



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:36 PM UTC

PDB ID : 5G1E / pdb_00005g1e
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 : 1.92 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

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>.

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

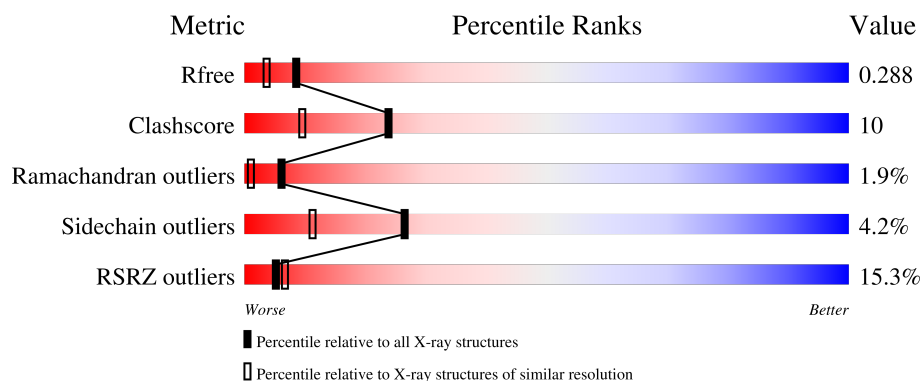
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 ≥ 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	201	 11% 66% 15% • 16%
1	B	201	 14% 63% 15% •• 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2697 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	169	Total	C	N	O	S	0	0	0
			1288	812	230	240	6			
1	B	164	Total	C	N	O	S	0	0	0
			1262	797	225	234	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 water.

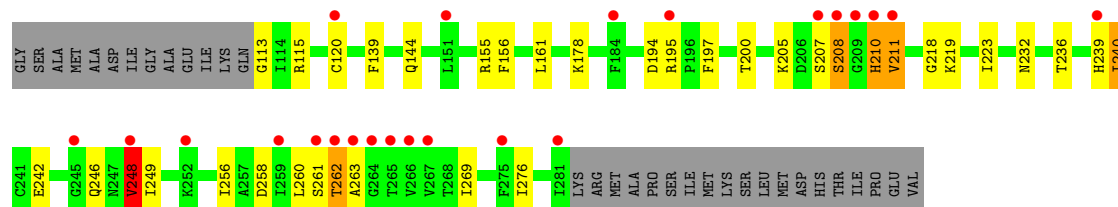
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total	O	0	0
			85	85		
2	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

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.

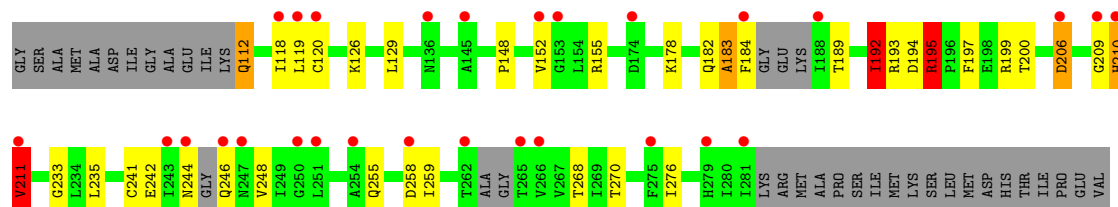
• Molecule 1: SYNTENIN-1

Chain A: 



• Molecule 1: SYNTENIN-1

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.74Å 63.32Å 103.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.03 – 1.92 54.03 – 1.92	Depositor EDS
% Data completeness (in resolution range)	95.9 (54.03-1.92) 96.0 (54.03-1.92)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.43 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.232 , 0.280 (Not available) , 0.288	Depositor DCC
R_{free} test set	1288 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2697	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.17	1/1306 (0.1%)	1.11	5/1759 (0.3%)
1	B	1.11	1/1277 (0.1%)	1.11	6/1717 (0.3%)
All	All	1.14	2/2583 (0.1%)	1.11	11/3476 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	CYS	C-N	-9.56	1.20	1.33
1	B	120	CYS	C-N	-7.29	1.24	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	CYS	O-C-N	-12.24	107.71	123.13
1	B	119	LEU	CA-C-N	8.87	135.47	123.05
1	B	119	LEU	C-N-CA	8.87	135.47	123.05
1	B	210	HIS	N-CA-C	7.63	122.48	112.72
1	A	248	VAL	N-CA-C	-6.06	107.22	113.10
1	A	120	CYS	CA-C-N	5.93	129.26	120.90
1	A	120	CYS	C-N-CA	5.93	129.26	120.90
1	B	195	ARG	CA-C-N	-5.37	114.29	119.87
1	B	195	ARG	C-N-CA	-5.37	114.29	119.87
1	A	210	HIS	N-CA-C	5.37	120.48	113.88
1	B	192	ILE	N-CA-C	5.06	115.99	108.46

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	1288	0	1321	23	0
1	B	1262	0	1293	32	0
2	A	85	0	0	2	0
2	B	62	0	0	6	0
All	All	2697	0	2614	52	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 10.

All (52) 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:B:155:ARG:NH1	2:B:2019:HOH:O	2.04	0.90
1:B:194:ASP:OD1	1:B:195:ARG:HD3	1.90	0.71
1:B:244:ASN:O	2:B:2058:HOH:O	2.10	0.70
1:A:248:VAL:HG22	1:A:256:ILE:HG12	1.73	0.69
1:B:178:LYS:HE3	1:B:182:GLN:HE21	1.60	0.67
1:A:155:ARG:HD2	1:A:195:ARG:NH1	2.13	0.63
1:A:258:ASP:O	1:A:262:THR:HG23	1.98	0.62
1:B:258:ASP:OD1	1:B:259:ILE:N	2.32	0.62
1:B:242:GLU:HB3	1:B:244:ASN:HD21	1.65	0.61
1:B:241:CYS:O	1:B:242:GLU:HG3	2.04	0.58
1:A:218:GLY:O	1:A:240:ILE:HG22	2.03	0.57
1:B:199:ARG:NH2	1:B:235:LEU:HD12	2.19	0.57
1:B:255:GLN:O	1:B:258:ASP:OD1	2.22	0.56
1:A:240:ILE:HD13	1:A:269:ILE:HB	1.88	0.56
1:A:115:ARG:NH1	1:A:194:ASP:OD1	2.39	0.56
1:A:223:ILE:CD1	1:A:236:THR:HG23	2.37	0.55
1:B:270:THR:HG23	2:B:2057:HOH:O	2.06	0.55
1:B:244:ASN:HA	1:B:246:GLN:N	2.23	0.54
1:B:241:CYS:C	1:B:242:GLU:HG3	2.33	0.54
1:A:248:VAL:CG2	1:A:256:ILE:HG12	2.38	0.53
1:B:242:GLU:HB2	1:B:270:THR:OG1	2.09	0.53
1:A:223:ILE:HD12	1:A:236:THR:HG23	1.91	0.52
1:B:126:LYS:NZ	2:B:2008:HOH:O	2.41	0.52
1:A:240:ILE:HD11	1:A:242:GLU:O	2.13	0.49
1:B:197:PHE:CD1	1:B:276:ILE:HD13	2.48	0.48
1:B:148:PRO:O	1:B:152:VAL:HG23	2.14	0.47
1:B:242:GLU:HB3	1:B:244:ASN:ND2	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LYS:HG3	2:A:2057:HOH:O	2.15	0.47
1:B:155:ARG:HD2	1:B:195:ARG:HD2	1.97	0.46
1:B:210:HIS:O	1:B:211:VAL:HB	2.14	0.46
1:A:207:SER:O	1:A:208:SER:OG	2.29	0.46
1:A:197:PHE:CD1	1:A:276:ILE:HD13	2.52	0.45
1:B:183:ALA:O	1:B:184:PHE:C	2.59	0.45
1:B:209:GLY:C	1:B:210:HIS:HD2	2.25	0.45
1:A:161:LEU:HD22	1:B:233:GLY:HA3	1.98	0.45
1:B:189:THR:HG23	2:B:2023:HOH:O	2.17	0.45
1:B:112:GLN:HG3	1:B:194:ASP:HB3	1.98	0.44
1:A:261:SER:O	1:A:263:ALA:N	2.50	0.44
1:A:219:LYS:HG3	1:A:239:HIS:HD2	1.82	0.44
1:B:126:LYS:HE2	2:B:2005:HOH:O	2.18	0.43
1:A:156:PHE:CD2	1:A:249:ILE:CD1	3.01	0.43
1:A:232:ASN:O	1:B:193:ARG:NH1	2.51	0.43
1:B:200:THR:HG23	1:B:268:THR:HG23	2.00	0.43
1:B:118:ILE:HD12	1:B:118:ILE:N	2.35	0.42
1:A:139:PHE:HZ	1:B:235:LEU:HD11	1.84	0.42
1:A:210:HIS:O	1:A:211:VAL:HB	2.19	0.42
1:A:205:LYS:NZ	1:A:260:LEU:O	2.51	0.42
1:A:205:LYS:NZ	1:A:263:ALA:HA	2.35	0.41
1:B:194:ASP:O	1:B:195:ARG:C	2.62	0.41
1:B:192:ILE:O	1:B:192:ILE:HG13	2.18	0.40
1:B:209:GLY:C	1:B:210:HIS:CD2	3.00	0.40
1:A:113:GLY:HA3	2:A:2001:HOH:O	2.22	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	167/201 (83%)	158 (95%)	6 (4%)	3 (2%)	6 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	156/201 (78%)	150 (96%)	3 (2%)	3 (2%)	6	1
All	All	323/402 (80%)	308 (95%)	9 (3%)	6 (2%)	6	1

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	SER
1	A	262	THR
1	B	206	ASP
1	A	246	GLN
1	B	183	ALA
1	B	211	VAL

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%)	137 (96%)	5 (4%)	32	16
1	B	141/168 (84%)	134 (95%)	7 (5%)	22	8
All	All	283/336 (84%)	271 (96%)	12 (4%)	26	11

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	A	200	THR
1	A	211	VAL
1	A	240	ILE
1	A	248	VAL
1	B	112	GLN
1	B	129	LEU
1	B	192	ILE
1	B	195	ARG
1	B	206	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	211	VAL
1	B	248	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	182	GLN
1	B	210	HIS

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, 95th 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 ²)	Q<0.9
1	A	169/201 (84%)	0.85	23 (13%) 7 9	11, 26, 51, 69	0
1	B	164/201 (81%)	1.06	28 (17%) 4 6	14, 28, 49, 75	0
All	All	333/402 (82%)	0.96	51 (15%) 5 7	11, 28, 52, 75	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	PHE	6.3
1	A	207	SER	6.0
1	A	262	THR	5.8
1	A	263	ALA	5.3
1	B	258	ASP	4.5
1	B	244	ASN	4.4
1	B	120	CYS	4.4
1	B	247	ASN	4.3
1	A	184	PHE	4.2
1	B	210	HIS	4.2
1	B	206	ASP	3.9
1	A	195	ARG	3.8
1	A	265	THR	3.8
1	B	262	THR	3.7
1	B	211	VAL	3.7
1	A	266	VAL	3.6
1	A	208	SER	3.4
1	A	264	GLY	3.4
1	B	250	GLY	3.4
1	A	261	SER	3.4
1	B	265	THR	3.3
1	A	120	CYS	3.2
1	B	281	ILE	3.1
1	B	188	ILE	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	243	ILE	2.9
1	B	251	LEU	2.8
1	B	279	HIS	2.7
1	A	281	ILE	2.6
1	B	119	LEU	2.5
1	A	151	LEU	2.5
1	B	246	GLN	2.5
1	A	211	VAL	2.5
1	A	267	VAL	2.5
1	A	245	GLY	2.4
1	B	275	PHE	2.4
1	A	239	HIS	2.4
1	B	174	ASP	2.4
1	B	145	ALA	2.4
1	A	209	GLY	2.4
1	A	275	PHE	2.3
1	B	152	VAL	2.3
1	B	153	GLY	2.2
1	B	254	ALA	2.2
1	B	136	ASN	2.1
1	B	209	GLY	2.1
1	A	210	HIS	2.1
1	A	252	LYS	2.1
1	B	266	VAL	2.1
1	B	118	ILE	2.0
1	A	259	ILE	2.0
1	A	248	VAL	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.