



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 06:08 PM JST

PDB ID : 9VA9 / pdb\_00009va9  
Title : Crystal structure of the PDZ tandem of syntenin  
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Deposited on : 2025-06-03  
Resolution : 1.81 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

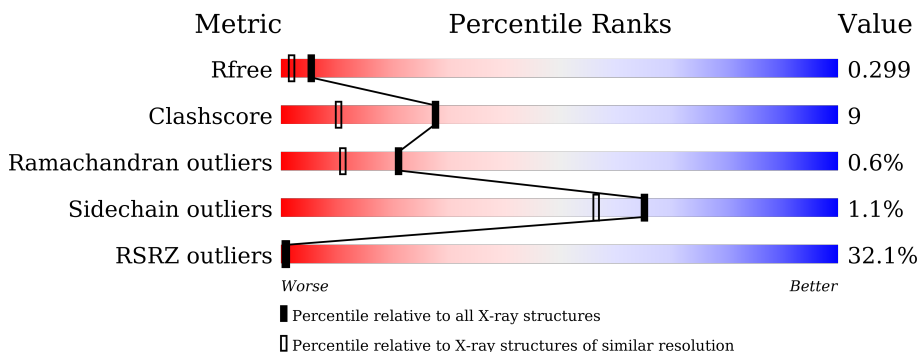
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.81 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))
$R_{free}$	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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>23%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	166	<div> <div>41%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2609 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	164	Total	C	N	O	S	0	1	0
			1256	788	226	236	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

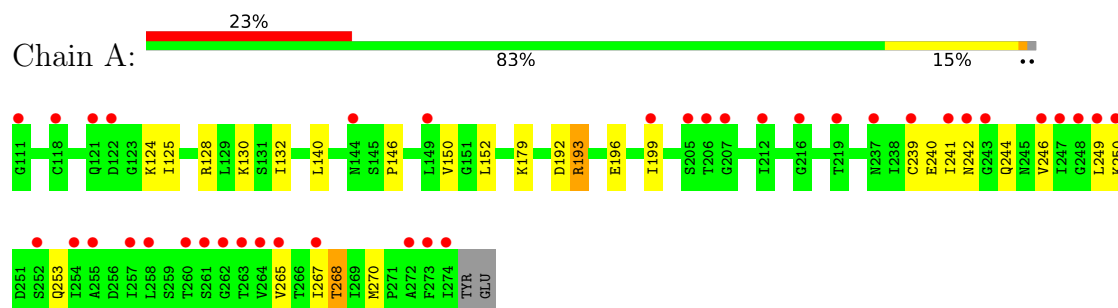
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	46	Total	O	0	0
			46	46		
2	B	37	Total	O	0	0
			37	37		

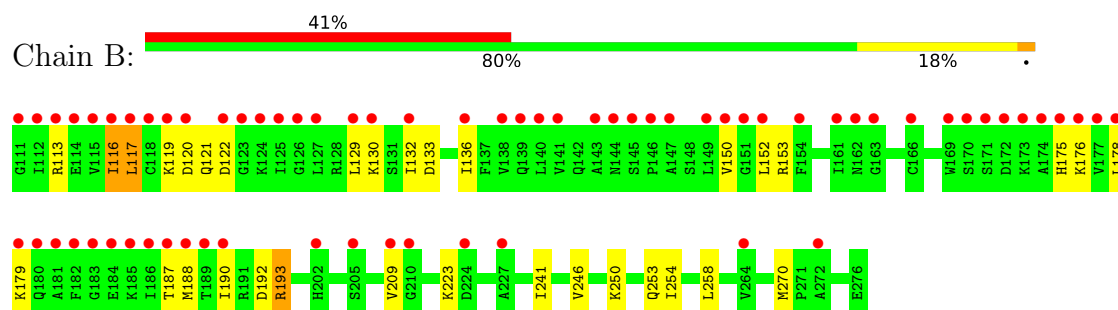
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Syntenin-1



#### • Molecule 1: Syntenin-1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.61Å 56.61Å 150.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.62 – 1.81 46.62 – 1.81	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.62-1.81) 95.1 (46.62-1.81)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.259 , 0.299 0.259 , 0.299	Depositor DCC
$R_{free}$ test set	1332 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.60% 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	0.21	0/1274	0.34	0/1714
1	B	0.17	0/1286	0.40	0/1730
All	All	0.19	0/2560	0.37	0/3444

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

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	1256	0	1298	23	0
1	B	1270	0	1300	23	0
2	A	46	0	0	0	0
2	B	37	0	0	0	0
All	All	2609	0	2598	46	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 9.

All (46) 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:250:LYS:HD2	1:A:253:GLN:OE1	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ARG:HG3	1:B:193:ARG:HD3	1.67	0.74
1:B:250:LYS:H	1:B:253:GLN:HE21	1.36	0.73
1:B:121:GLN:HG2	1:B:122:ASP:H	1.59	0.67
1:A:239:CYS:HB2	1:A:268:THR:HG22	1.77	0.66
1:A:130:LYS:HE3	1:A:132:ILE:HD11	1.79	0.65
1:B:175:HIS:HA	1:B:178:LEU:HG	1.79	0.64
1:B:152:LEU:HD11	1:B:188:MET:HE1	1.80	0.62
1:B:241:ILE:HD12	1:B:246:VAL:HG11	1.81	0.61
1:B:117:LEU:HA	1:B:150:VAL:HG11	1.84	0.59
1:A:241:ILE:HD12	1:A:246:VAL:HG11	1.85	0.58
1:A:193:ARG:HB3	1:A:196:GLU:HB2	1.85	0.58
1:A:128[B]:ARG:NH1	1:A:140:LEU:CB	2.68	0.56
1:B:179:LYS:O	1:B:179:LYS:HD2	2.06	0.56
1:A:128[B]:ARG:NH1	1:A:140:LEU:HB2	2.24	0.53
1:B:193:ARG:HD2	1:B:270:MET:HE1	1.89	0.53
1:B:209:VAL:HG11	1:B:258:LEU:HD22	1.90	0.52
1:B:241:ILE:HD11	1:B:254:ILE:HG23	1.92	0.51
1:A:128[B]:ARG:NH2	1:A:140:LEU:HD22	2.26	0.51
1:B:132:ILE:HG22	1:B:133:ASP:CG	2.37	0.50
1:A:239:CYS:SG	1:A:270:MET:HE3	2.52	0.49
1:B:116:ILE:HG23	1:B:187:THR:HG22	1.94	0.49
1:A:249:LEU:HD22	1:A:253:GLN:NE2	2.27	0.49
1:B:250:LYS:H	1:B:253:GLN:NE2	2.07	0.49
1:B:129:LEU:HD13	1:B:136:ILE:CG2	2.43	0.49
1:B:176:LYS:HD3	1:B:176:LYS:N	2.28	0.49
1:B:223:LYS:N	1:B:223:LYS:HD3	2.27	0.48
1:B:113:ARG:HB3	1:B:190:ILE:HB	1.95	0.48
1:B:121:GLN:HG2	1:B:122:ASP:N	2.26	0.47
1:B:119:LYS:HD3	1:B:120:ASP:H	1.79	0.47
1:A:240:GLU:HB2	1:A:268:THR:HB	1.97	0.46
1:A:150:VAL:HG23	1:A:152:LEU:HG	1.98	0.44
1:A:124:LYS:HA	1:A:124:LYS:HD3	1.81	0.44
1:A:179:LYS:HD3	1:A:179:LYS:HA	1.72	0.44
1:A:128[B]:ARG:NH1	1:A:140:LEU:HD22	2.33	0.43
1:A:125:ILE:HA	1:A:146:PRO:HG2	1.99	0.43
1:B:130:LYS:HG2	1:B:132:ILE:HD11	2.00	0.43
1:A:192:ASP:O	1:A:193:ARG:C	2.61	0.42
1:B:192:ASP:O	1:B:193:ARG:C	2.62	0.42
1:B:119:LYS:CG	1:B:120:ASP:H	2.32	0.42
1:A:199:ILE:HG23	1:A:267:ILE:HG13	2.01	0.42
1:A:242:ASN:HD21	1:A:265:VAL:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128[B]:ARG:HH22	1:A:140:LEU:HD22	1.85	0.41
1:A:240:GLU:HA	1:A:244:GLN:O	2.20	0.41
1:A:244:GLN:O	1:A:246:VAL:HG13	2.20	0.40
1:A:128[B]:ARG:CZ	1:A:140:LEU:HD22	2.51	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	163/166 (98%)	157 (96%)	5 (3%)	1 (1%)	21	11
1	B	164/166 (99%)	157 (96%)	6 (4%)	1 (1%)	21	11
All	All	327/332 (98%)	314 (96%)	11 (3%)	2 (1%)	21	11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	193	ARG
1	A	193	ARG

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/141 (99%)	139 (99%)	1 (1%)	76	70
1	B	141/141 (100%)	139 (99%)	2 (1%)	59	49
All	All	281/282 (100%)	278 (99%)	3 (1%)	65	56

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	THR
1	B	116	ILE
1	B	117	LEU

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	139	GLN
1	A	242	ASN
1	B	202	HIS
1	B	253	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	164/166 (98%)	1.24	38 (23%)	2 2	21, 38, 57, 66	1 (0%)
1	B	166/166 (100%)	2.01	68 (40%)	0 0	24, 44, 92, 109	0
All	All	330/332 (99%)	1.63	106 (32%)	1 1	21, 41, 80, 109	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	LEU	8.8
1	B	186	ILE	7.9
1	B	116	ILE	7.6
1	B	178	LEU	6.3
1	B	149	LEU	5.3
1	B	125	ILE	5.3
1	B	146	PRO	5.3
1	B	115	VAL	5.0
1	B	147	ALA	4.6
1	B	177	VAL	4.6
1	B	171	SER	4.5
1	A	205	SER	4.5
1	B	174	ALA	4.5
1	B	162	ASN	4.4
1	A	274	ILE	4.4
1	B	181	ALA	4.4
1	B	150	VAL	4.4
1	B	123	GLY	4.1
1	B	118	CYS	4.1
1	B	182	PHE	4.0
1	B	140	LEU	4.0
1	B	179	LYS	3.8
1	B	161	ILE	3.8
1	A	247	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	172	ASP	3.7
1	A	273	PHE	3.7
1	B	111	GLY	3.7
1	A	261	SER	3.6
1	B	124	LYS	3.6
1	B	202	HIS	3.6
1	A	118	CYS	3.5
1	B	129	LEU	3.5
1	B	120	ASP	3.5
1	B	138	VAL	3.4
1	A	199	ILE	3.4
1	B	209	VAL	3.4
1	A	267	ILE	3.4
1	A	272	ALA	3.3
1	B	184	GLU	3.3
1	B	163	GLY	3.2
1	A	262	GLY	3.2
1	B	183	GLY	3.2
1	B	187	THR	3.1
1	B	188	MET	3.1
1	B	122	ASP	3.1
1	B	127	LEU	3.1
1	B	144	ASN	3.1
1	B	119	LYS	3.1
1	B	141	VAL	3.0
1	A	260	THR	3.0
1	B	151	GLY	3.0
1	B	176	LYS	2.9
1	A	257	ILE	2.9
1	A	248	GLY	2.9
1	B	175	HIS	2.9
1	A	249	LEU	2.9
1	A	111	GLY	2.9
1	B	272	ALA	2.8
1	A	216	GLY	2.8
1	A	265	VAL	2.8
1	B	170	SER	2.7
1	A	255	ALA	2.7
1	B	189	THR	2.7
1	B	113	ARG	2.6
1	B	205	SER	2.6
1	A	206	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	152	LEU	2.6
1	A	263	THR	2.6
1	A	258	LEU	2.6
1	B	173	LYS	2.6
1	B	166	CYS	2.5
1	B	126	GLY	2.5
1	A	237	ASN	2.5
1	B	190	ILE	2.5
1	B	185	LYS	2.5
1	A	243	GLY	2.4
1	B	139	GLN	2.4
1	A	246	VAL	2.4
1	A	254	ILE	2.4
1	A	242	ASN	2.4
1	A	252	SER	2.3
1	B	224	ASP	2.3
1	B	112	ILE	2.3
1	A	250	LYS	2.3
1	A	219	THR	2.3
1	A	212	ILE	2.3
1	A	122	ASP	2.3
1	B	132	ILE	2.2
1	B	180	GLN	2.2
1	A	264	VAL	2.2
1	B	264	VAL	2.2
1	A	239	CYS	2.2
1	B	145	SER	2.2
1	A	241	ILE	2.2
1	A	207	GLY	2.2
1	B	143	ALA	2.2
1	B	114	GLU	2.1
1	B	154	PHE	2.1
1	A	121	GLN	2.1
1	A	149	LEU	2.1
1	B	136	ILE	2.1
1	B	169	TRP	2.1
1	A	144	ASN	2.1
1	B	130	LYS	2.0
1	B	210	GLY	2.0
1	B	227	ALA	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.