



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2022 – 12:04 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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	:	2.27
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)	:	2.27

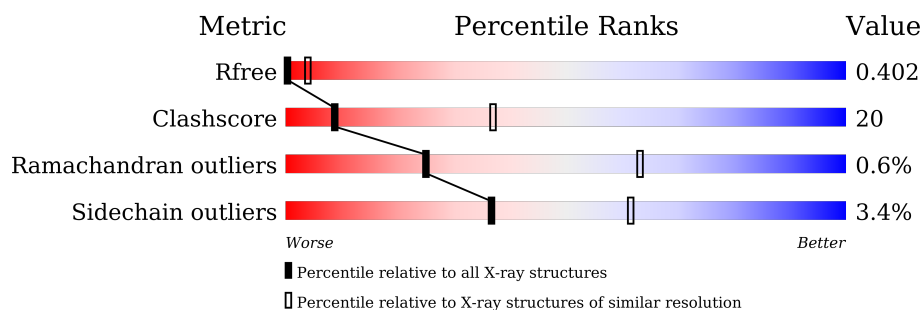
1 Overall quality at a glance

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 ≥ 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	
1	B	750	

2 Entry composition

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
1	A	727	Total	C	N	O	S	0	0	0
			5000	3215	830	947	8			
1	B	684	Total	C	N	O	S	0	0	0
			4852	3140	801	900	11			

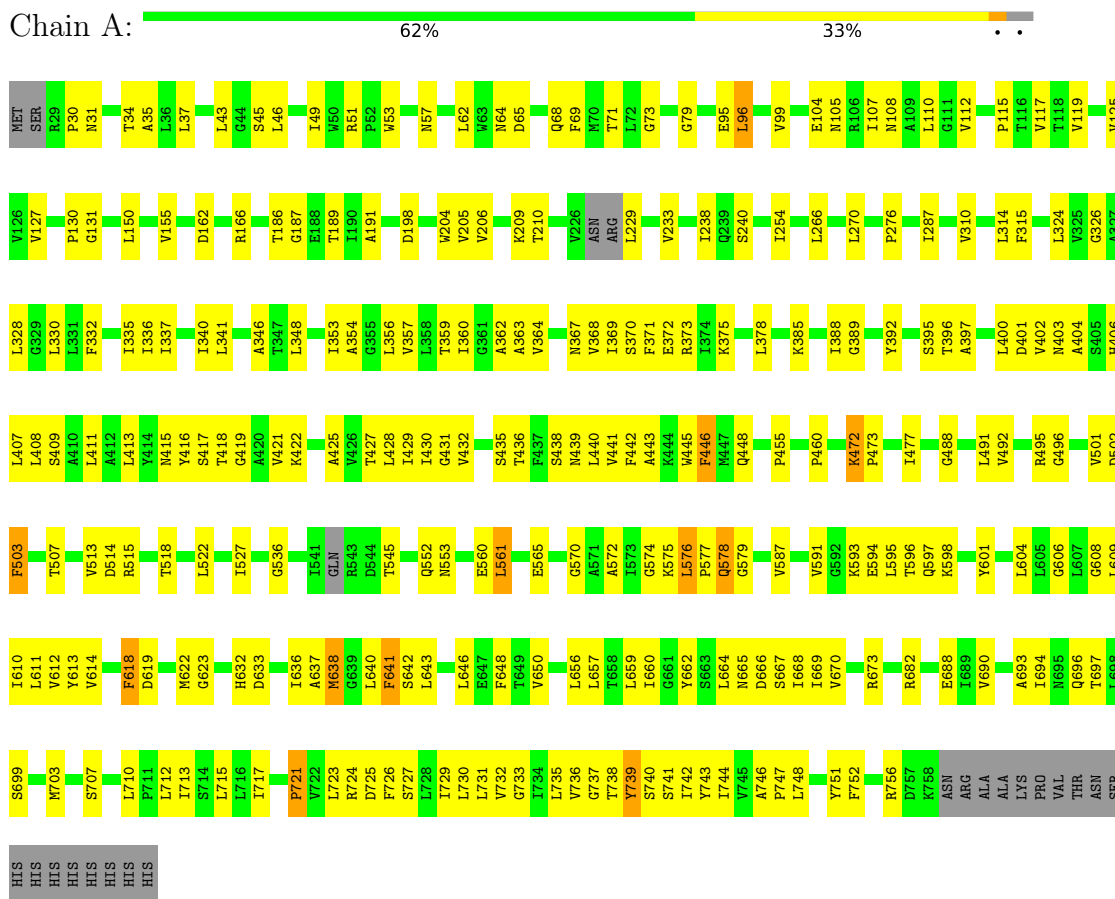
There are 18 discrepancies between the modelled and reference sequences:

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

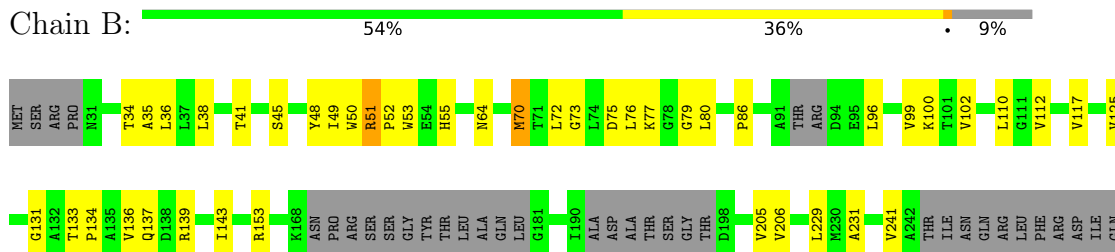
3 Residue-property plots

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	I527	T436	ILE
LYS	V690		V531	F437	SER
ASN	N691	F616		S438	GLY
ARG		R617	S532	N439	N257
ALA	I694	F618	K533	L440	L268
LYS	N695	D619	V534	V441	
PRO	Q696		T535	F442	I277
VAL	T697	L624	G536	A443	K278
THR	L698		T540	K444	I279
ASN	S699	I627	ILE	W445	
THR	R700	I628	GLN	F446	R265
SER	T701	A629	ARG	R447	S286
HIS	H702	A630	ASP	Q448	
HIS	H703	I631	THR		
HIS		H632	T546	P460	S290
HIS	L710	D633			L291
HIS	F711	V634	Q550	I463	G292
HIS	L712	A635		K464	A293
HIS	L713	I636	G551	H465	
HIS	S714	A637	Q552		R297
	L715	N638		D469	
	L716	G639	K557	K472	A302
	L717	L640		P473	A303
	F718	F641	L561		L304
	G719	S642		V476	V305
	G720		E565	I477	G306
		L646	V566	T478	I307
	L723	E647		T479	G308
	R724	F648	I569		V310
	D725		G570	A485	F311
	F726	V650	A571	L486	R312
	F727	A651	A572	A487	M313
	L728	S652		L491	
	L729		K575		Y317
	L730	A655	L576		Y318
	L731		P577	R495	G319
		L659	Q578		
	L734	I660	G579	Y499	F322
	L735	G661		F503	V325
	V736	Y662	L582	A504	G326
	G737	S663		P505	A327
	T738	L664	T586	G506	L328
	Y739	N665	V587	T507	G329
	S740	D666	G588	T508	L330
	S741	S667		R512	L331
	I742	I668	V591	V513	F332
	Y743	I669	L595	D514	
	I744	V670	T596	R515	I337
	V745	S671	Q597		
	A746	L672	K598	T518	G342
	P747	R673	T599	E520	G343
	L748	I674	I600	Q521	L348
	V749	R675	Y601	L522	T349
	V750	E676		S525	L350
	Y751	N677	L607	V526	P351
	E752	M678			G352
	E753		I610		I353
	E754	Y686	L611		
	TRP	R687	V612		
	ARG	E688			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.88Å)	Xtriage
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 ²)	150.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.19 , 176.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	9852	wwPDB-VP
Average B, all atoms (Å ²)	242.0	wwPDB-VP

Xtriage'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.*

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](#)

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 ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

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.