



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:17 pm BST

PDB ID : 5GW0  
Title : Crystal structure of SNX16 PX-Coiled coil  
Authors : Xu, J.; Liu, J.  
Deposited on : 2016-09-08  
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

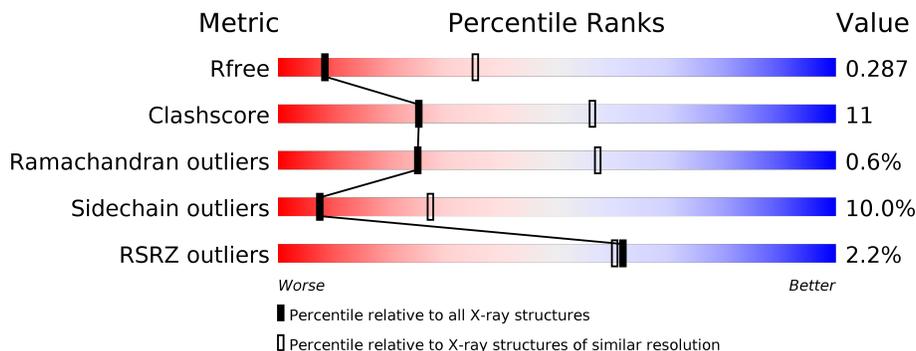
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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))
$R_{free}$	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 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	179	
1	B	179	
1	C	179	
1	D	179	
1	E	179	
1	F	179	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8558 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 Sorting nexin-16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	173	1446	926	246	268	3	3	0	0	0
1	B	170	1419	911	240	262	3	3	0	0	0
1	C	173	1446	926	246	268	3	3	0	0	0
1	D	170	1417	906	242	263	3	3	0	0	0
1	E	171	1428	915	241	266	3	3	0	0	0
1	F	168	1402	898	237	261	3	3	0	0	0





- Molecule 1: Sorting nexin-16



- Molecule 1: Sorting nexin-16



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.38Å 196.78Å 72.96Å 90.00° 111.75° 90.00°	Depositor
Resolution (Å)	19.99 – 3.30 54.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.99-3.30) 98.1 (54.45-3.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.236 , 0.288 0.236 , 0.287	Depositor DCC
$R_{free}$ test set	1364 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.3	Xtrriage
Anisotropy	0.270	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.056 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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	0.49	0/1473	0.70	0/1979
1	B	0.43	0/1445	0.66	0/1938
1	C	0.48	0/1473	0.73	0/1979
1	D	0.46	0/1442	0.66	1/1937 (0.1%)
1	E	0.39	0/1454	0.64	1/1953 (0.1%)
1	F	0.35	0/1424	0.68	1/1908 (0.1%)
All	All	0.44	0/8711	0.68	3/11694 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	166	LEU	C-N-CD	-7.86	103.30	120.60
1	E	275	LEU	CA-CB-CG	6.12	129.39	115.30
1	D	122	ALA	N-CA-C	-5.44	96.32	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	E	119	GLU	Peptide
1	F	119	GLU	Peptide

## 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	1446	0	1455	22	0
1	B	1419	0	1430	30	0
1	C	1446	0	1455	36	0
1	D	1417	0	1426	45	0
1	E	1428	0	1435	43	0
1	F	1402	0	1413	33	0
All	All	8558	0	8614	184	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 11.

The worst 5 of 184 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:F:164:LEU:HD22	1:F:194:ASN:HB3	1.53	0.90
1:C:150:ARG:HH21	1:C:231:GLU:HB2	1.40	0.85
1:D:238:TYR:OH	1:E:198:HIS:NE2	2.13	0.81
1:D:111:THR:HA	1:D:189:GLN:HE22	1.51	0.74
1:E:170:ARG:NH2	1:E:174:ASP:O	2.21	0.73

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	171/179 (96%)	167 (98%)	4 (2%)	0	100	100
1	B	166/179 (93%)	157 (95%)	8 (5%)	1 (1%)	25	57
1	C	171/179 (96%)	167 (98%)	4 (2%)	0	100	100
1	D	166/179 (93%)	160 (96%)	6 (4%)	0	100	100
1	E	169/179 (94%)	162 (96%)	6 (4%)	1 (1%)	25	57
1	F	162/179 (90%)	151 (93%)	7 (4%)	4 (2%)	5	27
All	All	1005/1074 (94%)	964 (96%)	35 (4%)	6 (1%)	25	57

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	121	ARG
1	F	121	ARG
1	B	122	ALA
1	F	135	PRO
1	F	166	LEU

### 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	161/164 (98%)	147 (91%)	14 (9%)	10	34
1	B	158/164 (96%)	142 (90%)	16 (10%)	7	27
1	C	161/164 (98%)	144 (89%)	17 (11%)	6	25
1	D	158/164 (96%)	144 (91%)	14 (9%)	9	32
1	E	159/164 (97%)	144 (91%)	15 (9%)	8	30
1	F	156/164 (95%)	137 (88%)	19 (12%)	5	20
All	All	953/984 (97%)	858 (90%)	95 (10%)	7	27

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	248	GLN
1	D	193	GLN
1	F	188	LEU
1	C	257	LEU
1	D	121	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	194	ASN

### 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 [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	170/179 (94%)	0.11	0 <b>100</b> <b>100</b>	42, 75, 111, 129	0
1	B	167/179 (93%)	0.17	2 (1%) <b>79</b> <b>78</b>	59, 87, 142, 163	0
1	C	170/179 (94%)	0.16	2 (1%) <b>79</b> <b>78</b>	35, 69, 113, 131	0
1	D	167/179 (93%)	0.05	3 (1%) <b>68</b> <b>67</b>	45, 81, 120, 168	0
1	E	168/179 (93%)	0.24	6 (3%) <b>42</b> <b>40</b>	65, 113, 155, 169	0
1	F	165/179 (92%)	0.18	9 (5%) <b>25</b> <b>23</b>	57, 133, 183, 190	0
All	All	1007/1074 (93%)	0.15	22 (2%) <b>62</b> <b>60</b>	35, 87, 162, 190	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	219	PRO	7.0
1	F	195	LEU	4.6
1	C	107	PRO	3.9
1	D	171	TRP	3.1
1	B	219	PRO	3.1

### 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

There are no such residues in this entry.