



# Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5YPR  
Title : Crystal Structure of PSD-95 SH3-GK domain in complex with a synthesized inhibitor  
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Deposited on : 2017-11-02  
Resolution : 2.35 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

<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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

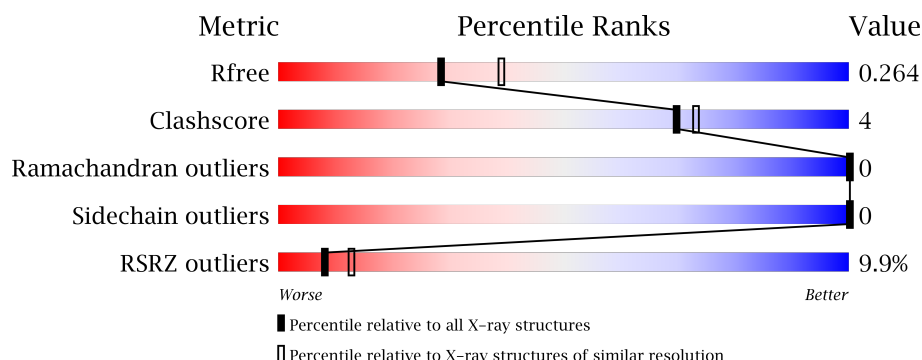
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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))
$R_{free}$	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (2.36-2.32)

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.

Mol	Chain	Length	Quality of chain
1	A	318	<div> <div>7%</div> <div>77%</div> <div>7%</div> <div>16%</div> </div>
2	B	16	<div> <div>31%</div> <div>81%</div> <div>19%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2257 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 Disks large homolog 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2077	1320	361	390	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	404	MET	-	expression tag	UNP P31016
A	405	HIS	-	expression tag	UNP P31016
A	406	HIS	-	expression tag	UNP P31016
A	407	HIS	-	expression tag	UNP P31016
A	408	HIS	-	expression tag	UNP P31016
A	409	HIS	-	expression tag	UNP P31016
A	410	HIS	-	expression tag	UNP P31016
A	411	SER	-	expression tag	UNP P31016
A	412	SER	-	expression tag	UNP P31016
A	413	GLY	-	expression tag	UNP P31016
A	414	LEU	-	expression tag	UNP P31016
A	415	GLU	-	expression tag	UNP P31016
A	416	VAL	-	expression tag	UNP P31016
A	417	LEU	-	expression tag	UNP P31016
A	418	PHE	-	expression tag	UNP P31016
A	419	GLN	-	expression tag	UNP P31016
A	420	GLY	-	expression tag	UNP P31016
A	421	PRO	-	expression tag	UNP P31016
A	422	GLY	-	expression tag	UNP P31016
A	423	SER	-	expression tag	UNP P31016
A	424	GLU	-	expression tag	UNP P31016
A	425	PHE	-	expression tag	UNP P31016

- Molecule 2 is a protein called Synthesized GK inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	0	0
			138	84	30	24			

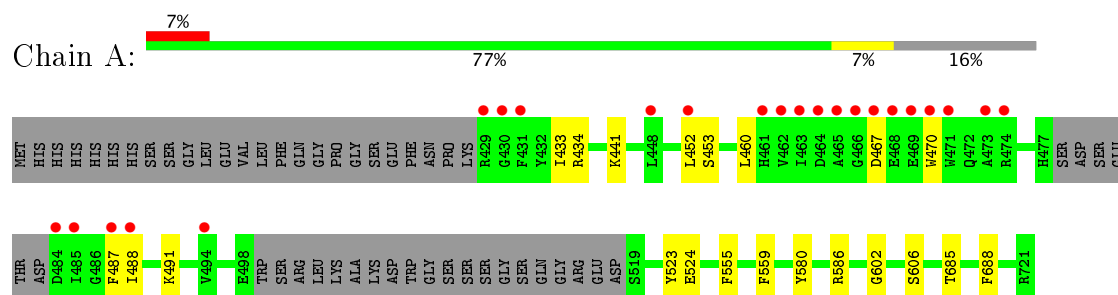
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		

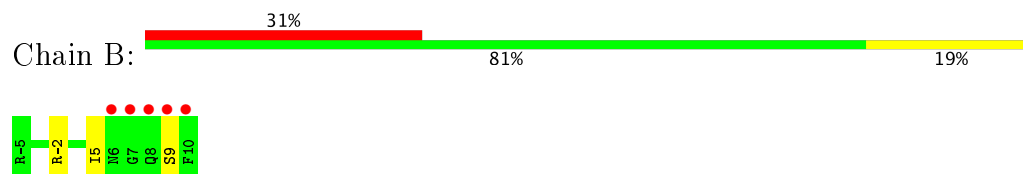
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: Disks large homolog 4



- Molecule 2: Synthesized GK inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.03Å 45.74Å 86.36Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	38.46 – 2.35 38.46 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.46-2.35) 98.7 (38.46-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, $R_{free}$	0.222 , 0.264 0.221 , 0.264	Depositor DCC
$R_{free}$ test set	974 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.5	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	2257	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.30% 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	0.24	0/2124	0.39	0/2879
2	B	0.22	0/139	0.38	0/183
All	All	0.24	0/2263	0.39	0/3062

There are no bond length outliers.

There are no bond angle outliers.

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	2077	0	1930	17	0
2	B	138	0	135	3	0
3	A	42	0	0	0	0
All	All	2257	0	2065	18	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 4.

All (18) 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)
2:B:5:ILE:O	2:B:9:SER:OG	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:TRP:HB3	1:A:487:PHE:CZ	2.40	0.56
1:A:467:ASP:HB3	1:A:470:TRP:O	2.08	0.54
1:A:555:PHE:HB2	1:A:559:PHE:HD2	1.75	0.51
1:A:470:TRP:HB3	1:A:487:PHE:HZ	1.77	0.50
1:A:470:TRP:CB	1:A:487:PHE:HZ	2.25	0.49
1:A:433:ILE:HG13	1:A:523:TYR:HB3	1.93	0.49
1:A:586:ARG:NH1	1:A:606:SER:O	2.44	0.49
1:A:433:ILE:HG22	1:A:460:LEU:HB2	1.96	0.47
1:A:460:LEU:HD13	1:A:488:ILE:HG21	1.96	0.47
1:A:441:LYS:HG3	1:A:453:SER:OG	2.17	0.44
1:A:452:LEU:N	1:A:487:PHE:O	2.51	0.43
1:A:602:GLY:HA2	2:B:9:SER:HA	2.01	0.42
1:A:555:PHE:HB2	1:A:559:PHE:CD2	2.53	0.42
1:A:580:TYR:OH	2:B:-2:ARG:HB3	2.20	0.42
1:A:685:THR:HA	1:A:688:PHE:CD2	2.55	0.41
1:A:434:ARG:NH1	1:A:524:GLU:OE1	2.48	0.41
1:A:491:LYS:HE3	1:A:491:LYS:HB2	1.85	0.41

There are no symmetry-related clashes.

## 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	261/318 (82%)	253 (97%)	8 (3%)	0	100	100
2	B	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
All	All	275/334 (82%)	266 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.



### 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	207/279 (74%)	207 (100%)	0	100	100
2	B	13/14 (93%)	13 (100%)	0	100	100
All	All	220/293 (75%)	220 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 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 ⓘ

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	267/318 (83%)	0.62	23 (8%)	11 16	36, 59, 108, 128	0
2	B	16/16 (100%)	2.27	5 (31%)	0 0	55, 75, 111, 119	0
All	All	283/334 (84%)	0.71	28 (9%)	8 13	36, 60, 109, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	9	SER	10.8
2	B	10	PHE	7.4
2	B	8	GLN	6.5
1	A	466	GLY	6.3
1	A	485	ILE	4.9
1	A	448	LEU	4.7
1	A	484	ASP	4.5
2	B	7	GLY	4.5
1	A	473	ALA	4.4
1	A	470	TRP	4.4
1	A	469	GLU	3.7
1	A	461	HIS	3.4
1	A	431	PHE	3.3
1	A	430	GLY	3.2
1	A	487	PHE	3.2
1	A	468	GLU	3.1
1	A	452	LEU	3.0
1	A	463	ILE	2.9
2	B	6	ASN	2.7
1	A	488	ILE	2.6
1	A	467	ASP	2.5
1	A	464	ASP	2.4
1	A	471	TRP	2.3
1	A	465	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	494	VAL	2.2
1	A	462	VAL	2.2
1	A	474	ARG	2.1
1	A	429	ARG	2.1

## 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.