



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2026 – 12:44 PM JST

PDB ID : 9UVE / pdb\_00009uve  
Title : Crystal structure of Sec23a/24a/22b bound to STING FpS motif  
Authors : Ma, W.F.  
Deposited on : 2025-05-10  
Resolution : 2.60 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.

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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

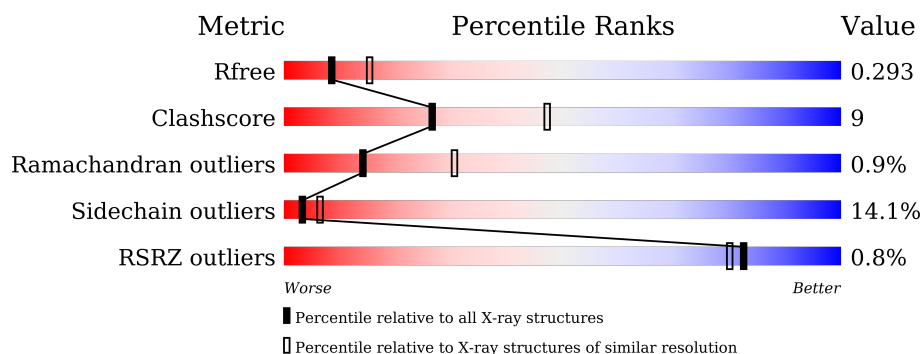
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	765	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 68%, green 22%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>68%</span> <span>22%</span> <span>• 7%</span> </div> </div>
2	B	747	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 62%, green 31%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>62%</span> <span>31%</span> <span>• •</span> </div> </div>
3	C	157	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 61%, green 20%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>61%</span> <span>20%</span> <span>• • 17%</span> </div> </div>
4	D	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 50%, yellow 50%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span></span> <span>50%</span> <span>50%</span> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12479 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5609	3577	960	1032	40			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5715	3649	963	1069	34			

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	131	Total	C	N	O	S	0	0	0
			1044	674	166	196	8			

- Molecule 4 is a protein called PHE-SEP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	2	Total	C	N	O	P	0	0	0
			22	12	2	7	1			

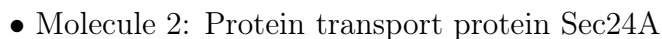
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

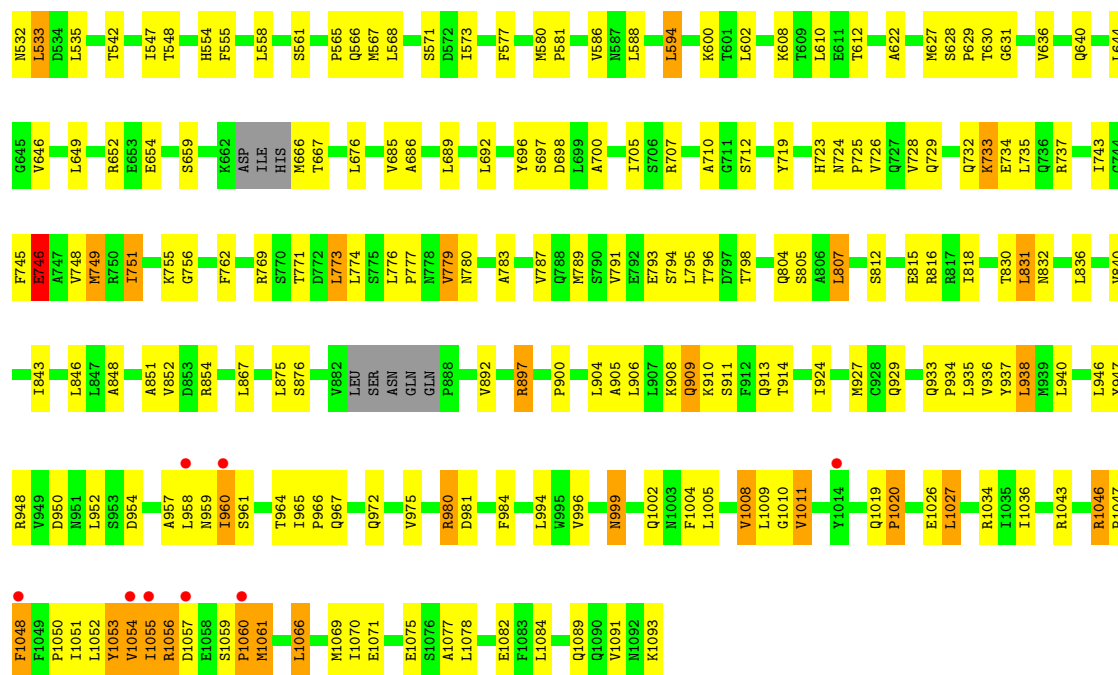
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

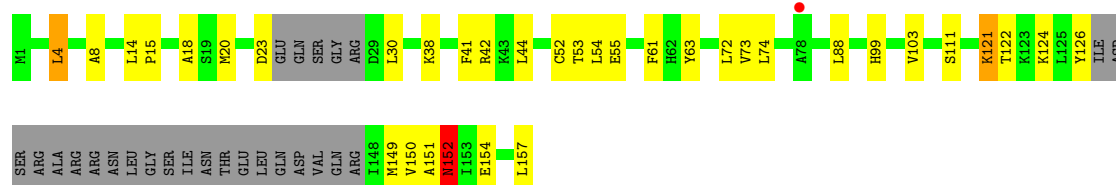
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	41	Total 41	O 41	0	0
6	B	43	Total 43	O 43	0	0
6	C	3	Total 3	O 3	0	0

- Molecule 1: Protein transport protein Sec23A





• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: PHE-SEP



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.26Å 98.17Å 130.12Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	19.88 – 2.60 19.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.88-2.60) 97.3 (19.88-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.07 (at 2.59Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.233 , 0.291 0.239 , 0.293	Depositor DCC
$R_{free}$ test set	1997 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.1	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 71.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12479	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, ZN

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	0.40	0/5740	0.63	0/7777
2	B	0.34	0/5837	0.57	2/7943 (0.0%)
3	C	0.38	0/1063	0.61	0/1434
4	D	0.10	0/11	0.20	0/13
All	All	0.37	0/12651	0.60	2/17167 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1053	TYR	CB-CA-C	5.93	122.23	110.42
2	B	1053	TYR	CA-CB-CG	5.47	123.75	113.90

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	5609	0	5519	91	0
2	B	5715	0	5711	122	0
3	C	1044	0	1036	21	0
4	D	22	0	14	0	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
6	A	41	0	0	2	0
6	B	43	0	0	1	0
6	C	3	0	0	0	0
All	All	12479	0	12280	230	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.

The worst 5 of 230 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)
3:C:15:PRO:HG3	3:C:38:LYS:HZ1	1.39	0.86
2:B:980:ARG:H	2:B:980:ARG:HE	1.26	0.82
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.62	0.81
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.64	0.80
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.68	0.76

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	702/765 (92%)	631 (90%)	67 (10%)	4 (1%)	21	42
2	B	724/747 (97%)	658 (91%)	57 (8%)	9 (1%)	10	23
3	C	125/157 (80%)	106 (85%)	18 (14%)	1 (1%)	16	34
All	All	1551/1669 (93%)	1395 (90%)	142 (9%)	14 (1%)	14	30

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1056	ARG
3	C	152	ASN
2	B	961	SER
1	A	255	PRO
2	B	1055	ILE

### 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	611/666 (92%)	534 (87%)	77 (13%)	4	9
2	B	648/678 (96%)	542 (84%)	106 (16%)	2	4
3	C	113/138 (82%)	103 (91%)	10 (9%)	9	21
4	D	1/1 (100%)	1 (100%)	0	100	100
All	All	1373/1483 (93%)	1180 (86%)	193 (14%)	3	6

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	630	THR
2	B	798	THR
2	B	659	SER
2	B	743	ILE
2	B	897	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	917	ASN
2	B	1003	ASN
3	C	152	ASN
2	B	1064	ASN
2	B	1002	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	SEP	D	1	4	9,10,10	1.56	2 (22%)	12,14,14	1.65	3 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SEP	D	1	4	-	4/10/10/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1	SEP	P-O1P	3.26	1.61	1.50
4	D	1	SEP	OXT-C	-2.17	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1	SEP	P-OG-CB	-3.28	109.26	118.30
4	D	1	SEP	OG-CB-CA	2.74	110.44	108.06
4	D	1	SEP	OXT-C-O	-2.47	118.47	124.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	SEP	N-CA-CB-OG
4	D	1	SEP	CB-OG-P-O1P
4	D	1	SEP	CB-OG-P-O2P
4	D	1	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	712/765 (93%)	-0.18	4 (0%) 85 83	58, 83, 122, 224	0
2	B	732/747 (97%)	-0.22	8 (1%) 78 74	30, 79, 118, 144	0
3	C	131/157 (83%)	0.09	1 (0%) 82 80	72, 108, 151, 169	0
4	D	1/2 (50%)	0.50	0 100 100	110, 110, 110, 110	0
All	All	1576/1671 (94%)	-0.17	13 (0%) 82 80	30, 83, 127, 224	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1060	PRO	4.6
2	B	958	LEU	3.0
2	B	960	ILE	2.9
2	B	1055	ILE	2.8
1	A	667	TRP	2.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SEP	D	1	11/11	0.85	0.10	122,125,128,148	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	A	801	1/1	0.88	0.15	201,201,201,201	0
5	ZN	B	1101	1/1	0.99	0.03	98,98,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.