



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:22 am BST

PDB ID : 3VHL
Title : Crystal structure of the DHR-2 domain of DOCK8 in complex with Cdc42 (T17N mutant)
Authors : Hanawa-Suetsugu, K.; Kukimoto-Niino, M.; Nishizak, T.; Terada, T.; Shirouzu, M.; Fukui, Y.; Yokoyama, S.
Deposited on : 2011-08-26
Resolution : 2.08 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

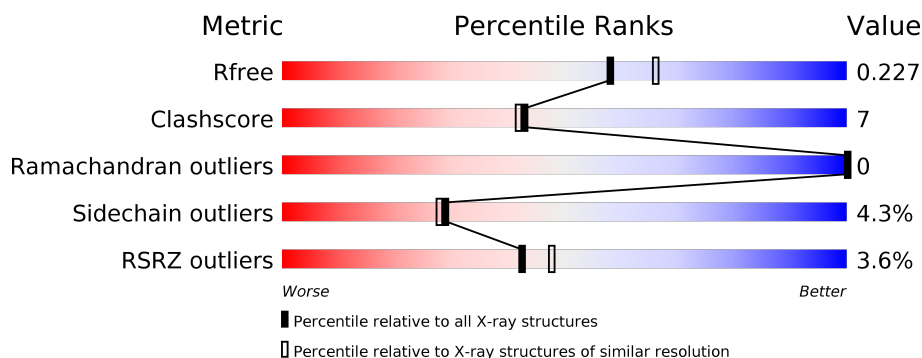
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	288	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>
2	B	195	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3781 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 Dedicator of cytokinesis protein 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2188	1402	380	395	11	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1780	GLY	-	EXPRESSION TAG	UNP Q8C147
A	1781	SER	-	EXPRESSION TAG	UNP Q8C147
A	1782	SER	-	EXPRESSION TAG	UNP Q8C147
A	1783	GLY	-	EXPRESSION TAG	UNP Q8C147
A	1784	SER	-	EXPRESSION TAG	UNP Q8C147
A	1785	SER	-	EXPRESSION TAG	UNP Q8C147
A	1786	GLY	-	EXPRESSION TAG	UNP Q8C147

- Molecule 2 is a protein called Cell division control protein 42 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	1389	893	222	267	7	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	GLY	-	EXPRESSION TAG	UNP P60953
B	-5	SER	-	EXPRESSION TAG	UNP P60953
B	-4	SER	-	EXPRESSION TAG	UNP P60953
B	-3	GLY	-	EXPRESSION TAG	UNP P60953
B	-2	SER	-	EXPRESSION TAG	UNP P60953
B	-1	SER	-	EXPRESSION TAG	UNP P60953
B	0	GLY	-	EXPRESSION TAG	UNP P60953
B	17	ASN	THR	ENGINEERED MUTATION	UNP P60953
B	188	SER	CYS	ENGINEERED MUTATION	UNP P60953

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

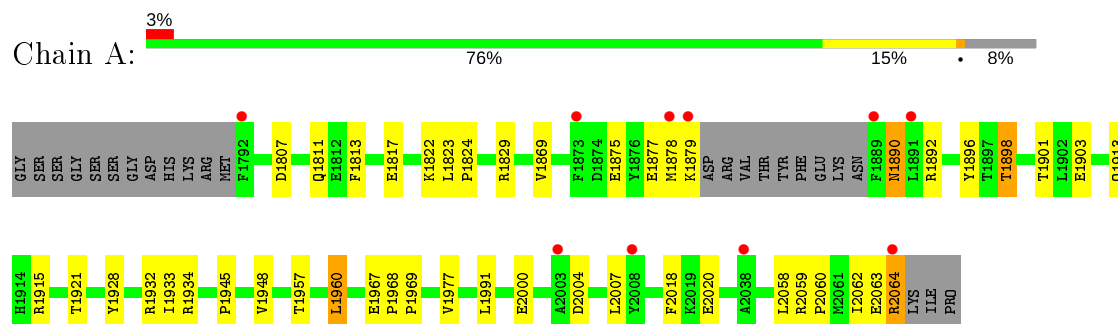
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total	O	0	0
			113	113		
4	B	81	Total	O	0	0
			81	81		

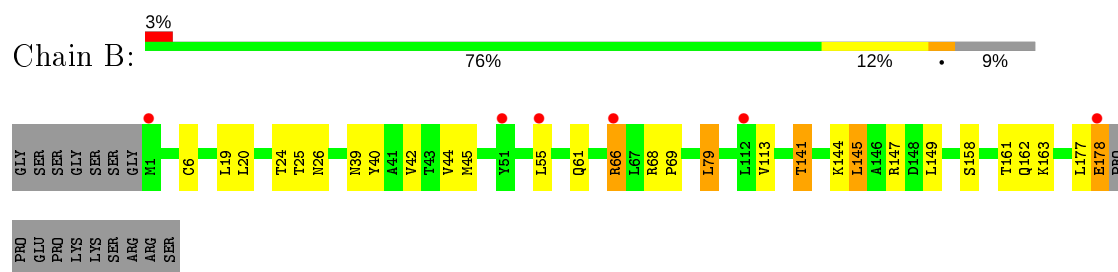
3 Residue-property plots [i](#)

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: Deducator of cytokinesis protein 8



- Molecule 2: Cell division control protein 42 homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.19 Å 73.28 Å 65.03 Å 90.00° 104.82° 90.00°	Depositor
Resolution (Å)	29.68 – 2.08 29.68 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.68-2.08) 93.2 (29.68-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 2.08 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.178 , 0.232 0.173 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (7.12%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3781	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.48	0/2238	0.63	0/3013
2	B	0.48	0/1419	0.64	0/1931
All	All	0.48	0/3657	0.63	0/4944

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	2188	0	2187	31	0
2	B	1389	0	1404	19	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	113	0	0	1	0
4	B	81	0	0	2	0
All	All	3781	0	3591	49	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 7.

All (49) 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:2063:GLU:O	1:A:2064:ARG:HG2	1.95	0.67
1:A:2059:ARG:HB3	1:A:2060:PRO:HD3	1.81	0.62
2:B:161:THR:O	2:B:162:GLN:HB2	2.02	0.60
2:B:145:LEU:HD22	2:B:149:LEU:HG	1.83	0.60
1:A:1813:PHE:CE1	1:A:1934:ARG:HG2	2.42	0.55
1:A:1898:THR:HG23	4:A:1:HOH:O	2.06	0.55
2:B:177:LEU:O	2:B:178:GLU:HB2	2.07	0.54
1:A:2004:ASP:HB3	1:A:2007:LEU:HD22	1.90	0.53
1:A:1901:THR:HB	1:A:1903:GLU:OE2	2.09	0.53
2:B:6:CYS:HB3	2:B:55:LEU:HD23	1.90	0.53
2:B:39:ASN:C	2:B:40:TYR:CD2	2.84	0.51
2:B:39:ASN:C	2:B:40:TYR:CG	2.85	0.50
1:A:2018:PHE:HB3	1:A:2062:ILE:HD12	1.94	0.49
1:A:1822:LYS:HE2	2:B:26:ASN:OD1	2.12	0.49
1:A:1913:GLN:O	1:A:1945:PRO:HA	2.13	0.48
2:B:61:GLN:H	2:B:61:GLN:CD	2.16	0.47
2:B:158:SER:HB3	2:B:161:THR:OG1	2.15	0.47
1:A:1957:THR:HG21	1:A:2020:GLU:HG3	1.97	0.46
2:B:79:LEU:HG	2:B:113:VAL:HG21	1.96	0.46
1:A:1890:ASN:C	1:A:1890:ASN:HD22	2.19	0.46
1:A:1915:ARG:HB2	1:A:1948:VAL:HG22	1.98	0.46
1:A:1869:VAL:HG12	1:A:1896:TYR:HB3	1.98	0.45
2:B:68:ARG:HB3	2:B:69:PRO:HD3	1.98	0.45
1:A:1811:GLN:OE1	1:A:1934:ARG:NH2	2.49	0.45
2:B:24:THR:HG22	2:B:42:VAL:HB	1.98	0.45
1:A:2007:LEU:N	1:A:2007:LEU:CD1	2.79	0.45
1:A:2064:ARG:HD3	1:A:2064:ARG:HA	1.73	0.45
2:B:141:THR:HG21	4:B:205:HOH:O	2.17	0.45
1:A:2058:LEU:O	1:A:2062:ILE:HG12	2.16	0.44
1:A:1967:GLU:HA	1:A:1968:PRO:C	2.35	0.44
2:B:19:LEU:HD12	2:B:19:LEU:C	2.38	0.44
2:B:19:LEU:HD12	2:B:20:LEU:N	2.33	0.43
1:A:1967:GLU:OE2	1:A:1969:PRO:HD3	2.18	0.43
2:B:39:ASN:HA	2:B:40:TYR:CD2	2.53	0.43
1:A:1957:THR:HG21	1:A:2020:GLU:CG	2.49	0.42
1:A:1823:LEU:N	1:A:1824:PRO:HD2	2.34	0.42
1:A:1960:LEU:HG	1:A:1977:VAL:HG12	2.02	0.41
1:A:1877:GLU:O	1:A:1879:LYS:HG3	2.21	0.41
2:B:25:THR:O	2:B:26:ASN:HB2	2.20	0.41
1:A:1817:GLU:CD	1:A:1829:ARG:HH12	2.24	0.41
1:A:1890:ASN:C	1:A:1890:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1928:TYR:CD2	1:A:1933:ILE:HG12	2.55	0.41
2:B:144:LYS:O	2:B:147:ARG:HG2	2.21	0.41
2:B:66:ARG:O	4:B:265:HOH:O	2.22	0.41
1:A:1892:ARG:HG2	1:A:1921:THR:HG23	2.03	0.40
1:A:1960:LEU:HA	1:A:1977:VAL:HG11	2.03	0.40
1:A:2018:PHE:HB3	1:A:2062:ILE:CD1	2.51	0.40
1:A:1878:MET:O	1:A:1879:LYS:HB2	2.22	0.40
1:A:2063:GLU:O	1:A:2064:ARG:CG	2.68	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	260/288 (90%)	258 (99%)	2 (1%)	0	100	100
2	B	176/195 (90%)	172 (98%)	4 (2%)	0	100	100
All	All	436/483 (90%)	430 (99%)	6 (1%)	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	237/258 (92%)	228 (96%)	9 (4%)	33	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	158/172 (92%)	150 (95%)	8 (5%)	24	21
All	All	395/430 (92%)	378 (96%)	17 (4%)	29	28

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1807	ASP
1	A	1875	GLU
1	A	1890	ASN
1	A	1898	THR
1	A	1932	ARG
1	A	1960	LEU
1	A	1991	LEU
1	A	2000	GLU
1	A	2064	ARG
2	B	44	VAL
2	B	45	MET
2	B	66	ARG
2	B	79	LEU
2	B	141	THR
2	B	145	LEU
2	B	163	LYS
2	B	178	GLU

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	1890	ASN
1	A	1966	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	2	-	4,4,4	0.82	0	6,6,6	0.59	0
3	PO4	B	189	-	4,4,4	0.68	0	6,6,6	0.44	0

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 [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	264/288 (91%)	0.01	10 (3%) 40 45	19, 33, 67, 115	0
2	B	178/195 (91%)	-0.06	6 (3%) 45 50	23, 32, 52, 86	0
All	All	442/483 (91%)	-0.02	16 (3%) 42 48	19, 33, 60, 115	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1889	PHE	8.0
1	A	1792	PHE	7.5
1	A	2064	ARG	5.6
1	A	2003	ALA	4.2
2	B	66	ARG	3.2
1	A	1878	MET	3.0
2	B	178	GLU	3.0
2	B	1	MET	2.8
1	A	2038	ALA	2.2
1	A	2008	TYR	2.2
1	A	1879	LYS	2.1
1	A	1873	PHE	2.1
1	A	1891	LEU	2.1
2	B	112	LEU	2.1
2	B	55	LEU	2.0
2	B	51	TYR	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](#)

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. The B-factors column lists the minimum, median, 95th 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PO4	A	2	5/5	0.97	0.09	44,45,49,52	0
3	PO4	B	189	5/5	0.99	0.06	29,33,34,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.