



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 28, 2026 – 12:40 PM JST

PDB ID : 9UVD / pdb_00009uvd
Title : Crystal structure of Sec23a/24a/22b bound to STING pSGME motif
Authors : Ma, W.F.
Deposited on : 2025-05-10
Resolution : 2.98 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

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
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

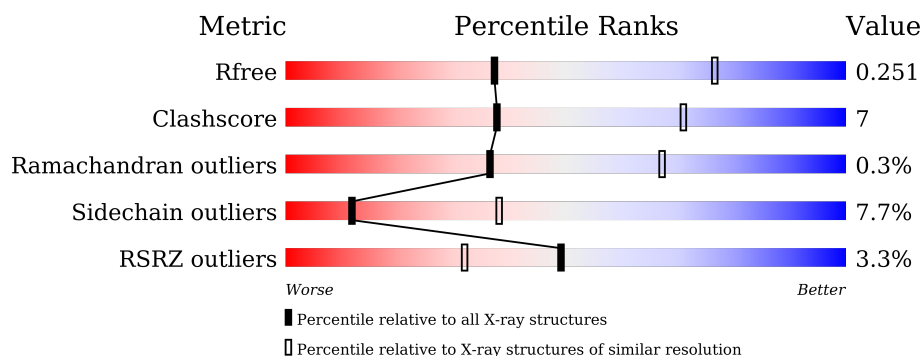
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	765	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	748	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>20%</div> <div>• •</div> </div> </div>
3	C	157	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>19%</div> <div>•</div> <div>15%</div> </div> </div>
4	D	5	<div> <div></div> <div> <div>20%</div> <div>60%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12340 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	704	Total	C	N	O	S	0	0	0
			5551	3545	940	1026	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5705	3643	965	1063	34			

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

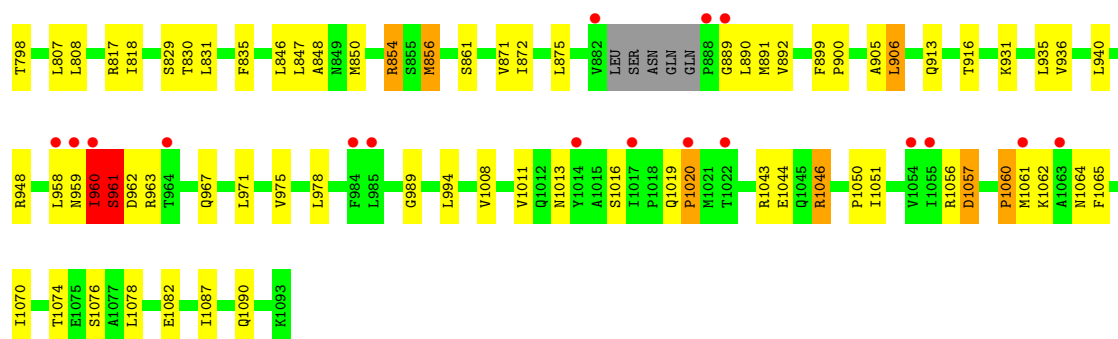
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	133	Total	C	N	O	S	0	0	0
			1046	676	165	197	8			

- Molecule 4 is a protein called ALA-SEP-GLY-MET-GLU.

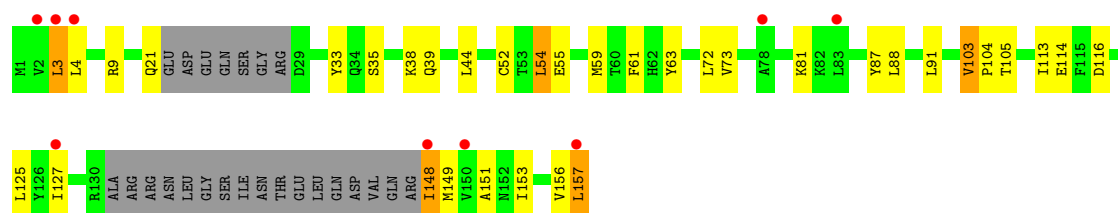
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	5	Total	C	N	O	P	S	0	0	0
			36	18	5	11	1	1			

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

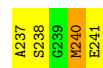
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		



• Molecule 3: Vesicle-trafficking protein SEC22b



• Molecule 4: ALA-SEP-GLY-MET-GLU



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.21Å 96.02Å 131.07Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	64.71 – 2.98 64.71 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (64.71-2.98) 99.6 (64.71-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.216 , 0.249 0.217 , 0.251	Depositor DCC
R_{free} test set	1996 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	65.8	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12340	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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](#)

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	0.17	0/5682	0.37	1/7701 (0.0%)
2	B	0.25	0/5827	0.47	5/7927 (0.1%)
3	C	0.22	0/1065	0.41	0/1438
4	D	0.72	0/24	1.30	0/28
All	All	0.22	0/12598	0.42	6/17094 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	VAL	CB-CA-C	-7.28	101.16	111.34
2	B	386	PHE	CB-CA-C	6.22	119.73	109.72
2	B	1064	ASN	N-CA-C	-5.94	105.89	113.02
2	B	447	GLN	N-CA-C	-5.39	105.73	114.09
2	B	1060	PRO	N-CA-C	-5.24	107.36	114.80

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	5551	0	5458	72	0
2	B	5705	0	5719	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1046	0	1030	18	0
4	D	36	0	25	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12340	0	12232	172	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 7.

The worst 5 of 172 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)
2:B:960:ILE:O	2:B:961:SER:HB2	1.76	0.86
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.61	0.82
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.66	0.77
2:B:960:ILE:O	2:B:961:SER:CB	2.32	0.73
1:A:621:PRO:HG3	1:A:652:THR:HG23	1.75	0.69

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	694/765 (91%)	664 (96%)	30 (4%)	0	100	100
2	B	721/748 (96%)	684 (95%)	33 (5%)	4 (1%)	21	53
3	C	127/157 (81%)	118 (93%)	9 (7%)	0	100	100
4	D	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1544/1675 (92%)	1468 (95%)	72 (5%)	4 (0%)	36	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	961	SER
2	B	1057	ASP
2	B	960	ILE
2	B	1020	PRO

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	607/666 (91%)	560 (92%)	47 (8%)	12	38
2	B	648/679 (95%)	604 (93%)	44 (7%)	14	43
3	C	112/138 (81%)	99 (88%)	13 (12%)	5	21
4	D	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	1369/1485 (92%)	1264 (92%)	105 (8%)	12	38

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	522	LEU
2	B	787	VAL
3	C	105	THR
2	B	561	SER
2	B	712	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	736	GLN
3	C	47	GLN
3	C	67	GLN
2	B	1064	ASN
1	A	655	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	238	4	8,9,10	0.61	0	8,12,14	0.63	0

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	238	4	-	5/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	238	SEP	N-CA-CB-OG
4	D	238	SEP	CB-OG-P-O2P
4	D	238	SEP	CB-OG-P-O3P
4	D	238	SEP	CB-OG-P-O1P
4	D	238	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	238	SEP	1	0

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, 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	704/765 (92%)	0.29	18 (2%) 57 38	43, 66, 117, 196	0
2	B	729/748 (97%)	0.23	25 (3%) 48 31	41, 63, 101, 128	0
3	C	133/157 (84%)	0.63	9 (6%) 23 14	48, 86, 121, 135	0
4	D	4/5 (80%)	0.79	0 100 100	81, 81, 86, 97	0
All	All	1570/1675 (93%)	0.29	52 (3%) 49 32	41, 66, 110, 196	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	888	PRO	3.5
2	B	1055	ILE	3.4
2	B	960	ILE	3.2
1	A	4	TYR	3.1
3	C	150	VAL	3.0

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, 95th 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 ²)	Q<0.9
4	SEP	D	238	10/11	0.74	0.20	73,85,90,101	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, 95th 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(\AA^2)	Q<0.9
5	ZN	A	801	1/1	0.98	0.05	85,85,85,85	0
5	ZN	B	1101	1/1	1.00	0.02	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.