



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 20, 2017 – 07:53 PM EST

PDB ID : 6Q21  
Title : MOLECULAR SWITCH FOR SIGNAL TRANSDUCTION: STRUCTURAL DIFFERENCES BETWEEN ACTIVE AND INACTIVE FORMS OF PROTOONCOGENIC RAS PROTEINS  
Authors : Kim, S.-H.  
Deposited on : unknown  
Resolution : 1.95 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

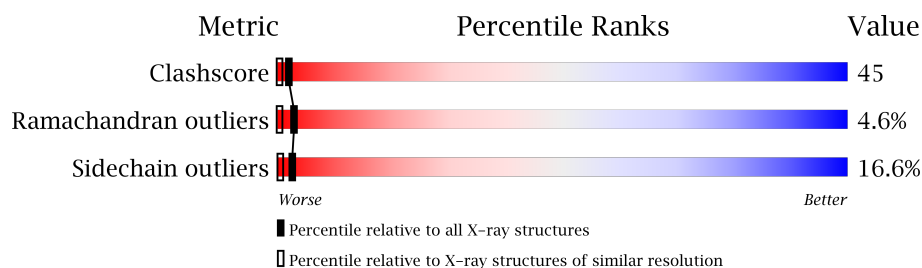
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)

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	171	
1	B	171	
1	C	171	
1	D	171	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6057 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.

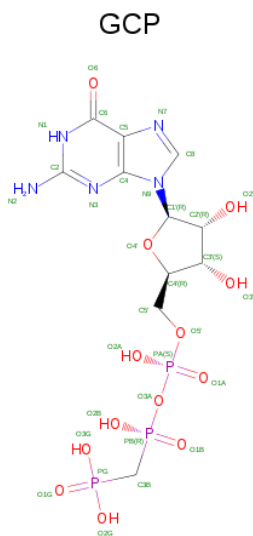
- Molecule 1 is a protein called C-H-RAS P21 PROTEIN CATALYTIC DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	B	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	C	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			
1	D	171	Total	C	N	O	S	0	0	0
			1368	854	238	269	7			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C<sub>11</sub>H<sub>18</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	B	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	C	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	D	1	Total 32	C 11	N 5	O 13	P 3	0	0

- Molecule 4 is water.

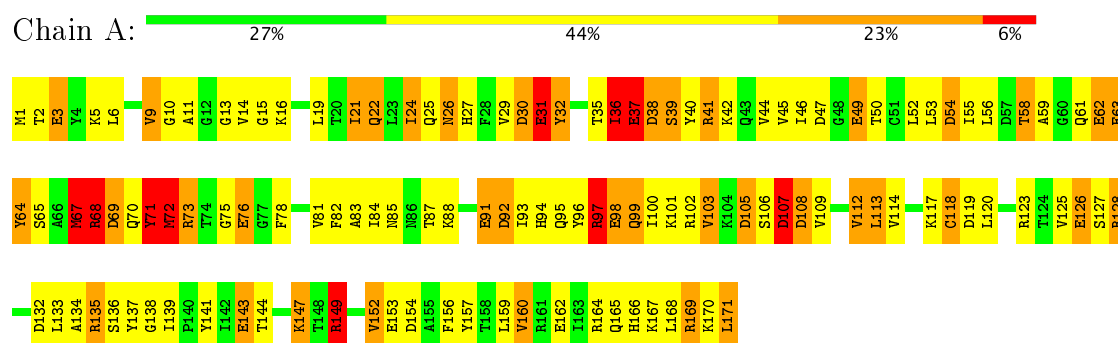
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	B	93	Total O 93 93	0	0
4	C	111	Total O 111 111	0	0
4	D	166	Total O 166 166	0	0

### 3 Residue-property plots [i](#)

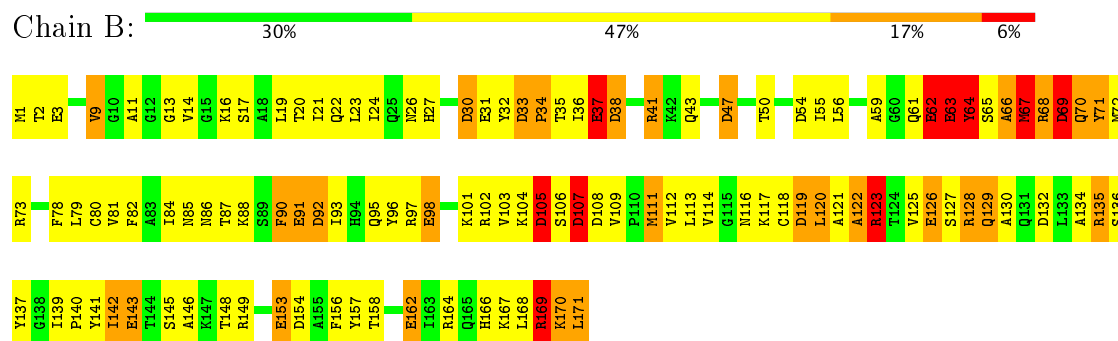
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

#### • Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



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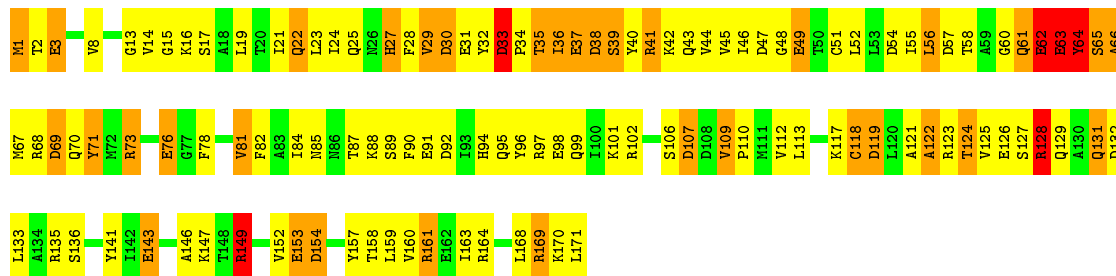


#### • Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN



● Molecule 1: C-H-RAS P21 PROTEIN CATALYTIC DOMAIN

Chain D: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.98Å 79.12Å 128.50Å 90.00° 90.00° 117.48°	Depositor
Resolution (Å)	(Not available) – 1.95	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.95)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.190 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6057	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, 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	1.06	13/1387 (0.9%)	1.69	30/1868 (1.6%)
1	B	1.06	11/1387 (0.8%)	1.63	33/1868 (1.8%)
1	C	1.11	11/1387 (0.8%)	1.62	27/1868 (1.4%)
1	D	1.11	13/1387 (0.9%)	1.67	31/1868 (1.7%)
All	All	1.08	48/5548 (0.9%)	1.65	121/7472 (1.6%)

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	2	0

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	GLU	CD-OE2	8.16	1.34	1.25
1	D	143	GLU	CD-OE2	8.05	1.34	1.25
1	C	126	GLU	CD-OE2	7.76	1.34	1.25
1	A	153	GLU	CD-OE2	7.70	1.34	1.25
1	B	126	GLU	CD-OE2	7.62	1.34	1.25

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	135	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	A	132	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	A	107	ASP	N-CA-CB	9.18	127.13	110.60
1	D	119	ASP	CB-CG-OD1	9.14	126.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	ARG	NE-CZ-NH1	8.93	124.77	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	64	TYR	CA
1	A	107	ASP	CA

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	1368	0	1357	132	0
1	B	1368	0	1355	151	0
1	C	1368	0	1355	70	0
1	D	1368	0	1356	160	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	32	0	14	6	0
3	B	32	0	14	2	0
3	C	32	0	14	4	0
3	D	32	0	14	5	0
4	A	83	0	0	18	0
4	B	93	0	0	14	0
4	C	111	0	0	16	0
4	D	166	0	0	58	0
All	All	6057	0	5479	502	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 45.

The worst 5 of 502 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:D:33:ASP:HB3	1:D:34:PRO:HD3	1.18	1.14
1:B:41:ARG:HD2	1:D:135:ARG:HD3	1.17	1.09
1:D:34:PRO:HB2	1:D:61:GLN:HG3	1.38	1.05
1:A:126:GLU:HB3	1:A:128:ARG:HE	1.24	1.02
1:D:13:GLY:H	3:D:180:GCP:H3B1	1.27	0.98

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	169/171 (99%)	135 (80%)	25 (15%)	9 (5%)	2	0
1	B	169/171 (99%)	150 (89%)	8 (5%)	11 (6%)	1	0
1	C	169/171 (99%)	159 (94%)	7 (4%)	3 (2%)	10	2
1	D	169/171 (99%)	149 (88%)	12 (7%)	8 (5%)	3	0
All	All	676/684 (99%)	593 (88%)	52 (8%)	31 (5%)	3	0

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	67	MET
1	A	69	ASP
1	A	73	ARG
1	B	34	PRO

### 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	149/149 (100%)	117 (78%)	32 (22%)	1	0
1	B	149/149 (100%)	125 (84%)	24 (16%)	3	0
1	C	149/149 (100%)	131 (88%)	18 (12%)	6	1
1	D	149/149 (100%)	124 (83%)	25 (17%)	2	0
All	All	596/596 (100%)	497 (83%)	99 (17%)	2	0

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	ILE
1	B	171	LEU
1	D	109	VAL
1	B	109	VAL
1	B	129	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	GLN
1	C	70	GLN
1	D	22	GLN
1	B	166	HIS
1	D	27	HIS

### 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	GCP	A	180	2	25,34,34	2.52	5 (20%)	28,54,54	2.01	9 (32%)
3	GCP	B	180	2	25,34,34	2.30	6 (24%)	28,54,54	2.03	8 (28%)
3	GCP	C	180	2	25,34,34	2.12	6 (24%)	28,54,54	2.21	7 (25%)
3	GCP	D	180	2	25,34,34	2.62	8 (32%)	28,54,54	1.43	4 (14%)

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
3	GCP	A	180	2	-	0/18/38/38	0/3/3/3
3	GCP	B	180	2	-	0/18/38/38	0/3/3/3
3	GCP	C	180	2	-	0/18/38/38	0/3/3/3
3	GCP	D	180	2	-	0/18/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	180	GCP	C5-C6	-7.53	1.39	1.53
3	A	180	GCP	C4-N9	-7.02	1.38	1.47
3	B	180	GCP	C4-N9	-6.95	1.38	1.47
3	A	180	GCP	C5-C6	-6.03	1.42	1.53
3	C	180	GCP	C4-N9	-5.87	1.39	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	180	GCP	O3G-PG-O1G	-4.62	99.93	112.32
3	A	180	GCP	O1B-PB-C3B	-4.37	98.18	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	C	180	GCP	O2B-PB-C3B	-4.08	89.20	106.54
3	C	180	GCP	O2G-PG-O1G	-4.00	101.60	112.32
3	B	180	GCP	O2B-PB-C3B	-3.28	92.59	106.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	180	GCP	6	0
3	B	180	GCP	2	0
3	C	180	GCP	4	0
3	D	180	GCP	5	0

## 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 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.