



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 06:07 PM JST

PDB ID : 9VAC / pdb\_00009vac  
Title : Crystal structure of the PDZ tandem of syntenin  
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Deposited on : 2025-06-03  
Resolution : 2.02 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

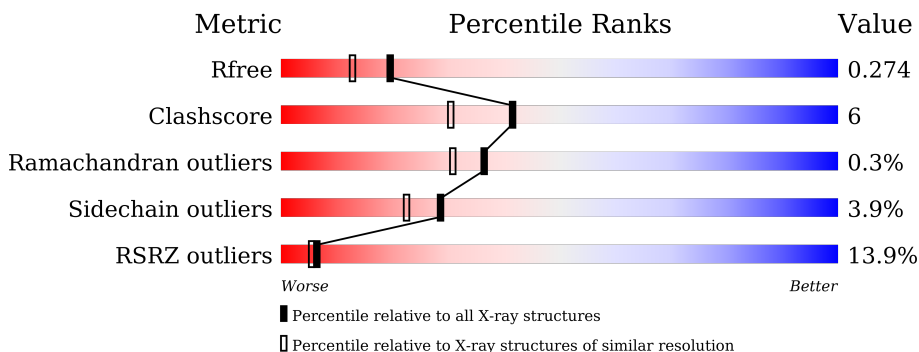
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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))
$R_{free}$	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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 of 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	166	<div> <div>7%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	B	166	<div> <div>21%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2635 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	166	Total	C	N	O	S	0	0	0
			1270	797	225	242	6			
1	B	166	Total	C	N	O	S	0	0	0
			1270	797	225	242	6			

There are 2 discrepancies between the modelled and reference sequences:

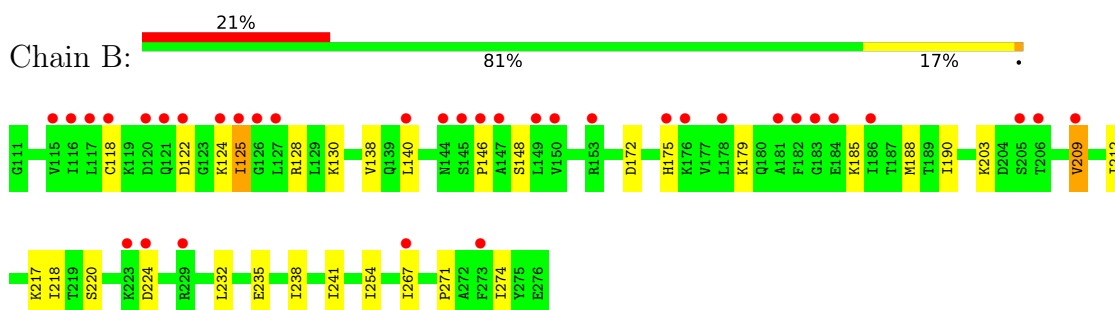
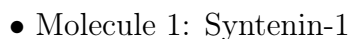
Chain	Residue	Modelled	Actual	Comment	Reference
A	275	TYR	PHE	engineered mutation	UNP O00560
B	275	TYR	PHE	engineered mutation	UNP O00560

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	57	Total	O	0	0
			57	57		
2	B	38	Total	O	0	0
			38	38		



- Molecule 1: Syntenin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.88Å 56.88Å 155.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.97 – 2.02 46.97 – 2.02	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.97-2.02) 92.3 (46.97-2.02)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.231 , 0.274 0.231 , 0.274	Depositor DCC
$R_{free}$ test set	994 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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	0.10	0/1286	0.29	0/1730
1	B	0.09	0/1286	0.28	0/1730
All	All	0.10	0/2572	0.29	0/3460

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	1270	0	1300	18	0
1	B	1270	0	1300	17	0
2	A	57	0	0	3	0
2	B	38	0	0	1	0
All	All	2635	0	2600	33	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 6.

All (33) 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:153:ARG:HH11	1:A:153:ARG:HG3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:CYS:SG	1:B:185:LYS:NZ	2.63	0.72
1:B:238:ILE:HG12	1:B:267:ILE:HD11	1.79	0.65
1:A:118:CYS:SG	2:A:355:HOH:O	2.57	0.60
1:B:130:LYS:HD3	1:B:274:ILE:HG23	1.84	0.59
1:A:130:LYS:HE3	1:A:132:ILE:HD11	1.84	0.59
1:A:129:LEU:H	1:A:175:HIS:CE1	2.24	0.56
1:A:128:ARG:HB2	1:A:140:LEU:HB3	1.91	0.53
1:A:238:ILE:HG12	1:A:267:ILE:HD11	1.90	0.52
1:A:246:VAL:HG13	1:A:254:ILE:HG12	1.93	0.49
1:A:130:LYS:NZ	1:A:275:TYR:O	2.45	0.49
1:A:217:LYS:NZ	1:A:235:GLU:OE2	2.40	0.49
1:B:203:LYS:HG2	1:B:209:VAL:HG13	1.94	0.49
1:B:175:HIS:O	1:B:179:LYS:HE2	2.14	0.48
1:A:154:PHE:HZ	1:A:275:TYR:HA	1.78	0.47
1:B:241:ILE:HD11	1:B:254:ILE:HG23	1.95	0.47
1:A:195:PHE:HE1	1:B:271:PRO:HG3	1.80	0.47
1:A:158:VAL:HA	1:A:190:ILE:HD13	1.97	0.46
1:B:125:ILE:HA	1:B:146:PRO:HG2	1.97	0.46
1:B:218:ILE:HD13	1:B:232:LEU:HD21	1.99	0.44
1:A:153:ARG:HG3	1:A:153:ARG:NH1	2.28	0.43
1:B:128:ARG:HG3	1:B:140:LEU:HB3	2.00	0.43
1:B:172:ASP:OD2	2:B:301:HOH:O	2.21	0.42
1:A:153:ARG:HH11	1:A:153:ARG:CG	2.29	0.42
1:A:249:LEU:O	2:A:301:HOH:O	2.22	0.41
1:B:179:LYS:HE3	1:B:179:LYS:HB2	1.84	0.41
1:B:122:ASP:CG	1:B:124:LYS:HE2	2.44	0.41
1:A:165:ASN:HD22	1:B:224:ASP:HA	1.84	0.41
1:B:217:LYS:NZ	1:B:235:GLU:OE2	2.40	0.41
1:B:212:ILE:HB	1:B:220:SER:HB3	2.03	0.41
1:A:128:ARG:HG3	1:A:140:LEU:HD22	2.03	0.40
1:A:215:ASN:ND2	2:A:302:HOH:O	2.39	0.40
1:B:188:MET:HB3	1:B:190:ILE:CD1	2.50	0.40

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	164/166 (99%)	157 (96%)	6 (4%)	1 (1%)	21	12
1	B	164/166 (99%)	155 (94%)	9 (6%)	0	100	100
All	All	328/332 (99%)	312 (95%)	15 (5%)	1 (0%)	36	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	ARG

### 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	141/141 (100%)	134 (95%)	7 (5%)	22	15
1	B	141/141 (100%)	137 (97%)	4 (3%)	38	35
All	All	282/282 (100%)	271 (96%)	11 (4%)	28	22

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	ARG
1	A	115	VAL
1	A	140	LEU
1	A	184	GLU
1	A	193	ARG
1	A	259	SER
1	A	263	THR
1	B	125	ILE
1	B	138	VAL
1	B	148	SER
1	B	209	VAL



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

Mol	Chain	Res	Type
1	A	237	ASN
1	A	244	GLN
1	B	134	ASN
1	B	160	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 oligosaccharides 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	166/166 (100%)	0.71	11 (6%) 24 23	19, 35, 53, 62	0
1	B	166/166 (100%)	1.13	35 (21%) 2 2	23, 38, 82, 101	0
All	All	332/332 (100%)	0.92	46 (13%) 6 5	19, 36, 66, 101	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	182	PHE	5.0
1	B	150	VAL	4.3
1	B	118	CYS	4.0
1	B	273	PHE	3.6
1	B	183	GLY	3.4
1	B	181	ALA	3.4
1	B	186	ILE	3.4
1	A	275	TYR	3.3
1	B	121	GLN	3.2
1	B	125	ILE	3.1
1	B	149	LEU	3.0
1	A	264	VAL	3.0
1	B	117	LEU	2.9
1	B	144	ASN	2.8
1	B	223	LYS	2.7
1	B	122	ASP	2.7
1	B	209	VAL	2.6
1	B	146	PRO	2.5
1	B	205	SER	2.5
1	B	140	LEU	2.5
1	A	245	ASN	2.3
1	A	249	LEU	2.3
1	B	184	GLU	2.3
1	A	266	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	120	ASP	2.3
1	A	261	SER	2.2
1	B	153	ARG	2.2
1	B	178	LEU	2.2
1	A	243	GLY	2.2
1	B	147	ALA	2.2
1	B	127	LEU	2.2
1	B	206	THR	2.2
1	A	205	SER	2.1
1	B	224	ASP	2.1
1	B	229	ARG	2.1
1	B	175	HIS	2.1
1	B	267	ILE	2.1
1	B	124	LYS	2.1
1	B	126	GLY	2.1
1	B	115	VAL	2.1
1	B	145	SER	2.1
1	A	118	CYS	2.0
1	B	176	LYS	2.0
1	B	116	ILE	2.0
1	A	263	THR	2.0
1	A	123	GLY	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 oligosaccharides 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.