



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1RGP / pdb_00001rgp
Title : GTPASE-ACTIVATION DOMAIN FROM RHOGAP
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Deposited on : 1996-12-05
Resolution : 2.00 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

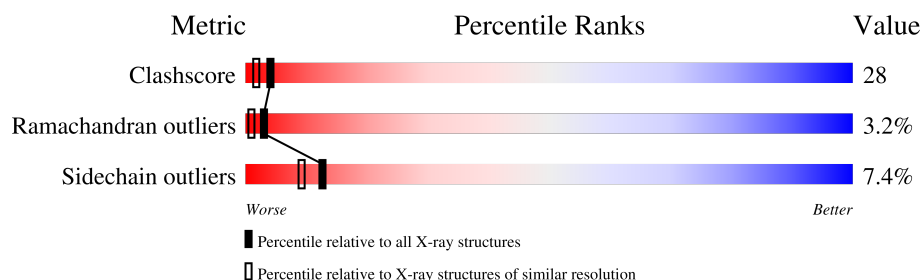
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 of 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	242	36% 25% 12% 5% 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1762 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 RHOGAP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1501	973	259	267	2			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	261	Total	O	6	0
			261	261		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	36.09Å 70.09Å 79.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.6 (20.00-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1762	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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	1.53	17/1539 (1.1%)	2.59	126/2103 (6.0%)

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	6

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	36	PRO	CA-C	-12.17	1.27	1.52
1	A	62	ILE	N-CA	10.85	1.54	1.46
1	A	36	PRO	C-N	-8.07	1.16	1.33
1	A	37	ARG	C-O	-7.21	1.15	1.24
1	A	192	ASN	C-N	6.65	1.42	1.33

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	GLU	CA-C-N	19.93	159.62	121.54
1	A	113	GLU	C-N-CA	19.93	159.62	121.54
1	A	36	PRO	O-C-N	14.88	146.81	123.00
1	A	132	LEU	O-C-N	-14.59	105.47	122.68
1	A	67	ARG	CD-NE-CZ	12.29	141.60	124.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	GLU	Peptide
1	A	115	HIS	Mainchain
1	A	132	LEU	Peptide,Mainchain
1	A	134	THR	Mainchain
1	A	193	THR	Mainchain

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	1501	0	1473	82	29
2	A	261	0	0	32	22
All	All	1762	0	1473	82	29

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 28.

The worst 5 of 82 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:36:PRO:O	1:A:38:PRO:CD	1.74	1.35
1:A:146:ASN:CG	2:A:416:HOH:O	1.88	1.11
1:A:37:ARG:CD	2:A:485:HOH:O	1.73	1.11
1:A:36:PRO:O	1:A:38:PRO:HD3	0.91	1.07
1:A:50:GLN:HE21	1:A:166:GLU:HG3	1.20	1.06

The worst 5 of 29 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:A:38:PRO:N	2:A:358:HOH:O[2_565]	0.44	1.76
1:A:38:PRO:CG	1:A:158:GLN:NE2[2_565]	0.54	1.66
1:A:37:ARG:CA	2:A:360:HOH:O[2_565]	0.56	1.64
1:A:36:PRO:CB	2:A:390:HOH:O[2_565]	0.62	1.58
1:A:37:ARG:C	2:A:358:HOH:O[2_565]	1.06	1.14

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	185/242 (76%)	174 (94%)	5 (3%)	6 (3%)	3 1

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	217	ASN
1	A	133	LEU
1	A	134	THR
1	A	113	GLU

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	162/219 (74%)	150 (93%)	12 (7%)	13 9

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	THR
1	A	185	SER
1	A	205	TRP
1	A	186	ASP
1	A	142	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	230	GLN
1	A	112	ASN
1	A	140	HIS
1	A	167	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 oligosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	36:PRO	C	37:ARG	N	1.16

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.