



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XCG  
Title : Crystal Structure of Human RhoA in complex with DH/PH fragment of PDZRHOGEF  
Authors : Derewenda, U.; Oleksy, A.; Stevenson, A.S.; Korczynska, J.; Dauter, Z.; Somlyo, A.P.; Otlewski, J.; Somlyo, A.V.; Derewenda, Z.S.  
Deposited on : 2004-09-01  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

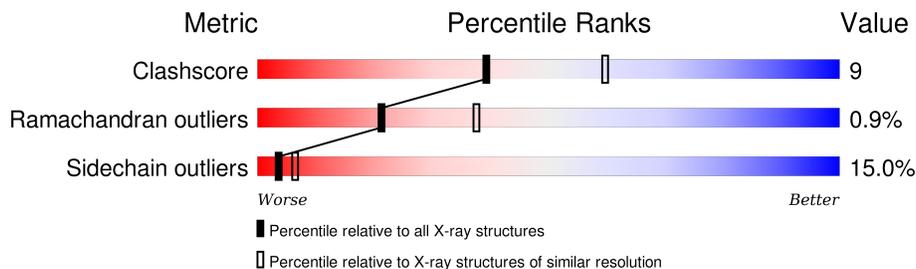
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	368	
1	E	368	
2	B	178	
2	F	178	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8750 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 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	355	2906	1837	519	535	15	0	0	0
1	E	358	2931	1852	525	539	15	0	0	0

- Molecule 2 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	1411	889	240	272	10	0	0	0
2	F	178	1411	889	240	272	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASN	PHE	ENGINEERED	UNP P61586
F	25	ASN	PHE	ENGINEERED	UNP P61586

- Molecule 3 is water.

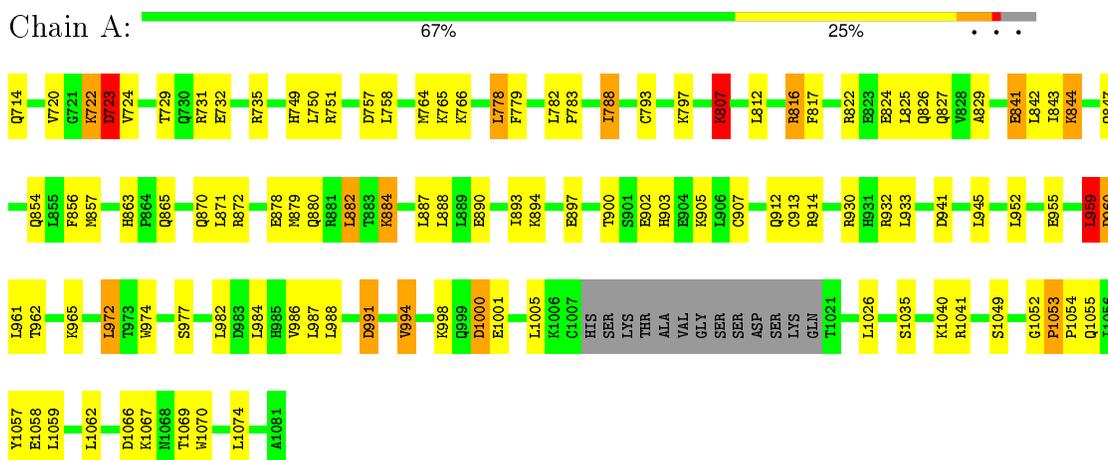
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	17	Total 17	O 17	0	0
3	E	30	Total 30	O 30	0	0
3	F	14	Total 14	O 14	0	0

### 3 Residue-property plots i

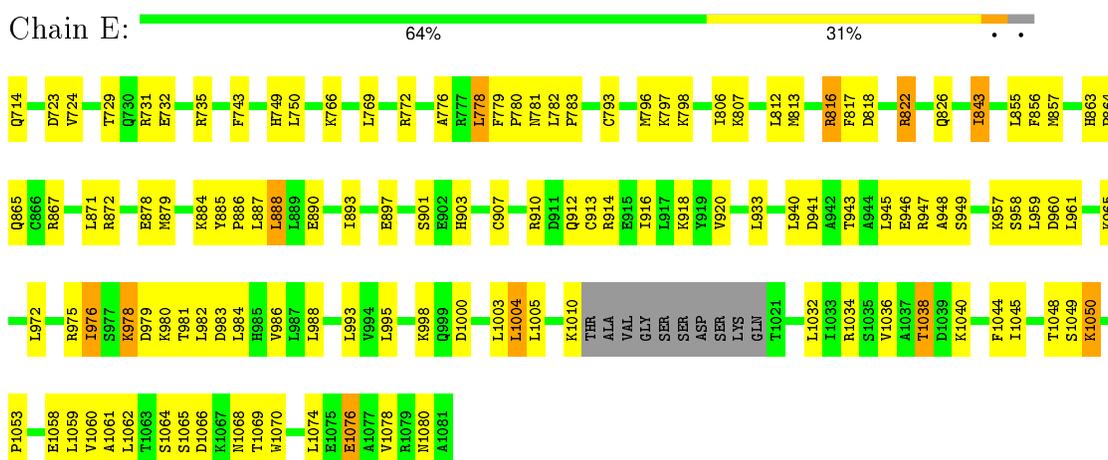
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: Rho guanine nucleotide exchange factor 11

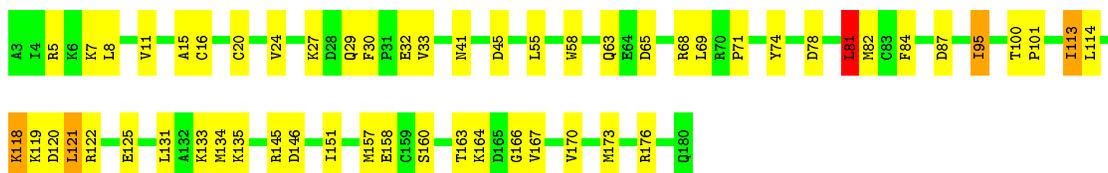


- Molecule 1: Rho guanine nucleotide exchange factor 11



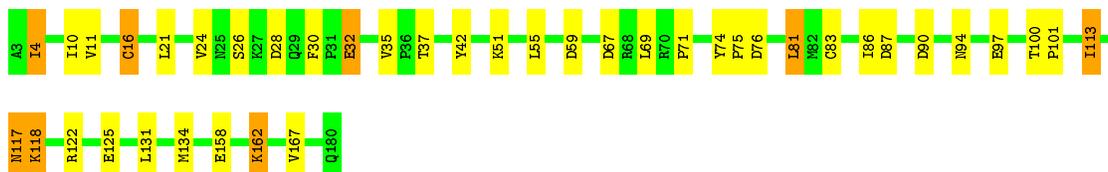
- Molecule 2: Transforming protein RhoA





- Molecule 2: Transforming protein RhoA

Chain F: 77% 19%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.24Å 118.78Å 90.13Å 90.00° 114.34° 90.00°	Depositor
Resolution (Å)	25.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.8 (25.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.224 , 0.281	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	8750	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

## 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	0.50	0/2950	0.74	7/3970 (0.2%)
1	E	0.51	0/2976	0.78	6/4004 (0.1%)
2	B	0.56	0/1438	0.82	6/1944 (0.3%)
2	F	0.56	0/1438	0.81	6/1944 (0.3%)
All	All	0.52	0/8802	0.78	25/11862 (0.2%)

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	ASP	CB-CG-OD2	7.30	124.87	118.30
1	E	723	ASP	CB-CG-OD2	7.13	124.72	118.30
2	F	90	ASP	CB-CG-OD2	6.61	124.25	118.30
2	B	81	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	1000	ASP	CB-CG-OD2	6.02	123.72	118.30

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	2906	0	2997	55	0
1	E	2931	0	3022	62	0
2	B	1411	0	1402	28	0
2	F	1411	0	1402	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	0	4	0
3	B	17	0	0	0	0
3	E	30	0	0	2	0
3	F	14	0	0	1	0
All	All	8750	0	8823	156	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 9.

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:A:879:MET:HE3	2:B:69:LEU:HB3	1.48	0.94
1:E:822:ARG:HH11	1:E:826:GLN:HE22	1.05	0.93
1:A:879:MET:CE	2:B:69:LEU:HB3	2.03	0.88
1:E:1061:ALA:HB1	1:E:1066:ASP:HB3	1.56	0.86
1:A:822:ARG:HH11	1:A:912:GLN:HE22	1.22	0.86

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	351/368 (95%)	333 (95%)	11 (3%)	7 (2%)	9 15
1	E	354/368 (96%)	335 (95%)	18 (5%)	1 (0%)	46 68
2	B	176/178 (99%)	165 (94%)	10 (6%)	1 (1%)	30 50
2	F	176/178 (99%)	169 (96%)	6 (3%)	1 (1%)	30 50
All	All	1057/1092 (97%)	1002 (95%)	45 (4%)	10 (1%)	21 37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1054	PRO
1	A	1000	ASP
1	A	1052	GLY
1	A	807	LYS
1	A	959	LEU

### 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	323/334 (97%)	272 (84%)	51 (16%)	3	5
1	E	326/334 (98%)	273 (84%)	53 (16%)	3	5
2	B	156/156 (100%)	133 (85%)	23 (15%)	4	7
2	F	156/156 (100%)	139 (89%)	17 (11%)	8	15
All	All	961/980 (98%)	817 (85%)	144 (15%)	3	6

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	119	LYS
1	E	778	LEU
2	F	35	VAL
2	B	125	GLU
2	B	160	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	749	HIS
1	E	826	GLN
1	E	985	HIS
1	E	714	GLN
1	E	715	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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers

EDS was not executed - this section will therefore be empty.