



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2016 – 11:22 AM EST

PDB ID : 5G1D  
Title : The complex structure of syntenin-1 PDZ domain with c-terminal extension  
Authors : Lee, I.; Kim, H.; Yun, J.H.; Lee, W.  
Deposited on : 2016-03-25  
Resolution : 2.81 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028320

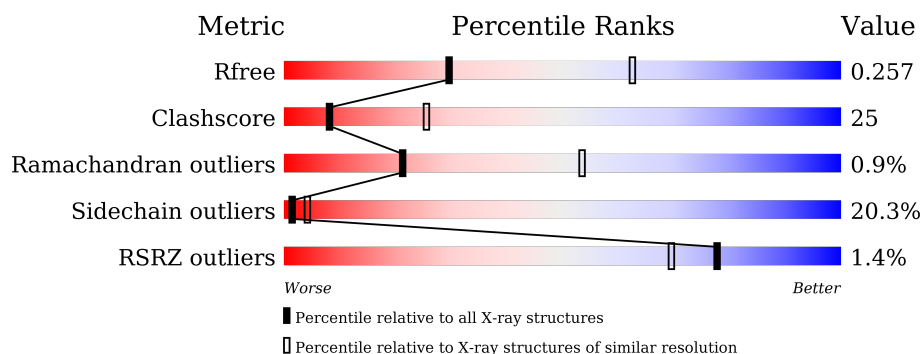
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	201	<div> <div>47%</div> <div>29%</div> <div>8%</div> <div>16%</div> </div>
1	B	201	<div>2%</div> <div>48%</div> <div>26%</div> <div>8%</div> <div>17%</div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2687 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 SYNTENIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1284	810	230	238	6			
1	B	167	Total	C	N	O	S	0	0	0
			1275	804	228	237	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLY	-	EXPRESSION TAG	UNP Q9JI92
A	101	SER	-	EXPRESSION TAG	UNP Q9JI92
A	102	ALA	-	EXPRESSION TAG	UNP Q9JI92
A	103	MET	-	EXPRESSION TAG	UNP Q9JI92
A	104	ALA	-	EXPRESSION TAG	UNP Q9JI92
A	105	ASP	-	EXPRESSION TAG	UNP Q9JI92
A	106	ILE	-	EXPRESSION TAG	UNP Q9JI92
A	107	GLY	-	EXPRESSION TAG	UNP Q9JI92
B	100	GLY	-	EXPRESSION TAG	UNP Q9JI92
B	101	SER	-	EXPRESSION TAG	UNP Q9JI92
B	102	ALA	-	EXPRESSION TAG	UNP Q9JI92
B	103	MET	-	EXPRESSION TAG	UNP Q9JI92
B	104	ALA	-	EXPRESSION TAG	UNP Q9JI92
B	105	ASP	-	EXPRESSION TAG	UNP Q9JI92
B	106	ILE	-	EXPRESSION TAG	UNP Q9JI92
B	107	GLY	-	EXPRESSION TAG	UNP Q9JI92

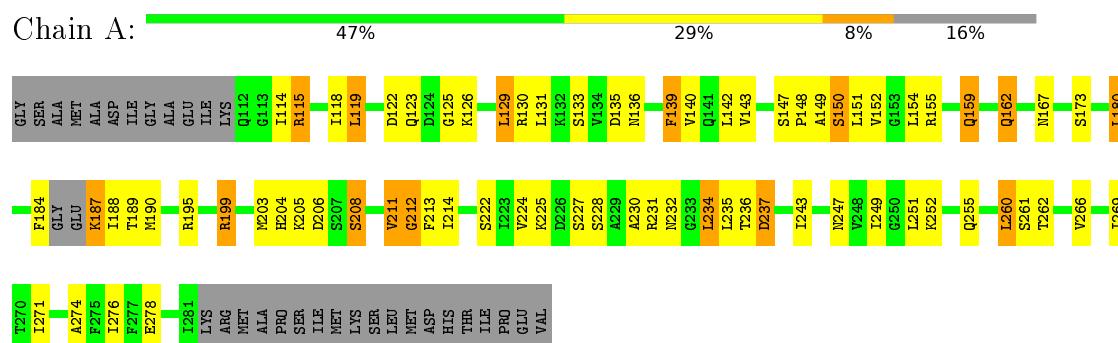
- Molecule 2 is a protein called SYNDECAN-4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			64	42	9	13			
2	D	8	Total	C	N	O	0	0	0
			64	42	9	13			

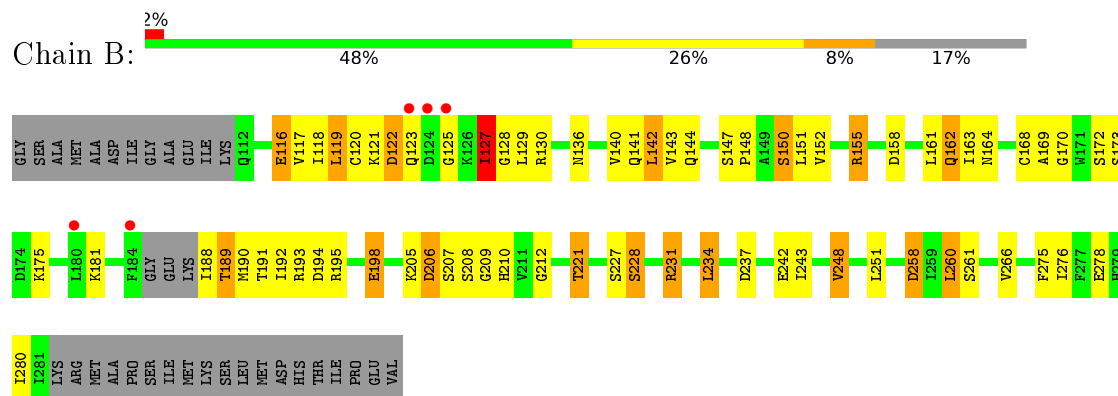
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

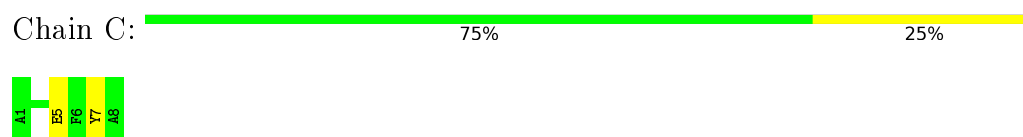
#### • Molecule 1: SYNTENIN-1



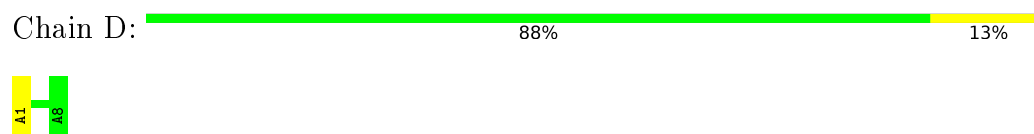
#### • Molecule 1: SYNTENIN-1



#### • Molecule 2: SYNDECAN-4



#### • Molecule 2: SYNDECAN-4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.53Å 88.53Å 90.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.81 34.57 – 2.81	Depositor EDS
% Data completeness (in resolution range)	96.3 (50.00-2.81) 96.4 (34.57-2.81)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.89 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.194 , 0.235 0.221 , 0.257	Depositor DCC
$R_{free}$ test set	666 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	2687	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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	1.30	4/1301 (0.3%)	0.79	1/1751 (0.1%)
1	B	1.43	8/1292 (0.6%)	1.06	2/1740 (0.1%)
2	C	1.82	1/66 (1.5%)	1.24	0/90
2	D	1.56	1/66 (1.5%)	1.08	0/90
All	All	1.38	14/2725 (0.5%)	0.95	3/3671 (0.1%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	168	CYS	CB-SG	-7.88	1.68	1.82
1	B	231	ARG	CZ-NH1	-7.48	1.23	1.33
1	B	198	GLU	CG-CD	6.30	1.61	1.51
1	A	139	PHE	CD2-CE2	-5.96	1.27	1.39
1	B	231	ARG	CZ-NH2	-5.93	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	193	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	B	206	ASP	CB-CG-OD1	-6.79	112.19	118.30
1	A	212	GLY	N-CA-C	6.23	128.67	113.10

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	1284	0	1319	85	0
1	B	1275	0	1306	48	0
2	C	64	0	56	1	0
2	D	64	0	56	0	0
All	All	2687	0	2737	133	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 25.

The worst 5 of 133 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:228:SER:HA	1:A:231:ARG:CD	1.77	1.14
1:A:139:PHE:CE2	1:A:159:GLN:HG3	1.83	1.12
1:A:162:GLN:NE2	1:A:167:ASN:OD1	1.79	1.12
1:A:228:SER:HA	1:A:231:ARG:HD3	1.39	1.01
1:A:139:PHE:CZ	1:A:159:GLN:HG3	2.00	0.95

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	164/201 (82%)	163 (99%)	1 (1%)	0	100	100
1	B	163/201 (81%)	153 (94%)	7 (4%)	3 (2%)	11	33
2	C	6/8 (75%)	6 (100%)	0	0	100	100
2	D	6/8 (75%)	6 (100%)	0	0	100	100
All	All	339/418 (81%)	328 (97%)	8 (2%)	3 (1%)	21	53

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	127	ILE
1	B	181	LYS
1	B	128	GLY

### 5.3.2 Protein sidechains ⓘ

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	142/168 (84%)	113 (80%)	29 (20%)	1	4
1	B	141/168 (84%)	110 (78%)	31 (22%)	1	3
2	C	6/6 (100%)	6 (100%)	0	100	100
2	D	6/6 (100%)	6 (100%)	0	100	100
All	All	295/348 (85%)	235 (80%)	60 (20%)	1	4

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	276	ILE
1	B	121	LYS
1	B	248	VAL
1	B	118	ILE
1	B	123	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	HIS
1	A	247	ASN
1	B	136	ASN
1	B	244	ASN

### 5.3.3 RNA ⓘ

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 [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	168/201 (83%)	-0.21	0 <span>100</span> <span>100</span>	9, 31, 58, 88	0
1	B	167/201 (83%)	-0.20	5 (2%) <span>54</span> <span>41</span>	10, 33, 88, 129	0
2	C	8/8 (100%)	-0.34	0 <span>100</span> <span>100</span>	22, 33, 38, 42	0
2	D	8/8 (100%)	-0.27	0 <span>100</span> <span>100</span>	26, 32, 39, 39	0
All	All	351/418 (83%)	-0.21	5 (1%) <span>78</span> <span>69</span>	9, 32, 69, 129	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	ASP	4.9
1	B	125	GLY	3.5
1	B	184	PHE	2.7
1	B	180	LEU	2.5
1	B	123	GLN	2.5

### 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.