



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 03:37 pm BST

PDB ID : 3ODW  
Title : Crystal Structure of the Linker-DH/PH domains of p115-RhoGEF  
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Deposited on : 2010-08-11  
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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
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

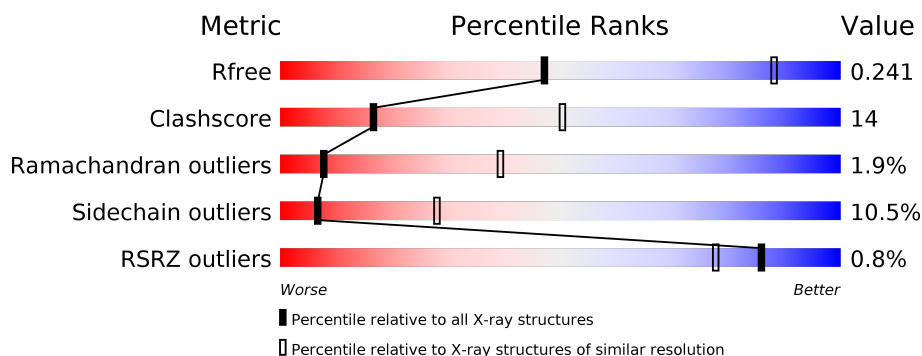
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	536	
1	B	536	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5416 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.

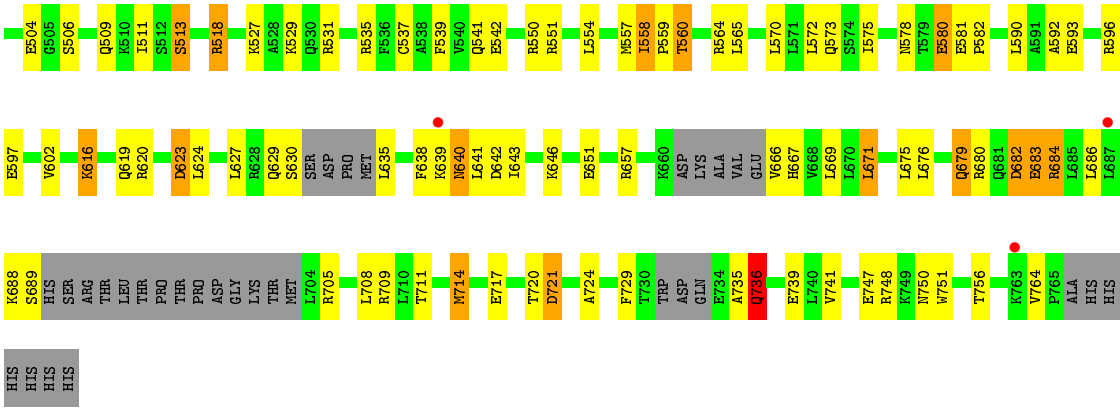
- Molecule 1 is a protein called Rho guanine nucleotide exchange factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2729	1730	490	493	16			
1	B	326	Total	C	N	O	S	0	0	0
			2687	1704	483	486	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	237	GLN	-	EXPRESSION TAG	UNP Q92888
A	238	THR	-	EXPRESSION TAG	UNP Q92888
A	239	SER	-	EXPRESSION TAG	UNP Q92888
A	767	HIS	-	EXPRESSION TAG	UNP Q92888
A	768	HIS	-	EXPRESSION TAG	UNP Q92888
A	769	HIS	-	EXPRESSION TAG	UNP Q92888
A	770	HIS	-	EXPRESSION TAG	UNP Q92888
A	771	HIS	-	EXPRESSION TAG	UNP Q92888
A	772	HIS	-	EXPRESSION TAG	UNP Q92888
B	237	GLN	-	EXPRESSION TAG	UNP Q92888
B	238	THR	-	EXPRESSION TAG	UNP Q92888
B	239	SER	-	EXPRESSION TAG	UNP Q92888
B	767	HIS	-	EXPRESSION TAG	UNP Q92888
B	768	HIS	-	EXPRESSION TAG	UNP Q92888
B	769	HIS	-	EXPRESSION TAG	UNP Q92888
B	770	HIS	-	EXPRESSION TAG	UNP Q92888
B	771	HIS	-	EXPRESSION TAG	UNP Q92888
B	772	HIS	-	EXPRESSION TAG	UNP Q92888





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.64Å 111.64Å 97.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.67 – 3.20 43.67 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.67-3.20) 99.5 (43.67-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.231 , 0.289 0.229 , 0.241	Depositor DCC
$R_{free}$ test set	1147 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.1	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.448 for h,-h-k,-l 0.012 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup> Theoretical 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

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	0.73	4/2770 (0.1%)	0.84	4/3721 (0.1%)
1	B	0.94	4/2727 (0.1%)	1.05	7/3664 (0.2%)
All	All	0.84	8/5497 (0.1%)	0.95	11/7385 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	684	ARG	CZ-NH1	16.19	1.54	1.33
1	A	684	ARG	CD-NE	13.16	1.68	1.46
1	B	623	ASP	CB-CG	11.23	1.75	1.51
1	A	684	ARG	CZ-NH1	-8.02	1.22	1.33
1	B	684	ARG	CZ-NH2	6.82	1.42	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	684	ARG	NE-CZ-NH1	-31.79	104.41	120.30
1	B	684	ARG	NH1-CZ-NH2	12.23	132.85	119.40
1	A	684	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	A	623	ASP	CB-CG-OD2	-11.42	108.02	118.30
1	A	623	ASP	CB-CG-OD1	10.73	127.96	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	684	ARG	Sidechain

## 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	2729	0	2802	66	0
1	B	2687	0	2762	94	1
All	All	5416	0	5564	156	1

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 14.

The worst 5 of 156 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:623:ASP:CB	1:B:623:ASP:CG	1.75	1.55
1:A:684:ARG:CD	1:A:684:ARG:NE	1.68	1.54
1:B:717:GLU:HG3	1:B:748:ARG:HH12	1.05	1.19
1:A:634:MET:HE2	1:A:635:LEU:HD12	1.31	1.12
1:B:717:GLU:HG3	1:B:748:ARG:NH1	1.67	1.09

All (1) 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)
1:B:504:GLU:OE1	1:B:535:ARG:NH1[2_654]	2.18	0.02

## 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	319/536 (60%)	285 (89%)	27 (8%)	7 (2%)	6	35
1	B	314/536 (59%)	265 (84%)	44 (14%)	5 (2%)	9	43
All	All	633/1072 (59%)	550 (87%)	71 (11%)	12 (2%)	8	39

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	635	LEU
1	A	721	ASP
1	B	490	GLU
1	B	721	ASP
1	A	565	LEU

### 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	306/476 (64%)	276 (90%)	30 (10%)	8	31
1	B	301/476 (63%)	267 (89%)	34 (11%)	6	25
All	All	607/952 (64%)	543 (90%)	64 (10%)	7	28

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	714	MET
1	B	490	GLU
1	B	711	THR
1	A	748	ARG
1	B	452	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	414	GLN
1	B	667	HIS
1	B	573	GLN
1	A	681	GLN
1	B	509	GLN

### 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, 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	331/536 (61%)	-0.02	1 (0%) 94 92	53, 85, 140, 199	0
1	B	326/536 (60%)	0.02	4 (1%) 79 67	62, 98, 145, 202	0
All	All	657/1072 (61%)	-0.00	5 (0%) 86 78	53, 95, 143, 202	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	763	LYS	2.8
1	B	639	LYS	2.5
1	B	687	LEU	2.3
1	A	628	ARG	2.3
1	B	499	ARG	2.1

### 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.