



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 12:50 PM GMT

PDB ID : 3DL8  
Title : Structure of the complex of aquifex aeolicus SecYEG and bacillus subtilis SecA  
Authors : Nam, Y.; Zimmer, J.; Rapoport, T.A.  
Deposited on : 2008-06-26  
Resolution : 7.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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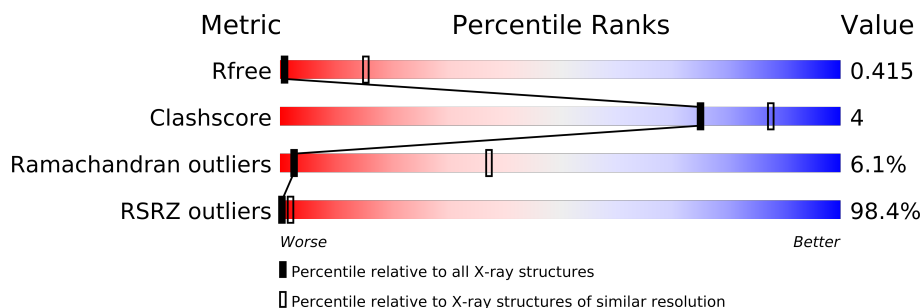
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 7.50 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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1301 (11.50-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	779	
1	B	779	
2	G	429	
2	H	429	
3	C	65	
3	D	65	
4	E	107	
4	F	107	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10232 atoms, of which 0 are hydrogen and 0 are deuterium.

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 secA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	0	0	0
			3092	1546	773	773			
1	B	773	Total	C	N	O	0	0	0
			3092	1546	773	773			

- Molecule 2 is a protein called Preprotein translocase subunit secY.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	406	Total	C	N	O	0	0	0
			1624	812	406	406			
2	H	406	Total	C	N	O	0	0	0
			1624	812	406	406			

- Molecule 3 is a protein called SecE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	35	Total	C	N	O	0	0	0
			140	70	35	35			
3	D	35	Total	C	N	O	0	0	0
			140	70	35	35			

- Molecule 4 is a protein called Protein-export membrane protein secG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	65	Total	C	N	O	0	0	0
			260	130	65	65			
4	F	65	Total	C	N	O	0	0	0
			260	130	65	65			

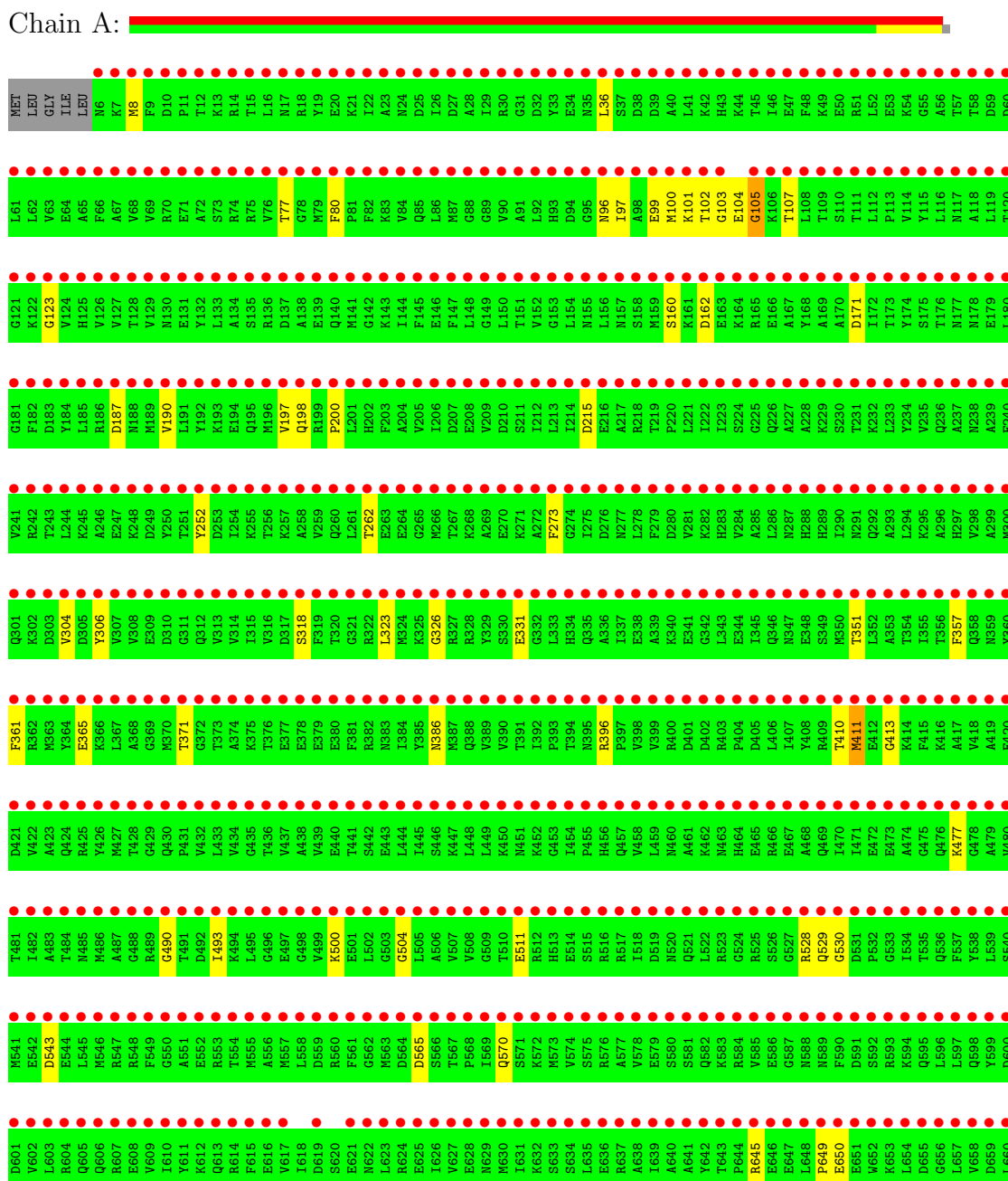
There are 14 discrepancies between the modelled and reference sequences:

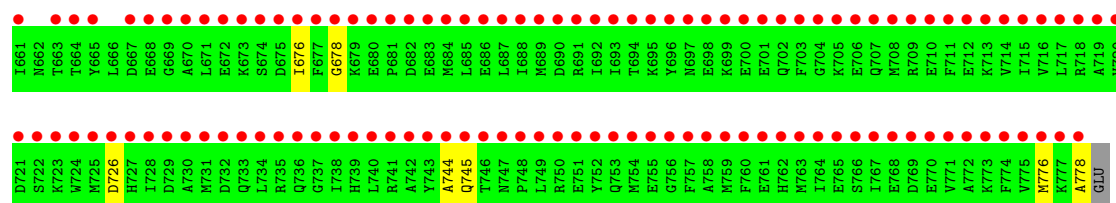
Chain	Residue	Modelled	Actual	Comment	Reference
E	101	GLY	-	EXPRESSION TAG	UNP O66505
E	102	HIS	-	EXPRESSION TAG	UNP O66505
E	103	HIS	-	INSERTION	UNP O66505
E	104	HIS	-	EXPRESSION TAG	UNP O66505
E	105	HIS	-	EXPRESSION TAG	UNP O66505
E	106	HIS	-	EXPRESSION TAG	UNP O66505
E	107	HIS	-	EXPRESSION TAG	UNP O66505
F	101	GLY	-	EXPRESSION TAG	UNP O66505
F	102	HIS	-	EXPRESSION TAG	UNP O66505
F	103	HIS	-	EXPRESSION TAG	UNP O66505
F	104	HIS	-	EXPRESSION TAG	UNP O66505
F	105	HIS	-	EXPRESSION TAG	UNP O66505
F	106	HIS	-	EXPRESSION TAG	UNP O66505
F	107	HIS	-	EXPRESSION TAG	UNP O66505

### 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 errors 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.

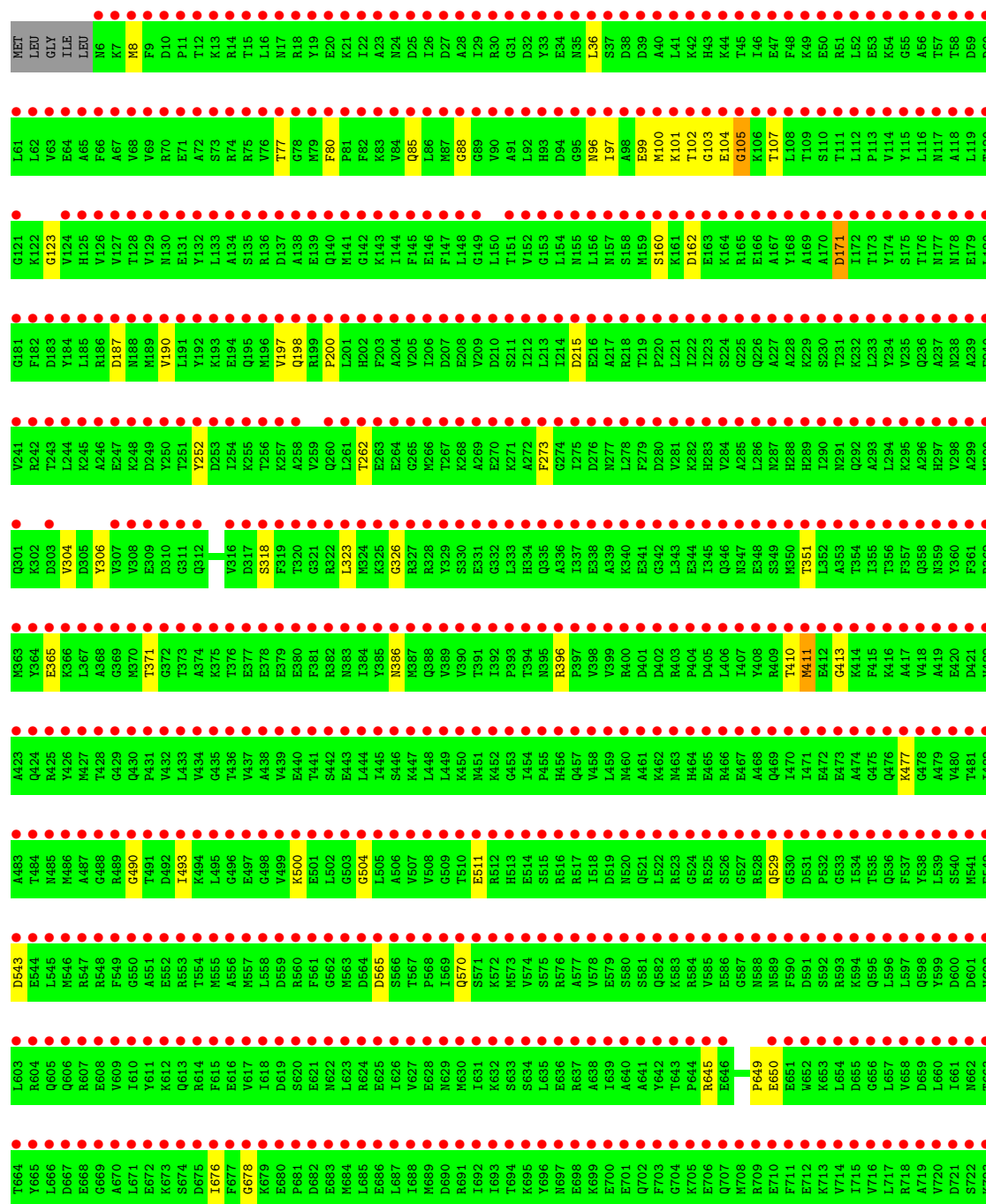
- Molecule 1: Protein translocase subunit secA

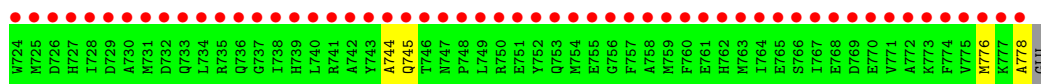




● Molecule 1: Protein translocase subunit secA

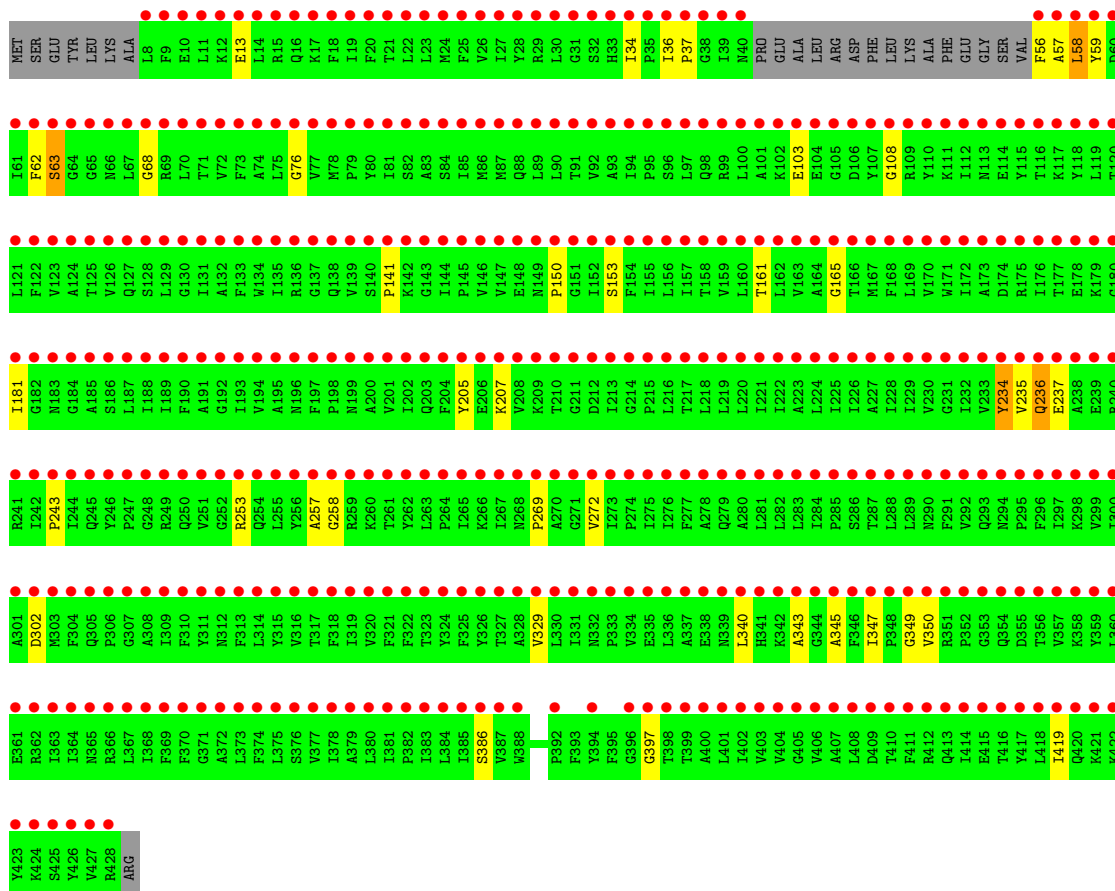
Chain B:





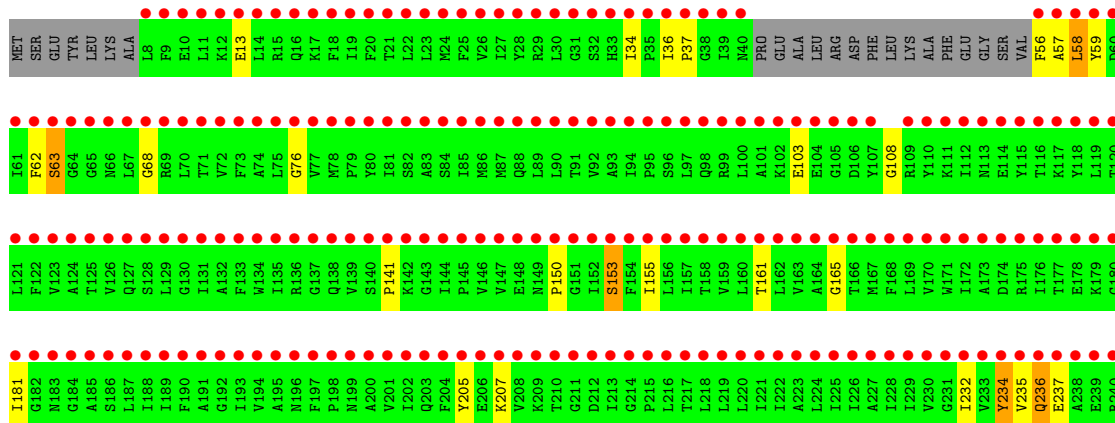
• Molecule 2: Preprotein translocase subunit secY

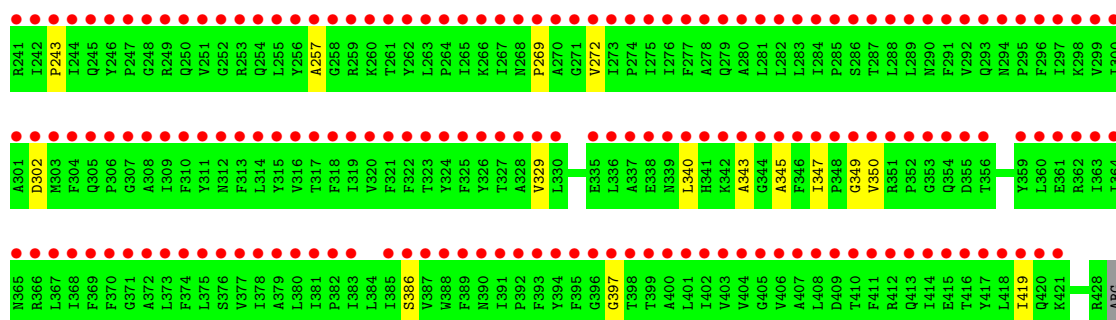
Chain G:



• Molecule 2: Preprotein translocase subunit secY

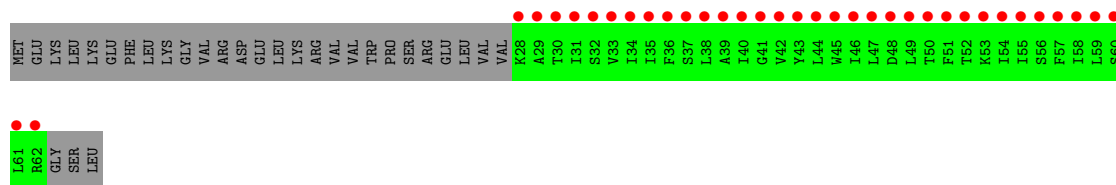
Chain H:





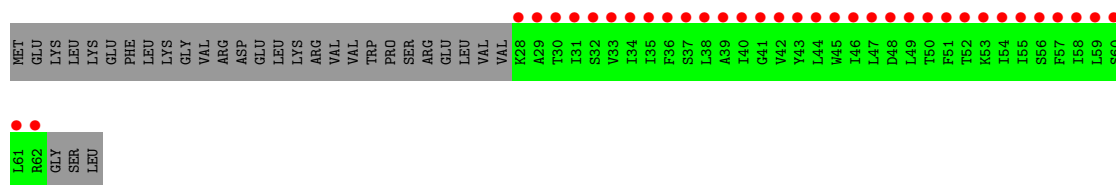
• Molecule 3: SecE

Chain C:



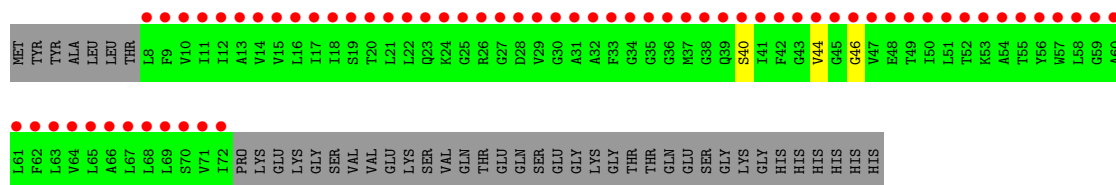
• Molecule 3: SecE

Chain D:



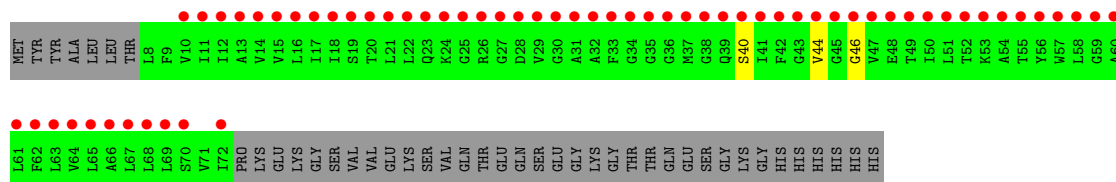
• Molecule 4: Protein-export membrane protein secG

Chain E:



• Molecule 4: Protein-export membrane protein secG

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.36Å 167.97Å 187.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.99 – 7.50 48.09 – 7.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.99-7.50) 99.0 (48.09-7.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 7.37Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.365 , 0.390 0.411 , 0.415	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	530.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	28.97 , 207.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 6217 reflections (0.016%)	Xtriage
$F_o, F_c$ correlation	0.62	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	452.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

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	0.88	0/3091	0.90	2/3862 (0.1%)
1	B	0.88	0/3091	0.90	2/3862 (0.1%)
2	G	0.98	0/1622	0.96	2/2024 (0.1%)
2	H	0.97	0/1622	0.96	2/2024 (0.1%)
3	C	0.94	0/139	0.75	0/172
3	D	0.94	0/139	0.75	0/172
4	E	1.02	0/259	0.93	0/322
4	F	1.02	0/259	0.93	0/322
All	All	0.92	0/10222	0.92	8/12760 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	SER	N-CA-C	-7.19	91.59	111.00
1	B	160	SER	N-CA-C	-7.17	91.63	111.00
1	A	304	VAL	C-N-CA	6.29	137.41	121.70
1	B	304	VAL	C-N-CA	6.25	137.31	121.70
2	H	302	ASP	C-N-CA	-5.36	108.31	121.70

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3092	0	856	18	0
1	B	3092	0	856	12	0
2	G	1624	0	446	17	0
2	H	1624	0	446	13	0
3	C	140	0	36	0	0
3	D	140	0	36	0	0
4	E	260	0	86	1	0
4	F	260	0	86	1	0
All	All	10232	0	2848	52	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

The worst 5 of 52 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:776:MET:O	1:B:778:ALA:O	1.54	1.25
1:A:776:MET:O	1:B:778:ALA:C	1.98	1.02
1:A:778:ALA:C	1:B:776:MET:O	1.99	1.00
1:A:778:ALA:O	1:B:776:MET:O	1.83	0.95
2:H:103:GLU:H	2:H:108:GLY:HA3	1.39	0.86

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	771/779 (99%)	638 (83%)	86 (11%)	47 (6%)	2	37
1	B	771/779 (99%)	638 (83%)	85 (11%)	48 (6%)	2	37
2	G	402/429 (94%)	321 (80%)	52 (13%)	29 (7%)	2	32
2	H	402/429 (94%)	319 (79%)	54 (13%)	29 (7%)	2	32
3	C	33/65 (51%)	33 (100%)	0	0	100	100
3	D	33/65 (51%)	33 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	14	71
4	F	63/107 (59%)	57 (90%)	5 (8%)	1 (2%)	14	71
All	All	2538/2760 (92%)	2096 (83%)	287 (11%)	155 (6%)	2	37

5 of 155 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	80	PHE
1	A	99	GLU
1	A	100	MET
1	A	101	LYS

### 5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	773/779 (99%)	15.31	768 (99%) 0 1	321, 444, 550, 648	0
1	B	773/779 (99%)	13.48	759 (98%) 0 2	340, 470, 540, 612	0
2	G	406/429 (94%)	15.20	401 (98%) 0 2	321, 409, 488, 512	0
2	H	406/429 (94%)	13.36	391 (96%) 0 2	372, 466, 536, 558	0
3	C	35/65 (53%)	22.79	35 (100%) 0 1	328, 363, 402, 405	0
3	D	35/65 (53%)	26.15	35 (100%) 0 1	383, 396, 463, 466	0
4	E	65/107 (60%)	12.29	65 (100%) 0 1	386, 446, 468, 473	0
4	F	65/107 (60%)	10.72	62 (95%) 0 2	477, 523, 550, 551	0
All	All	2558/2760 (92%)	14.49	2516 (98%) 0 2	321, 450, 541, 648	0

The worst 5 of 2516 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	117	LYS	61.3
1	A	50	GLU	57.8
1	A	51	ARG	56.3
1	A	120	THR	54.6
2	G	121	LEU	54.4

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.