



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:17 AM UTC

PDB ID : 8YA3 / pdb_00008ya3
EMDB ID : EMD-39090
Title : Structure of the SecA-SecY complex with the substrate FtsQ-LacY(+7C) treated with DTT
Authors : Ou, X.; Ma, C.; Sun, D.; Xu, J.; Wu, X.; Gao, N.; Li, L.
Deposited on : 2024-02-07
Resolution : 3.27 Å(reported)

This is a Full wwPDB EM Validation 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

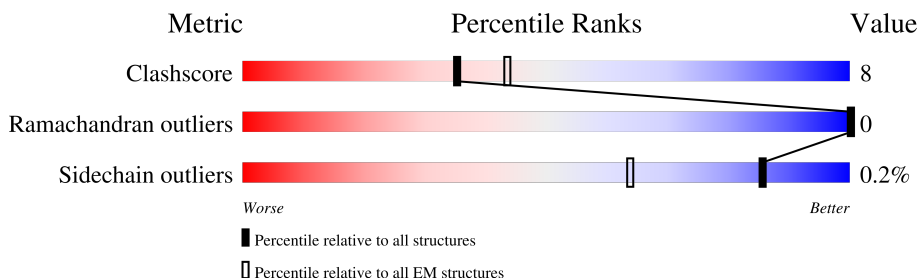
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.27 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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	Y	430	 81% 13% 6%
2	E	70	 71% 11% 17%
3	B	78	 60% 10% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4060 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Y	406	Total	C	N	O	S	0	0
			3165	2100	523	529	13		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	60	CYS	GLY	engineered mutation	UNP A4IJK8
Y	202	THR	GLN	engineered mutation	UNP A4IJK8
Y	211	THR	PHE	engineered mutation	UNP A4IJK8
Y	213	ASN	ARG	engineered mutation	UNP A4IJK8

- Molecule 2 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	58	Total	C	N	O	0	0
			480	322	80	78		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	61	GLY	-	expression tag	UNP A4IJH4
E	62	GLY	-	expression tag	UNP A4IJH4
E	63	HIS	-	expression tag	UNP A4IJH4
E	64	HIS	-	expression tag	UNP A4IJH4
E	65	HIS	-	expression tag	UNP A4IJH4
E	66	HIS	-	expression tag	UNP A4IJH4
E	67	HIS	-	expression tag	UNP A4IJH4
E	68	HIS	-	expression tag	UNP A4IJH4
E	69	HIS	-	expression tag	UNP A4IJH4
E	70	HIS	-	expression tag	UNP A4IJH4

- Molecule 3 is a protein called Cell division protein FtsQ, Lactose permease.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	55	Total	C	N	O	S	0	0
			415	278	65	70	2		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P06136
B	2	ALA	-	expression tag	UNP P06136
B	3	LYS	-	expression tag	UNP P06136
B	4	LYS	-	expression tag	UNP P06136
B	5	THR	-	expression tag	UNP P06136
B	26	ALA	-	linker	UNP P06136
B	27	GLN	-	linker	UNP P06136
B	28	TYR	-	linker	UNP P06136
B	29	GLU	-	linker	UNP P06136
B	30	ASP	-	linker	UNP P06136
B	31	GLY	-	linker	UNP P06136
B	32	CYS	-	linker	UNP P06136
B	33	SER	-	linker	UNP P06136
B	34	GLY	-	linker	UNP P06136
B	53	ALA	CYS	conflict	UNP P02920
B	55	SER	-	expression tag	UNP P02920
B	56	ILE	-	expression tag	UNP P02920
B	57	SER	-	expression tag	UNP P02920
B	58	GLY	-	expression tag	UNP P02920
B	59	ASP	-	expression tag	UNP P02920
B	60	GLY	-	expression tag	UNP P02920
B	61	ASP	-	expression tag	UNP P02920
B	62	SER	-	expression tag	UNP P02920
B	63	PRO	-	expression tag	UNP P02920
B	64	HIS	-	expression tag	UNP P02920
B	65	SER	-	expression tag	UNP P02920
B	66	TYR	-	expression tag	UNP P02920
B	67	HIS	-	expression tag	UNP P02920
B	68	SER	-	expression tag	UNP P02920
B	69	GLY	-	expression tag	UNP P02920
B	70	ASP	-	expression tag	UNP P02920
B	71	GLY	-	expression tag	UNP P02920
B	72	ASP	-	expression tag	UNP P02920
B	73	LYS	-	expression tag	UNP P02920
B	74	LEU	-	expression tag	UNP P02920
B	75	PRO	-	expression tag	UNP P02920
B	76	GLU	-	expression tag	UNP P02920

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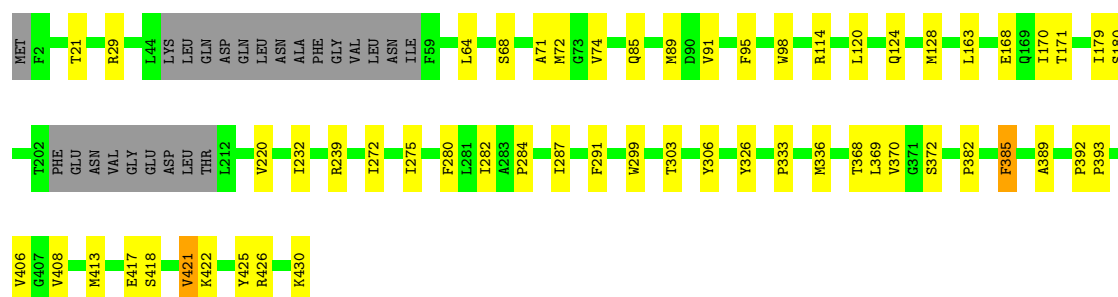
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	GLY	-	expression tag	UNP P02920
B	78	VAL	-	expression tag	UNP P02920

3 Residue-property plots [i](#)

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.

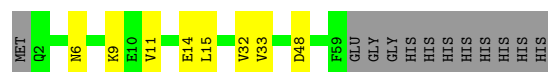
- Molecule 1: Protein translocase subunit SecY

Chain Y: 



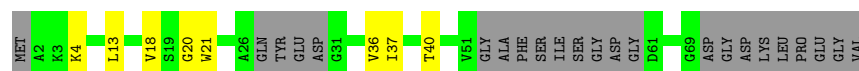
- Molecule 2: Protein translocase subunit SecE

Chain E: 



- Molecule 3: Cell division protein FtsQ, Lactose permease

Chain B: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	123581	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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	Y	0.38	0/3237	0.58	1/4400 (0.0%)
2	E	0.31	0/490	0.45	0/664
3	B	0.36	0/423	0.55	0/574
All	All	0.37	0/4150	0.56	1/5638 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Y	421	VAL	N-CA-C	6.16	118.75	111.05

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	Y	3165	0	3326	58	0
2	E	480	0	507	8	0
3	B	415	0	439	23	0
All	All	4060	0	4272	66	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 8.

All (66) 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:Y:280:PHE:CZ	3:B:13:LEU:CD1	2.34	1.11
1:Y:280:PHE:CE2	3:B:13:LEU:HD13	1.90	1.07
1:Y:280:PHE:CE2	3:B:13:LEU:CD1	2.38	1.06
1:Y:417:GLU:O	1:Y:421:VAL:HG13	1.74	0.87
1:Y:280:PHE:CE2	3:B:13:LEU:HD12	2.09	0.85
1:Y:282:ILE:HD12	3:B:37:ILE:HG12	1.57	0.84
1:Y:280:PHE:CZ	3:B:13:LEU:HD12	2.12	0.81
1:Y:280:PHE:CZ	3:B:13:LEU:HD13	2.08	0.80
1:Y:282:ILE:HD12	3:B:37:ILE:CG1	2.16	0.74
1:Y:418:SER:O	1:Y:421:VAL:HG22	1.89	0.71
1:Y:74:VAL:HG11	1:Y:179:ILE:HG23	1.75	0.68
1:Y:306:TYR:HE1	3:B:36:VAL:HG22	1.58	0.67
1:Y:306:TYR:CE1	3:B:36:VAL:HG22	2.30	0.66
1:Y:74:VAL:O	1:Y:74:VAL:HG12	1.97	0.65
1:Y:333:PRO:HA	1:Y:336:MET:HG2	1.82	0.62
1:Y:282:ILE:CD1	3:B:37:ILE:HG12	2.30	0.60
1:Y:306:TYR:CE1	3:B:36:VAL:CG2	2.85	0.60
1:Y:85:GLN:NE2	1:Y:326:TYR:OH	2.36	0.58
1:Y:287:ILE:O	1:Y:291:PHE:CD2	2.58	0.57
1:Y:120:LEU:HD22	3:B:18:VAL:HG11	1.87	0.56
1:Y:368:THR:O	1:Y:372:SER:HB2	2.07	0.54
3:B:36:VAL:HG12	3:B:36:VAL:O	2.07	0.54
1:Y:114:ARG:NH1	1:Y:168:GLU:OE2	2.41	0.54
1:Y:284:PRO:HA	1:Y:287:ILE:HG12	1.90	0.54
3:B:20:GLY:O	3:B:37:ILE:HD13	2.08	0.53
1:Y:422:LYS:O	1:Y:425:TYR:CD2	2.62	0.53
1:Y:272:ILE:HA	1:Y:275:ILE:HD12	1.92	0.52
1:Y:287:ILE:O	1:Y:291:PHE:HD2	1.93	0.52
1:Y:370:VAL:HG21	2:E:15:LEU:HD21	1.92	0.52
1:Y:180:SER:HB3	1:Y:408:VAL:HG22	1.92	0.52
1:Y:72:MET:HE1	1:Y:124:GLN:HB3	1.92	0.51
1:Y:406:VAL:HG22	2:E:33:VAL:HG21	1.93	0.51
1:Y:68:SER:H	1:Y:71:ALA:HB2	1.76	0.51
1:Y:426:ARG:HD3	1:Y:430:LYS:HE2	1.93	0.50
1:Y:21:THR:HG23	1:Y:170:ILE:HD11	1.94	0.50
1:Y:299:TRP:O	1:Y:303:THR:OG1	2.29	0.49
1:Y:418:SER:HA	1:Y:421:VAL:HG22	1.97	0.47
1:Y:418:SER:C	1:Y:421:VAL:HG22	2.40	0.47
1:Y:124:GLN:O	1:Y:128:MET:HB2	2.15	0.46
1:Y:220:VAL:HG21	1:Y:389:ALA:HB2	1.97	0.46
3:B:21:TRP:CZ2	3:B:37:ILE:CG2	2.99	0.46
3:B:37:ILE:HA	3:B:40:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:382:PRO:HA	1:Y:385:PHE:HB2	1.98	0.44
1:Y:392:PRO:HA	1:Y:393:PRO:HD3	1.89	0.43
3:B:21:TRP:CE2	3:B:37:ILE:CG2	3.01	0.43
1:Y:74:VAL:O	1:Y:74:VAL:CG1	2.65	0.43
1:Y:163:LEU:HD23	1:Y:163:LEU:HA	1.81	0.43
3:B:36:VAL:O	3:B:40:THR:N	2.47	0.43
1:Y:29:ARG:HA	1:Y:29:ARG:HD2	1.74	0.43
1:Y:95:PHE:HD1	1:Y:98:TRP:HD1	1.67	0.42
1:Y:168:GLU:HA	1:Y:171:THR:HG22	2.02	0.42
1:Y:91:VAL:HG22	3:B:4:LYS:HG3	2.02	0.42
3:B:36:VAL:O	3:B:36:VAL:CG1	2.67	0.42
1:Y:89:MET:HE2	1:Y:89:MET:HB2	1.72	0.42
1:Y:72:MET:HB3	1:Y:72:MET:HE3	1.76	0.42
1:Y:306:TYR:HE1	3:B:36:VAL:CG2	2.25	0.42
1:Y:418:SER:O	1:Y:421:VAL:CG2	2.63	0.42
1:Y:64:LEU:H	1:Y:64:LEU:HG	1.57	0.42
1:Y:239:ARG:NE	2:E:14:GLU:OE2	2.48	0.42
1:Y:120:LEU:HD23	1:Y:120:LEU:HA	1.87	0.41
2:E:6:ASN:OD1	2:E:9:LYS:NZ	2.40	0.41
1:Y:29:ARG:NH2	2:E:48:ASP:OD2	2.52	0.41
1:Y:369:LEU:HD23	2:E:11:VAL:HG21	2.02	0.41
1:Y:232:ILE:HD11	2:E:33:VAL:HG11	2.03	0.40
1:Y:413:MET:HG3	2:E:32:VAL:HG11	2.02	0.40
1:Y:280:PHE:CZ	3:B:13:LEU:HD11	2.44	0.40

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 PDB entries followed by that with respect to all EM entries.

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	Y	400/430 (93%)	369 (92%)	31 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	56/70 (80%)	55 (98%)	1 (2%)	0	100	100
3	B	49/78 (63%)	45 (92%)	4 (8%)	0	100	100
All	All	505/578 (87%)	469 (93%)	36 (7%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	Y	340/361 (94%)	339 (100%)	1 (0%)	86	86
2	E	53/63 (84%)	53 (100%)	0	100	100
3	B	48/65 (74%)	48 (100%)	0	100	100
All	All	441/489 (90%)	440 (100%)	1 (0%)	85	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	385	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	7	ASN
1	Y	65	GLN
1	Y	66	ASN
1	Y	85	GLN
1	Y	133	ASN
1	Y	134	ASN
1	Y	235	GLN
1	Y	267	ASN
1	Y	294	ASN
1	Y	387	ASN

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Mol	Chain	Res	Type
2	E	2	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 oligosaccharides 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 Map visualisation

This section contains visualisations of the EMDB entry EMD-39090. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.