



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:32 am GMT

PDB ID : 3EGD  
Title : Crystal structure of the mammalian COPII-coat protein Sec23a/24a complexed with the SNARE protein Sec22 and bound to the transport signal sequence of vesicular stomatitis virus glycoprotein  
Authors : Goldberg, J.; Mancias, J.D.  
Deposited on : 2008-09-10  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

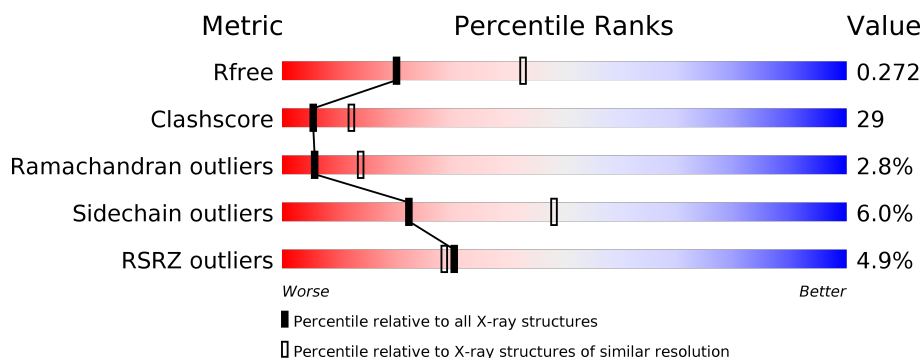
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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. 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	764	
2	B	748	
3	C	157	
4	D	10	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12754 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	711	Total	C	N	O	S	0	0	0
			5645	3597	971	1037	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5780	3690	983	1073	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	ALA	ARG	CONFLICT	UNP O95486

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1104	708	182	206	8			

- Molecule 4 is a protein called 10 residue peptide from VSV glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	S	0	0	0
			60	34	11	14	1			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

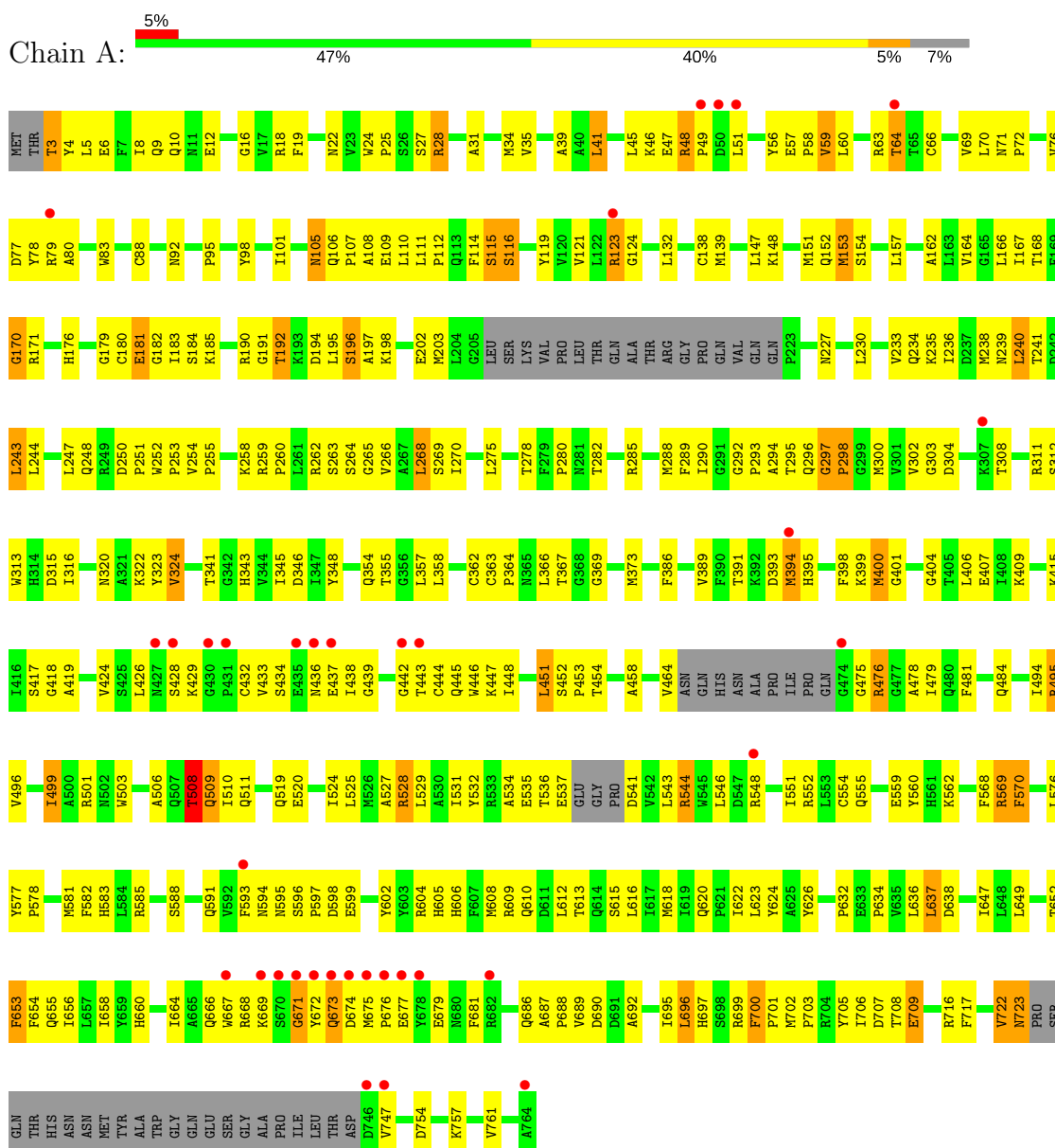
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	74	Total 74	O 74	0	0
6	B	84	Total 84	O 84	0	0
6	C	5	Total 5	O 5	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Protein transport protein Sec23A



#### • Molecule 2: Protein transport protein Sec24A



GLN	
ILE	
TYR	
T502	
D503	
I504	
E505	
M506	
N507	
R508	

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	147.75Å 97.63Å 129.12Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 91.7 (29.60-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.206 , 0.274 0.205 , 0.272	Depositor DCC
$R_{free}$ test set	2291 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12754	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: 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	0.38	0/5778	0.65	2/7824 (0.0%)
2	B	0.38	0/5904	0.65	0/8024
3	C	0.34	0/1123	0.57	0/1510
4	D	0.72	0/59	1.18	0/76
All	All	0.38	0/12864	0.65	2/17434 (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
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-7.96	89.51	111.00
1	A	170	GLY	N-CA-C	-5.23	100.03	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	937	TYR	Sidechain

## 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	5645	0	5591	334	0
2	B	5780	0	5835	318	0
3	C	1104	0	1109	77	0
4	D	60	0	55	16	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	74	0	0	24	0
6	B	84	0	0	29	0
6	C	5	0	0	0	0
All	All	12754	0	12590	721	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 29.

The worst 5 of 721 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:48:ARG:HB2	1:A:49:PRO:HD2	1.17	1.15
2:B:435:ARG:HH21	4:D:507:ASN:HB3	1.07	1.14
1:A:417:SER:HB3	1:A:438:ILE:HD13	1.31	1.08
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.31	1.07
1:A:48:ARG:HB2	1:A:49:PRO:CD	1.84	1.05

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	701/764 (92%)	620 (88%)	58 (8%)	23 (3%)	4	10
2	B	723/748 (97%)	648 (90%)	59 (8%)	16 (2%)	8	20
3	C	131/157 (83%)	106 (81%)	21 (16%)	4 (3%)	5	11
4	D	5/10 (50%)	2 (40%)	3 (60%)	0	100	100
All	All	1560/1679 (93%)	1376 (88%)	141 (9%)	43 (3%)	6	14

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	181	GLU
1	A	182	GLY
1	A	196	SER
1	A	653	PHE

### 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	621/666 (93%)	588 (95%)	33 (5%)	26	54
2	B	662/678 (98%)	620 (94%)	42 (6%)	21	46
3	C	120/138 (87%)	113 (94%)	7 (6%)	23	50
4	D	7/10 (70%)	4 (57%)	3 (43%)	0	0
All	All	1410/1492 (94%)	1325 (94%)	85 (6%)	22	48

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	412	HIS
2	B	614	SER
3	C	63	TYR
2	B	431	CYS
2	B	589	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	373	HIS
2	B	502	GLN
3	C	39	GLN
2	B	382	ASN
2	B	395	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 carbohydrates 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 ⓘ

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	711/764 (93%)	-0.03	35 (4%) 30 29	12, 36, 80, 119	0
2	B	731/748 (97%)	-0.19	23 (3%) 49 49	11, 30, 73, 102	0
3	C	137/157 (87%)	0.68	17 (12%) 4 4	27, 61, 92, 104	0
4	D	7/10 (70%)	2.04	3 (42%) 0 0	74, 87, 96, 103	0
All	All	1586/1679 (94%)	-0.03	78 (4%) 30 29	11, 35, 83, 119	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	MET	6.9
4	D	502	THR	6.1
1	A	672	TYR	5.4
2	B	1055	ILE	5.2
1	A	675	MET	4.5

### 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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ZN	A	765	1/1	0.98	0.07	-1.49	49,49,49,49	0
5	ZN	B	1094	1/1	0.99	0.06	-2.14	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.