



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:16 am BST

PDB ID : 5I6J  
Title : Crystal Structure of SRGAP2 F-BARx  
Authors : Sporny, M.; Guez-Haddad, J.; Isupov, M.N.; Opatowsky, Y.  
Deposited on : 2016-02-16  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

---

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

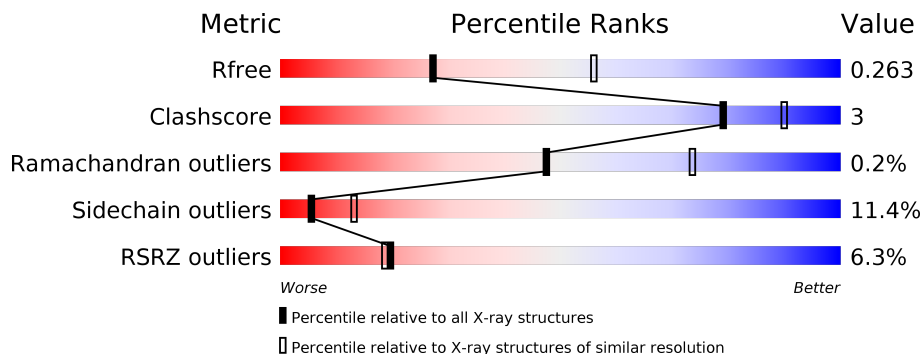
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	484	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3388 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 SLIT-ROBO Rho GTPase-activating protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3369	2108	582	657	22	0	2	0

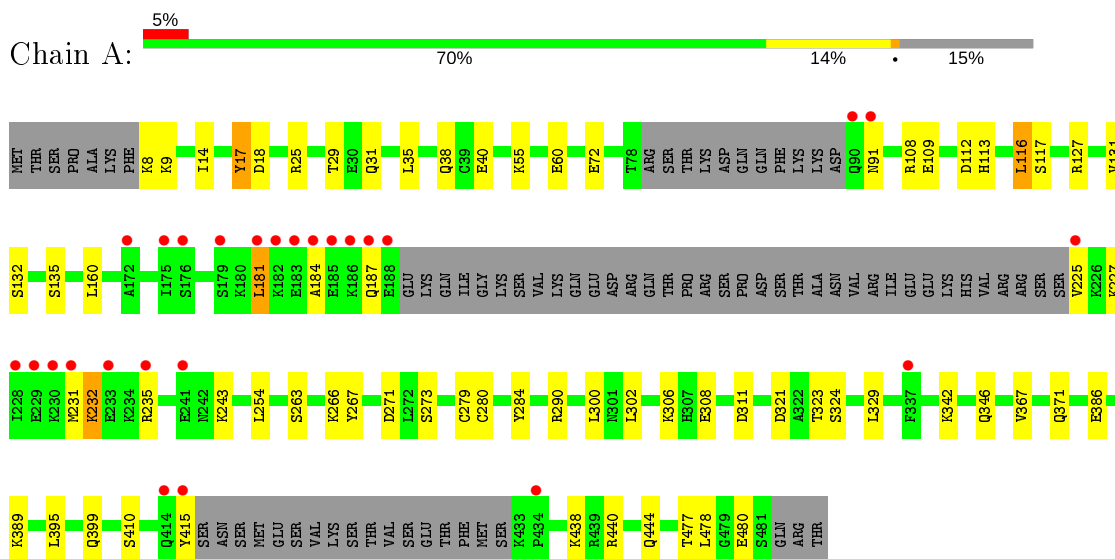
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		

### 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.

- Molecule 1: SLIT-ROBO Rho GTPase-activating protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.17Å 29.90Å 94.73Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	101.53 – 2.70 42.38 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (101.53-2.70) 98.9 (42.38-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.203 , 0.263 0.203 , 0.263	Depositor DCC
$R_{free}$ test set	800 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.7	Xtrriage
Anisotropy	0.777	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.00% 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 [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	0.65	0/3416	0.83	2/4579 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	290	ARG	NE-CZ-NH1	5.58	123.09	120.30

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	3369	0	3385	19	0
2	A	19	0	0	0	0
All	All	3388	0	3385	19	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 3.

All (19) 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:112:ASP:HB3	1:A:302:LEU:HD12	1.60	0.83
1:A:440:ARG:O	1:A:444:GLN:HG3	1.97	0.65
1:A:17:TYR:CE2	1:A:160:LEU:HD23	2.34	0.62
1:A:267:TYR:HA	1:A:271:ASP:HB2	1.86	0.55
1:A:184:ALA:HB1	1:A:232:LYS:HB2	1.91	0.53
1:A:109:GLU:O	1:A:113:HIS:HD2	1.93	0.52
1:A:280:CYS:HA	1:A:284:TYR:HB3	1.93	0.50
1:A:17:TYR:HE2	1:A:160:LEU:HD23	1.75	0.49
1:A:116:LEU:HD13	1:A:302:LEU:HD13	1.97	0.47
1:A:395:LEU:O	1:A:399:GLN:HG2	2.15	0.46
1:A:227:LYS:O	1:A:231:MET:HG2	2.18	0.44
1:A:127:ARG:O	1:A:131:VAL:HG23	2.19	0.43
1:A:112:ASP:HB3	1:A:302:LEU:CD1	2.38	0.42
1:A:321:ASP:OD2	1:A:324:SER:HB2	2.18	0.42
1:A:367:VAL:HG22	1:A:478:LEU:HD13	2.01	0.42
1:A:60:GLU:OE2	1:A:113:HIS:ND1	2.53	0.41
1:A:31:GLN:NE2	1:A:267:TYR:OH	2.53	0.41
1:A:60:GLU:HG3	1:A:116:LEU:HD23	2.02	0.41
1:A:181:LEU:HD12	1:A:235:ARG:HG3	2.02	0.40

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	404/484 (84%)	376 (93%)	27 (7%)	1 (0%)	47 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	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	379/448 (85%)	336 (89%)	43 (11%)	<b>6</b> <b>13</b>

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	9	LYS
1	A	14	ILE
1	A	17	TYR
1	A	18	ASP
1	A	25	ARG
1	A	29	THR
1	A	35	LEU
1	A	38	GLN
1	A	40	GLU
1	A	55	LYS
1	A	72	GLU
1	A	91	ASN
1	A	108	ARG
1	A	116	LEU
1	A	117	SER
1	A	132	SER
1	A	135	SER
1	A	181	LEU
1	A	187	GLN
1	A	225	VAL
1	A	232	LYS
1	A	243	LYS
1	A	254	LEU
1	A	263	SER
1	A	266	LYS
1	A	273	SER
1	A	279	CYS
1	A	300	LEU
1	A	306	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	308	GLU
1	A	311	ASP
1	A	323	THR
1	A	329	LEU
1	A	342	LYS
1	A	346	GLN
1	A	371	GLN
1	A	386	GLU
1	A	389	LYS
1	A	410	SER
1	A	415	TYR
1	A	438	LYS
1	A	477	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	168	HIS
1	A	178	GLN
1	A	236	GLN
1	A	285	HIS
1	A	304	GLN
1	A	334	ASN
1	A	444	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

### 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	410/484 (84%)	0.10	26 (6%) <b>20</b> <b>19</b>	33, 72, 143, 200	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	MET	4.9
1	A	182	LYS	4.3
1	A	188	GLU	4.3
1	A	183	GLU	4.1
1	A	225	VAL	3.8
1	A	175	ILE	3.7
1	A	415	TYR	3.5
1	A	181	LEU	3.5
1	A	184	ALA	3.3
1	A	91	ASN	3.2
1	A	235	ARG	3.2
1	A	90	GLN	3.2
1	A	187	GLN	3.2
1	A	228	ILE	3.2
1	A	337	PHE	3.0
1	A	414	GLN	2.9
1	A	185	GLU	2.9
1	A	241	GLU	2.9
1	A	172	ALA	2.6
1	A	434	PRO	2.6
1	A	186	LYS	2.5
1	A	233	GLU	2.4
1	A	229	GLU	2.4
1	A	230	LYS	2.3
1	A	176	SER	2.2
1	A	179	SER	2.0

## 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.