



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2023 – 01:23 PM JST

PDB ID : 5XAM  
Title : Crystal structure of SecDF in I form at 4 Å resolution  
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Deposited on : 2017-03-14  
Resolution : 4.00 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 : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

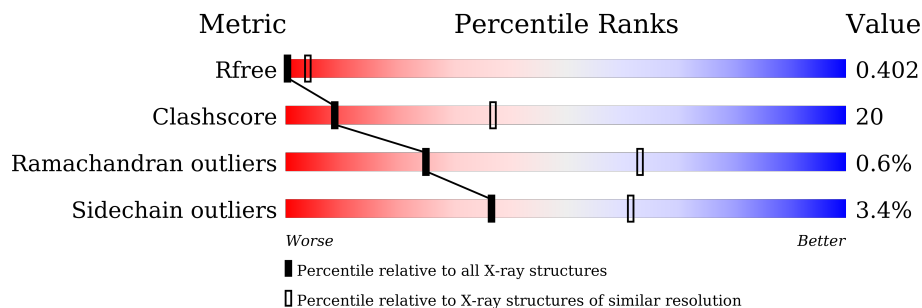
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)

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 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	750	 62% 33% . .
1	B	750	 54% 36% . 9%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 9852 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 translocase subunit SecD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	5000	3215	830	947	8	0	0	0
1	B	684	4852	3140	801	900	11	0	0	0

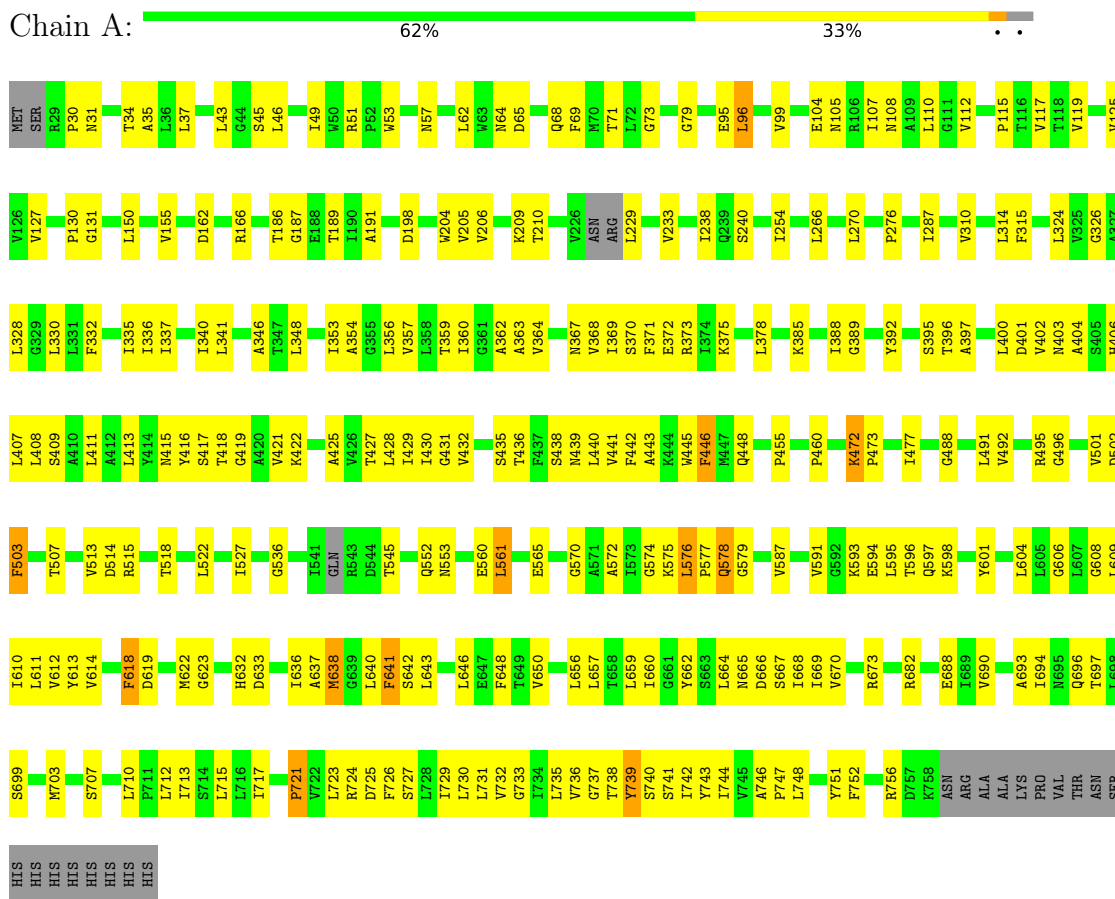
There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9RTE3
A	769	HIS	-	expression tag	UNP Q9RTE3
A	770	HIS	-	expression tag	UNP Q9RTE3
A	771	HIS	-	expression tag	UNP Q9RTE3
A	772	HIS	-	expression tag	UNP Q9RTE3
A	773	HIS	-	expression tag	UNP Q9RTE3
A	774	HIS	-	expression tag	UNP Q9RTE3
A	775	HIS	-	expression tag	UNP Q9RTE3
A	776	HIS	-	expression tag	UNP Q9RTE3
B	27	MET	-	expression tag	UNP Q9RTE3
B	769	HIS	-	expression tag	UNP Q9RTE3
B	770	HIS	-	expression tag	UNP Q9RTE3
B	771	HIS	-	expression tag	UNP Q9RTE3
B	772	HIS	-	expression tag	UNP Q9RTE3
B	773	HIS	-	expression tag	UNP Q9RTE3
B	774	HIS	-	expression tag	UNP Q9RTE3
B	775	HIS	-	expression tag	UNP Q9RTE3
B	776	HIS	-	expression tag	UNP Q9RTE3

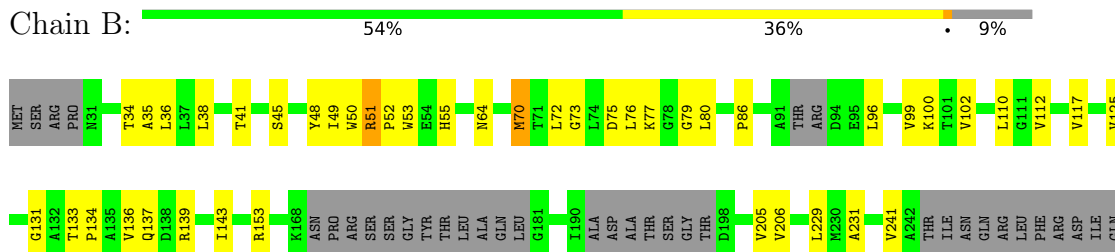
### 3 Residue-property plots

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. 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. 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 translocase subunit SecD



- Molecule 1: Protein translocase subunit SecD



ASP	I689	Y613	I627	T436	V357	ILE
LYS	V690	F616	V531	F437	SER	SER
ASN	N691	R617	S532	S438	GLY	GLY
ARG	I694	F618	K533	N439	N257	
ALA	N695	D619	V534	L440	L268	
LYS	Q696	L624	T535	V441	A362	
PRO	T697	L627	G536	F442	V364	
VAL	L698	I628	T540	A443	D365	
THR	S699	I629	I540	K444	I279	
ASN	R700	I628	ILE	W445	I279	
SER	T701	A629	GLN	F446	I369	
HIS	V702	A630	ARG	R447	S370	
HIS	N703	I631	ASP	Q448	F371	
HIS	L710	H632	THR	P460	E372	
HIS	F711	D633	T546	I463	R373	
HIS	L712	V634	Q550	I463	G292	
HIS	T713	I636	G551	K464	A293	
HIS	S714	A637	Q552	H465		
HIS	L715	N638	K557	D469	R297	
	L716	G639	L561	K472	A302	
	L717	L640	E565	P473	A303	
	F718	F641	V566	V476	L304	
	G719	S642	I569	I477	V305	
	G720	L646	G570	T479	G306	
	L723	F648	A571	A485	I307	
	R724	V650	A572	L486	G308	
	T649	A651	K575	A487	L309	
	F726	S652	L576	L491	V310	
	S727	A655	Q577	R495	F311	
	L728	L659	G579	Y499	R312	
	I729	G661	L582	F503	M313	
	L730	S663	T586	A504	Y317	
	L731	L664	V587	P505	G319	
	I734	N665	G588	G506	F322	
	L735	D666	V591	T507	V325	
	V736	S667	L595	T508	G326	
	G737	I668	T596	R512	A327	
	T738	V670	Q597	D514	L328	
	Y739	S671	K598	R515	G329	
	S740	T673	T599	T518	L330	
	S741	R674	I600	T519	L331	
	I742	R675	Y601	E520	F332	
	I743	R676	L607	Q521	L337	
	I744	M677	I610	L522	G342	
	V745	M678	L611	S525	G343	
	A746	E688	V612	V526	L348	
	P747	Y686	I612	A434	T349	
	L748	R687	L612	A433	L350	
	V749	E688	V612	S435	P351	
	V750				G352	
	Y751				I353	
	E752					
	E753					
	E754					
	TRP					
	ARG					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.32Å 62.26Å 181.71Å 90.00° 101.71° 90.00°	Depositor
Resolution (Å)	47.98 – 4.00 47.99 – 3.92	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.98-4.00) 93.3 (47.99-3.92)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 3.88Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.333 , 0.402 0.333 , 0.402	Depositor DCC
$R_{free}$ test set	1762 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	150.3	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.19 , 176.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	242.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.44% 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](#)

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	0.27	1/5071 (0.0%)	0.48	1/6964 (0.0%)
1	B	0.26	0/4926	0.48	0/6735
All	All	0.27	1/9997 (0.0%)	0.48	1/13699 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	ARG	C-N	7.32	1.48	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	LEU	CA-CB-CG	5.41	127.75	115.30

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	5000	0	4921	195	0
1	B	4852	0	4894	208	0
All	All	9852	0	9815	403	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 20.

The worst 5 of 403 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:30:PRO:HG2	1:A:448:GLN:HG2	1.48	0.92
1:B:690:VAL:HG21	1:B:750:VAL:HG11	1.60	0.83
1:B:561:LEU:HB2	1:B:565:GLU:HB3	1.61	0.82
1:A:34:THR:HA	1:A:37:LEU:HB3	1.60	0.82
1:A:404:ALA:HA	1:A:407:LEU:HB2	1.62	0.80

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	721/750 (96%)	656 (91%)	59 (8%)	6 (1%)	19	58
1	B	672/750 (90%)	622 (93%)	47 (7%)	3 (0%)	34	71
All	All	1393/1500 (93%)	1278 (92%)	106 (8%)	9 (1%)	25	63

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	578	GLN
1	A	721	PRO
1	B	51	ARG
1	A	446	PHE
1	B	420	ALA

### 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	481/603 (80%)	462 (96%)	19 (4%)	31	57
1	B	484/603 (80%)	470 (97%)	14 (3%)	42	65
All	All	965/1206 (80%)	932 (97%)	33 (3%)	37	61

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	676	GLU
1	B	678	MET
1	B	752	PHE
1	A	638	MET
1	A	618	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	137	GLN
1	B	448	GLN
1	B	465	HIS
1	A	108	ASN
1	A	66	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 monosaccharides 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.