



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:42 pm BST

PDB ID : 6A9Y  
Title : The crystal structure of Mu homology domain of SGIP1  
Authors : Feng, Y.; Liu, X.  
Deposited on : 2018-07-16  
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.

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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
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

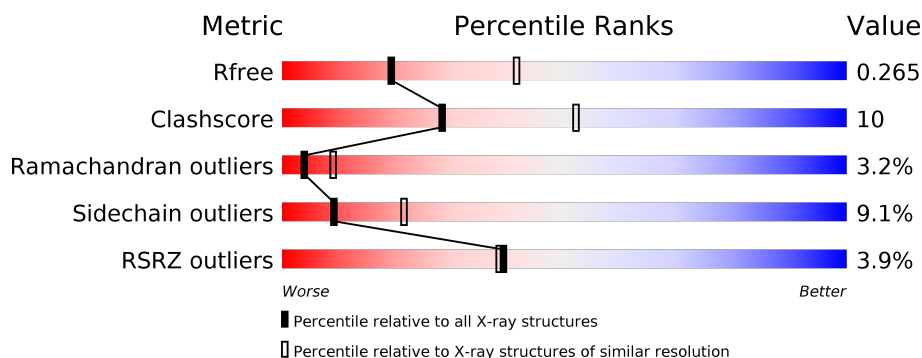
# 1 Overall quality at a glance

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	284	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2260 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 SH3-containing GRB2-like protein 3-interacting protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2199	1400	372	417	10			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	545	VAL	-	expression tag	UNP Q9BQI5
A	546	ASP	-	expression tag	UNP Q9BQI5
A	547	LEU	-	expression tag	UNP Q9BQI5
A	548	GLY	-	expression tag	UNP Q9BQI5
A	549	THR	-	expression tag	UNP Q9BQI5
A	550	GLU	-	expression tag	UNP Q9BQI5
A	551	ASN	-	expression tag	UNP Q9BQI5
A	552	LEU	-	expression tag	UNP Q9BQI5
A	553	TYR	-	expression tag	UNP Q9BQI5
A	554	PHE	-	expression tag	UNP Q9BQI5
A	555	GLN	-	expression tag	UNP Q9BQI5
A	556	SER	-	expression tag	UNP Q9BQI5
A	557	ALA	-	expression tag	UNP Q9BQI5

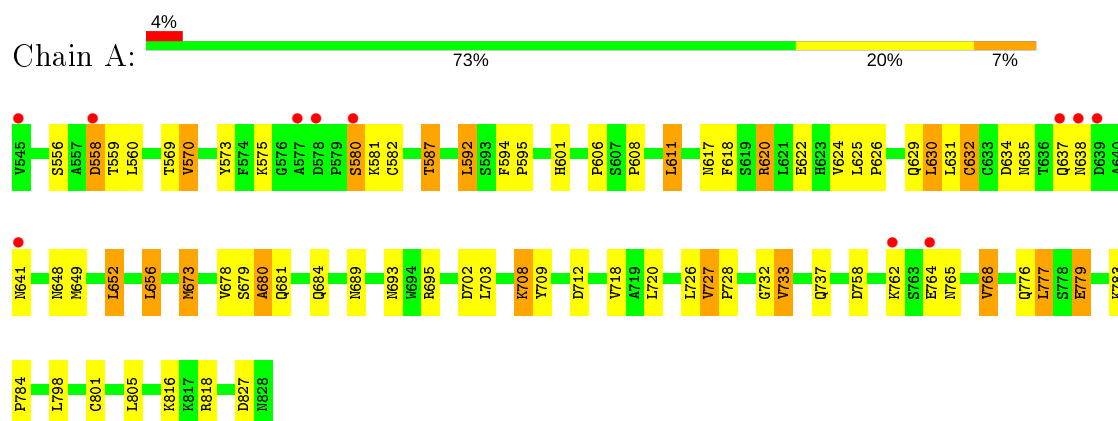
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		

### 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: SH3-containing GRB2-like protein 3-interacting protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.07Å 132.31Å 40.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.70 29.91 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.91-2.70) 99.8 (29.91-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	10.78 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.198 , 0.266 0.199 , 0.265	Depositor DCC
$R_{free}$ test set	524 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	1.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2260	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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

### 5.1 Standard geometry

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	0.42	0/2249	0.75	1/3064 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	632	CYS	CA-CB-SG	20.78	151.40	114.00

There are no chirality outliers.

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	2199	0	2187	43	1
2	A	61	0	0	4	0
All	All	2260	0	2187	43	1

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 10.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance ( $\text{\AA}$ )	Clash overlap ( $\text{\AA}$ )
1:A:611:LEU:H	1:A:649:MET:HE3	1.29	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:SER:HA	1:A:582:CYS:N	2.04	0.71
1:A:679:SER:HA	1:A:680:ALA:HB2	1.71	0.71
1:A:630:LEU:HA	1:A:648:ASN:HB3	1.78	0.66
1:A:575:LYS:NZ	2:A:905:HOH:O	2.30	0.64
1:A:689:ASN:HB2	1:A:708:LYS:HB2	1.82	0.62
1:A:652:LEU:HD22	1:A:656:LEU:HD22	1.82	0.61
1:A:783:LYS:NZ	1:A:784:PRO:O	2.28	0.60
1:A:816:LYS:HD2	1:A:818:ARG:HH12	1.65	0.59
1:A:617:ASN:HB3	1:A:620:ARG:HH21	1.67	0.59
1:A:689:ASN:ND2	2:A:907:HOH:O	2.35	0.58
1:A:560:LEU:HD21	1:A:601:HIS:CE1	2.40	0.57
1:A:678:VAL:HG12	1:A:679:SER:H	1.71	0.56
1:A:684:GLN:NE2	1:A:712:ASP:OD2	2.42	0.52
1:A:558:ASP:CG	1:A:559:THR:H	2.12	0.52
1:A:617:ASN:HB2	1:A:801:CYS:HA	1.91	0.51
1:A:570:VAL:HG22	1:A:798:LEU:HD11	1.92	0.51
1:A:733:VAL:H	1:A:777:LEU:HD12	1.77	0.50
1:A:709:TYR:OH	1:A:718:VAL:O	2.24	0.50
1:A:732:GLY:HA3	1:A:779:GLU:H	1.77	0.49
1:A:737:GLN:OE1	1:A:776:GLN:HG2	2.13	0.48
1:A:611:LEU:HB2	1:A:649:MET:HE1	1.95	0.47
1:A:765:ASN:HB3	1:A:768:VAL:O	2.13	0.47
1:A:764:GLU:HB2	2:A:903:HOH:O	2.15	0.47
1:A:606:PRO:O	1:A:608:PRO:HD3	2.16	0.45
1:A:573:TYR:O	1:A:582:CYS:HA	2.16	0.45
1:A:569:THR:HB	1:A:587:THR:HG22	1.99	0.45
1:A:611:LEU:HB2	1:A:649:MET:CE	2.47	0.45
1:A:637:GLN:HA	1:A:638:ASN:HA	1.72	0.45
1:A:617:ASN:HA	1:A:641:ASN:OD1	2.17	0.45
1:A:592:LEU:HD22	1:A:673:MET:HG2	1.99	0.45
1:A:709:TYR:HE2	1:A:720:LEU:HD13	1.81	0.44
1:A:625:LEU:HA	1:A:626:PRO:HD2	1.84	0.43
1:A:727:VAL:HA	1:A:728:PRO:HD3	1.73	0.43
1:A:560:LEU:HD21	1:A:601:HIS:NE2	2.35	0.42
1:A:720:LEU:O	1:A:758:ASP:HA	2.20	0.41
1:A:695:ARG:HB3	1:A:702:ASP:HB2	2.02	0.41
1:A:656:LEU:HD12	1:A:656:LEU:HA	1.95	0.41
1:A:594:PHE:HA	1:A:595:PRO:HD3	1.97	0.40
1:A:764:GLU:O	1:A:765:ASN:HB2	2.21	0.40
1:A:693:ASN:OD1	2:A:901:HOH:O	2.22	0.40
1:A:764:GLU:HG3	1:A:765:ASN:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:ASP:O	1:A:635:ASN:HB2	2.21	0.40

All (1) 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:632:CYS:CB	1:A:632:CYS:SG[2_555]	1.80	0.40

## 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	282/284 (99%)	253 (90%)	20 (7%)	9 (3%)	<b>4</b> <b>9</b>

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	680	ALA
1	A	681	GLN
1	A	779	GLU
1	A	558	ASP
1	A	581	LYS
1	A	733	VAL
1	A	618	PHE
1	A	622	GLU
1	A	580	SER

### 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	243/243 (100%)	221 (91%)	22 (9%)	9 21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	SER
1	A	570	VAL
1	A	587	THR
1	A	592	LEU
1	A	611	LEU
1	A	620	ARG
1	A	624	VAL
1	A	629	GLN
1	A	630	LEU
1	A	631	LEU
1	A	652	LEU
1	A	656	LEU
1	A	673	MET
1	A	703	LEU
1	A	708	LYS
1	A	726	LEU
1	A	727	VAL
1	A	762	LYS
1	A	768	VAL
1	A	777	LEU
1	A	805	LEU
1	A	827	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	284/284 (100%)	0.08	11 (3%) 39 38	1, 17, 59, 117	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	ASN	7.9
1	A	639	ASP	7.6
1	A	764	GLU	3.7
1	A	637	GLN	3.7
1	A	577	ALA	3.0
1	A	641	ASN	2.7
1	A	762	LYS	2.5
1	A	578	ASP	2.4
1	A	545	VAL	2.1
1	A	558	ASP	2.1
1	A	580	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

There are no such residues in this entry.