



# wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 11:30 PM GMT

PDB ID : 1CC0  
Title : CRYSTAL STRUCTURE OF THE RHOA.GDP-RHO GDI COMPLEX  
Authors : Longenecker, K.L.; Read, P.; Derewenda, U.; Dauter, Z.; Garrard, S.; Walker, L.; Somlyo, A.V.; Somlyo, A.P.; Nakamoto, R.K.; Derewenda, Z.S.  
Deposited on : 1999-03-03  
Resolution : 5.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

---

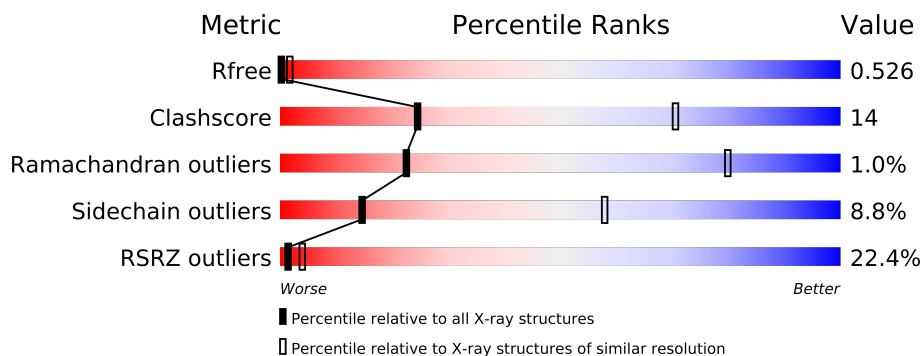
The following versions of software and data (see [references](#)) were used in the production of this report:

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 5.00 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	1052 (6.50-3.50)
Clashscore	79885	1327 (6.50-3.50)
Ramachandran outliers	78287	1242 (6.50-3.50)
Sidechain outliers	78261	1221 (6.50-3.50)
RSRZ outliers	66119	1051 (6.50-3.50)

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. 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	190	
1	C	190	
2	E	204	
2	F	204	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5174 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 transforming protein rhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	187	Total	C	N	O	S	0	0	10
			1415	896	239	270	10			
1	C	187	Total	C	N	O	S	0	0	10
			1415	896	239	270	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ASN	PHE	conflict	UNP P61586
C	25	ASN	PHE	conflict	UNP P61586

- Molecule 2 is a protein called rho GDP dissociation inhibitor alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	180	Total	C	N	O	S	0	0	44
			1143	748	183	208	4			
2	F	180	Total	C	N	O	S	0	0	44
			1143	748	183	208	4			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

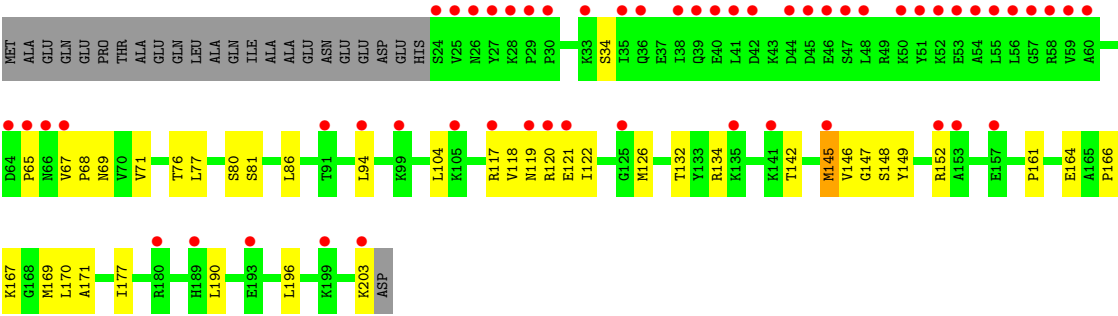
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
4	C	1	Total	C	N	O	P	0	0
			28	10	5	11	2		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.30Å 139.30Å 253.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 5.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-5.00) 99.2 (19.97-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 3.94Å)	Xtriage
Refinement program	O	Depositor
R, $R_{free}$	(Not available) , (Not available) 0.545 , 0.526	Depositor DCC
$R_{free}$ test set	642 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	138.6	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 12673 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.67	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.74% 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: GDP, 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	1.00	2/1432 (0.1%)	2.12	48/1937 (2.5%)
1	C	1.00	2/1432 (0.1%)	2.12	49/1937 (2.5%)
2	E	0.58	0/1124	0.93	1/1515 (0.1%)
2	F	0.59	0/1124	0.92	1/1515 (0.1%)
All	All	0.84	4/5112 (0.1%)	1.70	99/6904 (1.4%)

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	A	0	5
1	C	0	5
All	All	0	10

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	GLU	CD-OE2	5.85	1.32	1.25
1	C	93	GLU	CD-OE2	5.76	1.31	1.25
1	C	93	GLU	CG-CD	5.35	1.59	1.51
1	A	93	GLU	CG-CD	5.35	1.59	1.51

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	A	122	ARG	NE-CZ-NH2	-16.21	112.20	120.30
1	A	176	ARG	NE-CZ-NH2	-15.41	112.59	120.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	C	150	ARG	NE-CZ-NH2	-15.31	112.64	120.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	VAL	Peptide
1	A	49	ASP	Peptide
1	A	50	GLY	Peptide
1	A	62	GLY	Mainchain
1	A	64	GLU	Peptide

## 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	1415	0	1392	56	7
1	C	1415	0	1394	61	16
2	E	1143	0	1100	34	20
2	F	1143	0	1100	39	6
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	28	0	12	0	0
4	C	28	0	12	0	0
All	All	5174	0	5010	143	26

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 14.

The worst 5 of 143 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:67:VAL:CA	2:F:68:PRO:N	1.83	1.41
1:C:71:PRO:HB3	2:F:148:SER:OG	1.28	1.30
1:A:71:PRO:HB3	2:E:148:SER:OG	1.45	1.14

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:PRO:HB3	2:E:148:SER:CB	1.83	1.08
1:C:105:HIS:CD2	2:F:145:MET:CE	2.37	1.06

The worst 5 of 26 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	Distance(Å)	Clash(Å)
2:E:91:THR:O	1:C:34:TYR:CE2[6_554]	0.52	1.68
2:E:91:THR:O	1:C:34:TYR:CZ[6_554]	1.09	1.11
1:A:123:ASN:OD1	1:C:129:ARG:NH1[7_555]	1.17	1.03
2:E:80:SER:OG	2:E:80:SER:OG[10_665]	1.20	1.00
2:E:91:THR:O	1:C:34:TYR:CD2[6_554]	1.33	0.87

## 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	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	14	70
1	C	175/190 (92%)	164 (94%)	8 (5%)	3 (2%)	14	70
2	E	134/204 (66%)	132 (98%)	2 (2%)	0	100	100
2	F	134/204 (66%)	132 (98%)	2 (2%)	0	100	100
All	All	618/788 (78%)	592 (96%)	20 (3%)	6 (1%)	22	80

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	C	41	ASN
1	A	64	GLU
1	A	66	TYR
1	C	64	GLU

### 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	156/164 (95%)	143 (92%)	13 (8%)	16	61
1	C	156/164 (95%)	143 (92%)	13 (8%)	16	61
2	E	122/180 (68%)	111 (91%)	11 (9%)	14	56
2	F	122/180 (68%)	110 (90%)	12 (10%)	12	51
All	All	556/688 (81%)	507 (91%)	49 (9%)	14	58

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	170	LEU
1	C	68	ARG
2	F	161	PRO
1	C	29	GLN
1	C	69	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	180	GLN
2	F	130	GLN
2	F	100	GLN
2	E	119	ASN
2	F	69	ASN

### 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, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z  > 2$
4	GDP	A	201	3	30,30,30	1.53	5 (16%)	44,47,47	8.55	7 (15%)
4	GDP	C	202	3	30,30,30	1.53	5 (16%)	44,47,47	8.57	7 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GDP	A	201	3	-	0/16/32/32	0/1/3/3
4	GDP	C	202	3	-	0/16/32/32	0/1/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	GDP	C5-C4	-4.63	1.30	1.40
4	A	201	GDP	C5-C4	-4.59	1.30	1.40
4	A	201	GDP	C4-N3	-2.82	1.31	1.35
4	C	202	GDP	C4-N3	-2.81	1.31	1.35
4	C	202	GDP	C8-N9	2.63	1.40	1.36

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	GDP	C6-C5-N7	-55.86	126.62	134.14
4	A	201	GDP	C6-C5-N7	-55.72	126.64	134.14

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	202	GDP	C4-C5-N7	4.48	113.36	109.52
4	A	201	GDP	C4-C5-N7	4.44	113.32	109.52
4	A	201	GDP	O2'-C2'-C1'	-4.09	98.85	111.23

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	187/190 (98%)	1.04	23 (12%) 5 10	35, 35, 35, 35	0
1	C	187/190 (98%)	1.18	31 (16%) 2 6	35, 35, 35, 35	0
2	E	180/204 (88%)	1.87	56 (31%) 1 3	35, 35, 35, 35	0
2	F	180/204 (88%)	2.05	55 (30%) 1 3	35, 35, 35, 35	0
All	All	734/788 (93%)	1.53	165 (22%) 1 4	35, 35, 35, 35	0

The worst 5 of 165 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	LYS	17.4
2	F	36	GLN	13.0
1	A	186	LYS	12.0
2	E	57	GLY	11.6
2	F	39	GLN	11.4

### 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( $\text{\AA}^2$ )	Q<0.9
4	GDP	C	202	28/28	0.38	-	35,35,35,35	0
3	MG	C	302	1/1	0.48	-	35,35,35,35	0
3	MG	A	301	1/1	0.36	-	35,35,35,35	0
4	GDP	A	201	28/28	0.32	-	35,35,35,35	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.