	1:D:215:MET:CE	2.96	0.48
1:A:122:MET:CE	1:A:141:LEU:CA	2.92	0.48
1:C:48:ASP:OD2	1:C:48:ASP:N	2.48	0.46
1:B:80:ASN:ND2	3:B:5:HOH:O	2.49	0.46
1:B:298:PHE:CD1	1:B:315:ASN:O	2.70	0.45
1:A:126:PHE:O	1:A:127:PRO:C	2.55	0.44
1:D:47:THR:CG2	1:D:48:ASP:N	2.77	0.44
1:A:206:THR:N	1:A:207:PRO:CD	2.81	0.43
1:A:217:LYS:NZ	3:A:389:HOH:O	2.51	0.43
1:B:277:LEU:CD2	1:B:341:TYR:OH	2.68	0.42
1:C:122:MET:CE	1:C:141:LEU:O	2.67	0.42
1:B:341:TYR:CD1	1:B:342:ASP:N	2.88	0.41
1:B:337:LYS:NZ	3:B:423:HOH:O	2.53	0.41
1:A:55:GLY:N	1:A:62:ASP:OD2	2.53	0.41
1:C:140:GLN:O	1:C:140:GLN:CG	2.68	0.41
1:D:25:ARG:NH1	3:D:418:HOH:O	2.54	0.41
1:D:41:TYR:O	1:D:47:THR:OG1	2.39	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:104:MET:CE	1:C:105:PHE:CZ	3.04	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	233/341 (68%)	226 (97%)	7 (3%)	0	100	100
1	B	296/341 (87%)	288 (97%)	7 (2%)	1 (0%)	50	60
1	C	224/341 (66%)	215 (96%)	7 (3%)	2 (1%)	25	26
1	D	228/341 (67%)	218 (96%)	6 (3%)	4 (2%)	13	10
All	All	981/1364 (72%)	947 (96%)	27 (3%)	7 (1%)	30	34

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ASP
1	D	48	ASP
1	D	209	ARG
1	D	212	LYS
1	B	296	PRO
1	D	202	GLY
1	C	202	GLY

### 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 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	218/310 (70%)	212 (97%)	6 (3%)	56	73
1	B	275/310 (89%)	258 (94%)	17 (6%)	26	33
1	C	209/310 (67%)	196 (94%)	13 (6%)	26	33
1	D	213/310 (69%)	205 (96%)	8 (4%)	44	59
All	All	915/1240 (74%)	871 (95%)	44 (5%)	35	46

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	56	THR
1	A	71	LEU
1	A	170	ASN
1	A	213	ASP
1	A	218	ARG
1	B	16	ASN
1	B	48	ASP
1	B	52	LEU
1	B	88	ASP
1	B	104	MET
1	B	139	THR
1	B	152	SER
1	B	165	ARG
1	B	170	ASN
1	B	266	LEU
1	B	267	ASN
1	B	274	LEU
1	B	302	VAL
1	B	308	LEU
1	B	315	ASN
1	B	326	MET
1	B	342	ASP
1	C	17	GLU
1	C	47	THR
1	C	48	ASP
1	C	51	VAL
1	C	56	THR
1	C	71	LEU
1	C	81	ARG
1	C	139	THR
1	C	140	GLN
1	C	141	LEU

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Mol	Chain	Res	Type
1	C	171	GLU
1	C	218	ARG
1	C	237	THR
1	D	48	ASP
1	D	51	VAL
1	D	52	LEU
1	D	88	ASP
1	D	180	SER
1	D	198	LYS
1	D	237	THR
1	D	248	GLU

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 chains 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 4 ligands modelled in this entry, 4 are 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.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	239/341 (70%)	-0.10	14 (5%)	22 30	14, 32, 98, 144	0
1	B	304/341 (89%)	0.45	44 (14%)	3 5	11, 38, 127, 170	0
1	C	228/341 (66%)	0.11	20 (8%)	10 16	14, 36, 105, 147	0
1	D	232/341 (68%)	-0.02	14 (6%)	21 30	15, 37, 104, 137	0
All	All	1003/1364 (73%)	0.13	92 (9%)	9 15	11, 36, 109, 170	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TYR	12.2
1	C	54	LEU	8.4
1	B	343	LEU	7.9
1	B	293	THR	6.5
1	D	56	THR	6.2
1	B	296	PRO	6.0
1	C	48	ASP	5.9
1	A	206	THR	5.8
1	D	58	GLU	5.7
1	B	323	ARG	5.6
1	A	260	MET	5.5
1	A	207	PRO	5.5
1	C	50	ASN	5.4
1	B	317	ILE	5.4
1	B	214	LYS	5.3
1	A	215	MET	5.2
1	D	258	SER	5.2
1	A	258	SER	5.2
1	B	215	MET	5.2
1	B	292	LEU	5.2
1	B	299	ARG	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	213	ASP	5.2
1	C	53	ASN	5.2
1	B	140	GLN	5.1
1	B	319	GLU	5.1
1	A	127	PRO	5.0
1	B	298	PHE	5.0
1	B	270	ALA	4.9
1	C	200	LEU	4.8
1	C	209	ARG	4.8
1	B	295	MET	4.7
1	B	136	ALA	4.7
1	B	266	LEU	4.7
1	B	342	ASP	4.6
1	B	269	ASN	4.5
1	B	318	ARG	4.3
1	C	55	GLY	4.1
1	C	139	THR	4.1
1	C	56	THR	4.1
1	B	297	PRO	4.0
1	D	15	SER	4.0
1	B	315	ASN	3.9
1	D	54	LEU	3.9
1	D	48	ASP	3.8
1	C	59	ASN	3.7
1	B	294	GLU	3.7
1	B	265	PRO	3.7
1	D	139	THR	3.6
1	D	257	SER	3.6
1	C	51	VAL	3.6
1	D	57	ALA	3.6
1	B	320	ALA	3.5
1	B	268	LYS	3.4
1	C	214	LYS	3.2
1	A	259	GLN	3.2
1	B	137	GLN	3.2
1	B	300	VAL	3.1
1	B	291	LYS	3.1
1	C	252	LYS	3.0
1	B	273	GLU	2.9
1	B	277	LEU	2.9
1	B	316	SER	2.8
1	A	216	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	322	HIS	2.8
1	C	206	THR	2.8
1	B	330	GLU	2.7
1	A	214	LYS	2.7
1	D	210	VAL	2.7
1	A	126	PHE	2.7
1	B	314	GLY	2.7
1	C	49	GLN	2.6
1	C	140	GLN	2.6
1	B	138	LYS	2.5
1	D	51	VAL	2.5
1	B	267	ASN	2.5
1	D	256	LYS	2.4
1	B	313	GLU	2.4
1	A	257	SER	2.4
1	B	256	LYS	2.3
1	A	256	LYS	2.3
1	A	173	MET	2.2
1	C	207	PRO	2.2
1	C	208	THR	2.2
1	C	255	ALA	2.2
1	A	136	ALA	2.2
1	D	18	LEU	2.2
1	B	135	ASP	2.2
1	D	176	GLN	2.1
1	B	48	ASP	2.1
1	C	256	LYS	2.0
1	B	312	ALA	2.0
1	B	139	THR	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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	1	1/1	0.07	-2.15	45,45,45,45	0
2	MG	B	3	1/1	0.06	-2.98	49,49,49,49	0
2	MG	D	2	1/1	0.07	-3.05	56,56,56,56	0
2	MG	C	4	1/1	0.05	-3.88	40,40,40,40	0

## 6.5 Other polymers

There are no such residues in this entry.