



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 14, 2017 – 11:04 AM EST

PDB ID : 5WQ7
EMDB ID: : EMD-6675
Title : CryoEM structure of type II secretion system secretin GspD in E.coli K12
Authors : Yan, Z.; Yin, M.; Li, X.
Deposited on : 2016-11-23
Resolution : 3.04 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

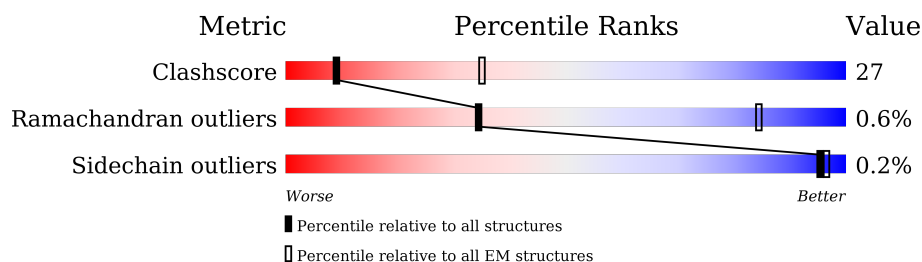
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.04 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.





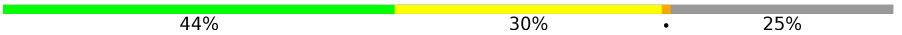
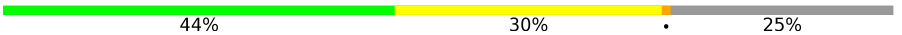
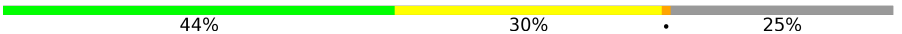
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	627	
1	B	627	
1	C	627	
1	D	627	
1	E	627	
1	F	627	
1	G	627	
1	H	627	
1	I	627	

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Mol	Chain	Length	Quality of chain
1	J	627	 44% 31% • 25%
1	K	627	 45% 30% • 25%
1	L	627	 45% 30% • 25%
1	M	627	 44% 30% • 25%
1	N	627	 44% 30% • 25%
1	O	627	 44% 30% • 25%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 54480 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.

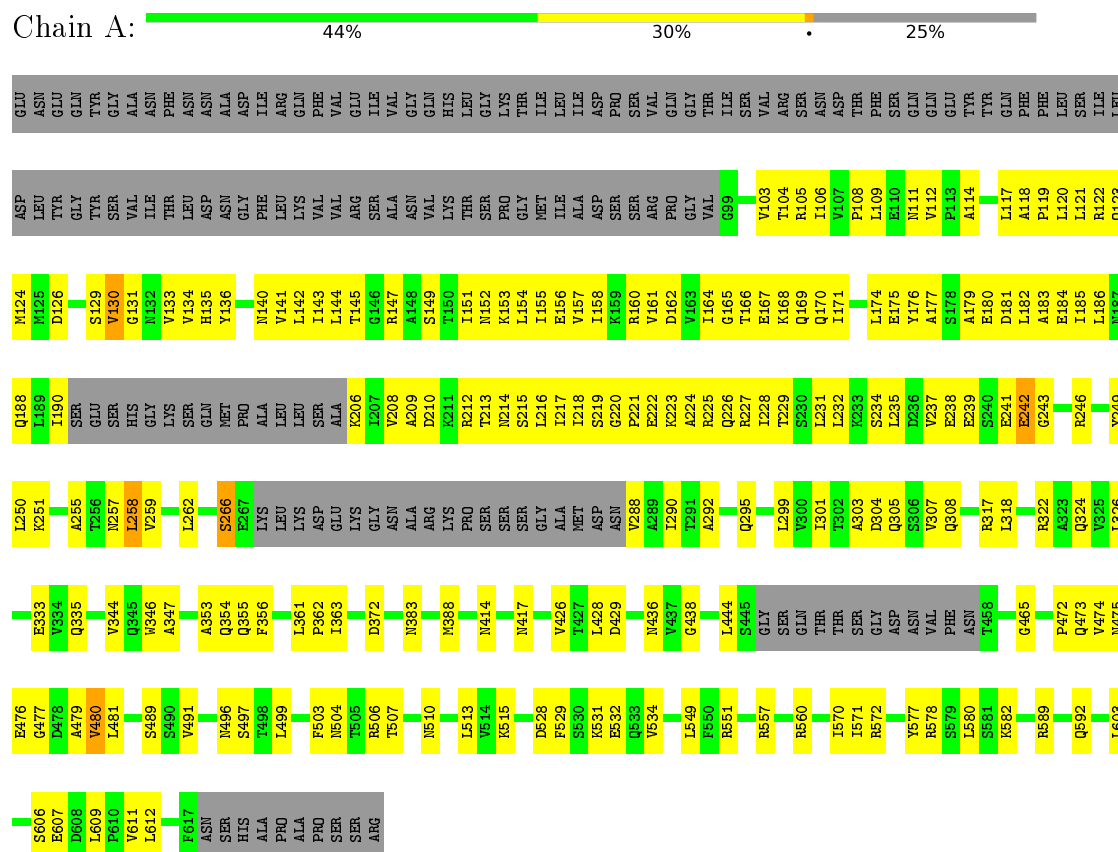
- Molecule 1 is a protein called Putative type II secretion system protein D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	B	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	C	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	D	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	E	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	F	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	G	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	H	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	I	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	J	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	K	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	L	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	M	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	N	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		
1	O	472	Total	C	N	O	S	0	0
			3632	2279	628	720	5		

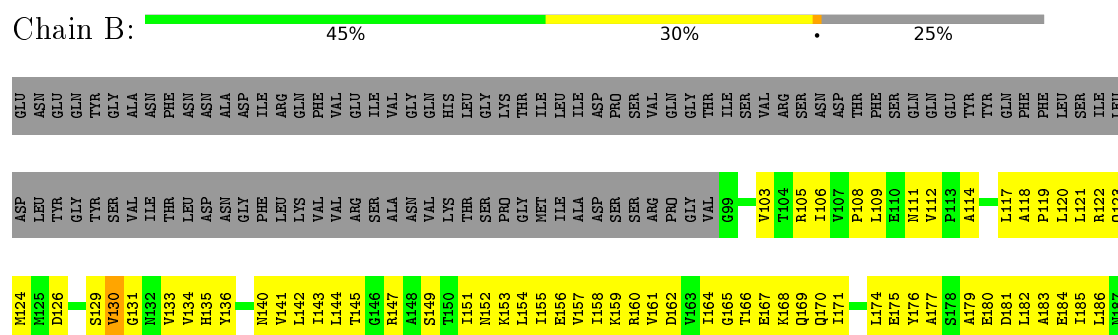
3 Residue-property plots

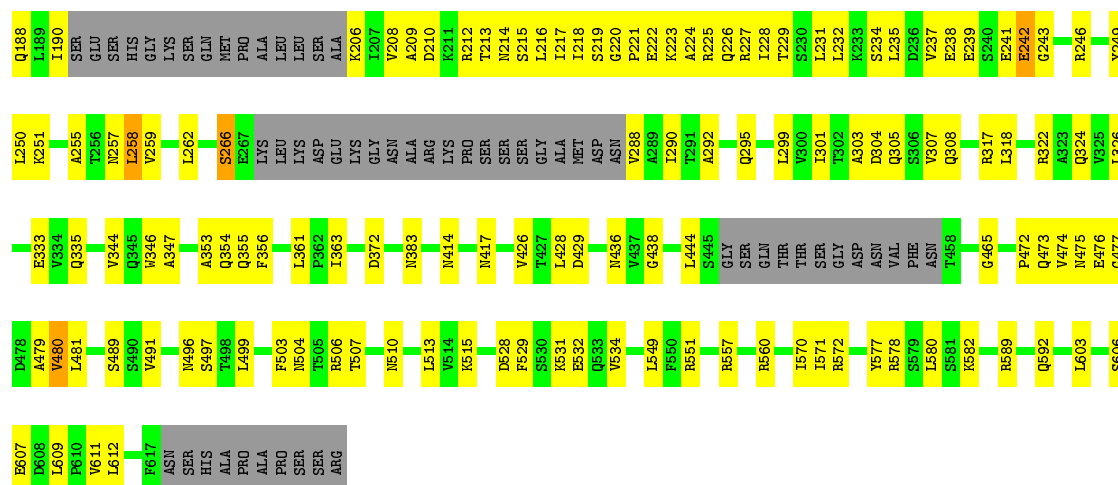
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric 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: Putative type II secretion system protein D



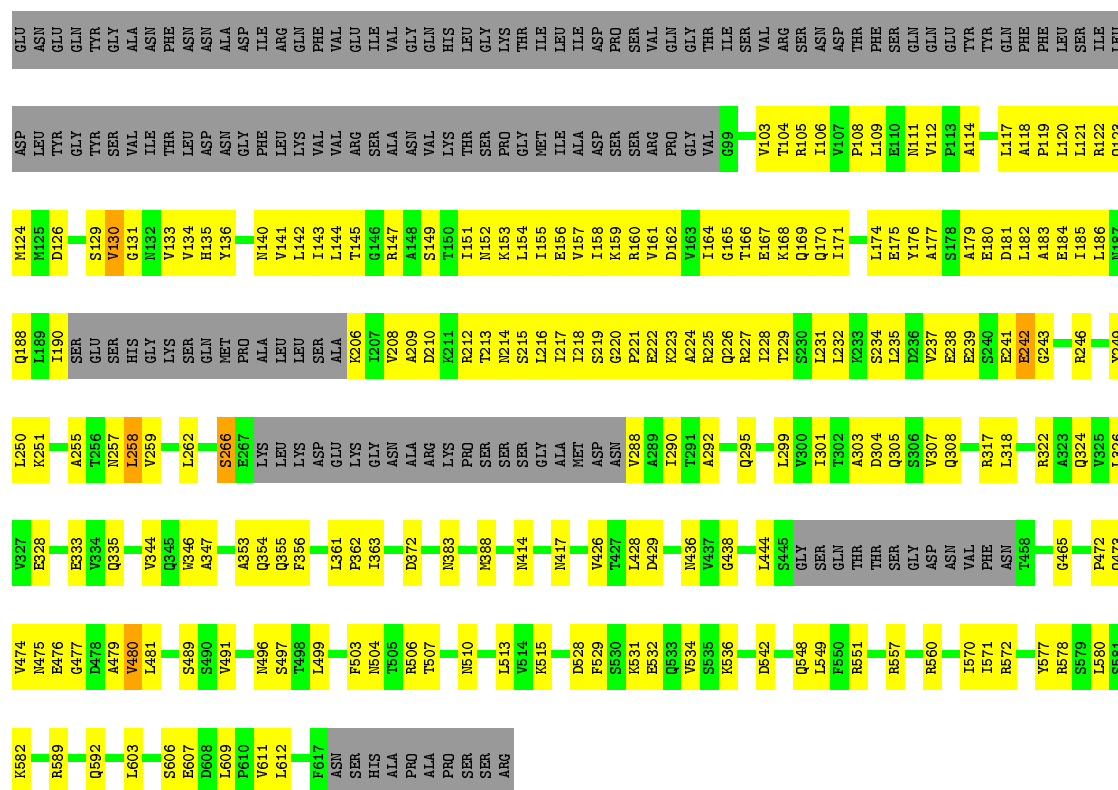
- Molecule 1: Putative type II secretion system protein D





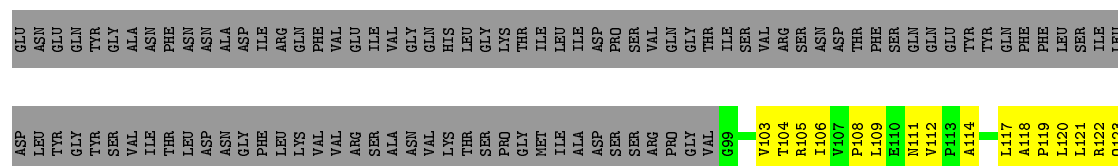
• Molecule 1: Putative type II secretion system protein D

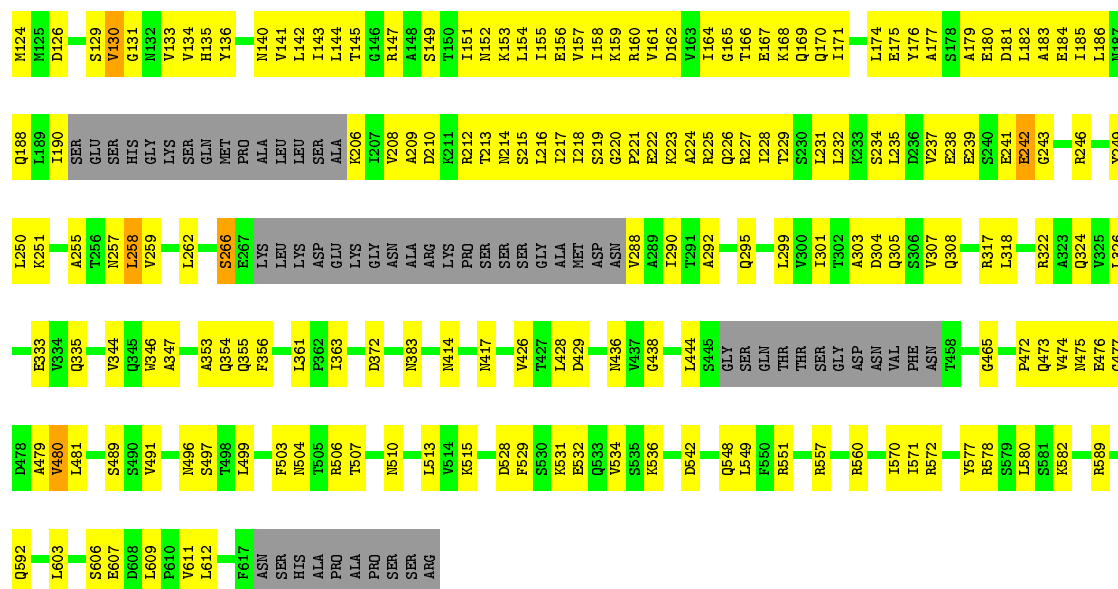
Chain C: 44% 31% 25%



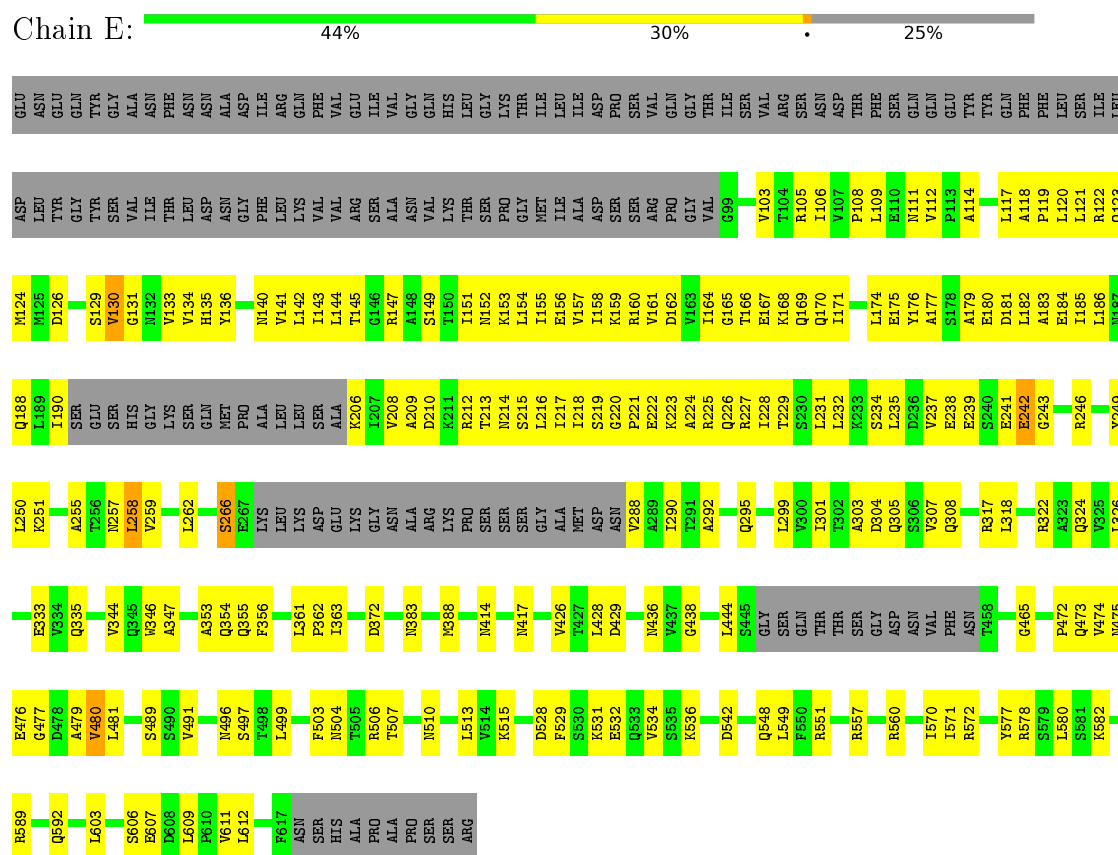
• Molecule 1: Putative type II secretion system protein D

Chain D: 44% 30% 25%

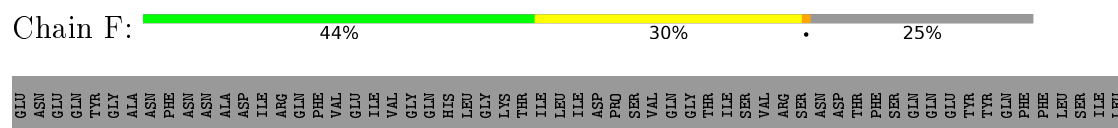


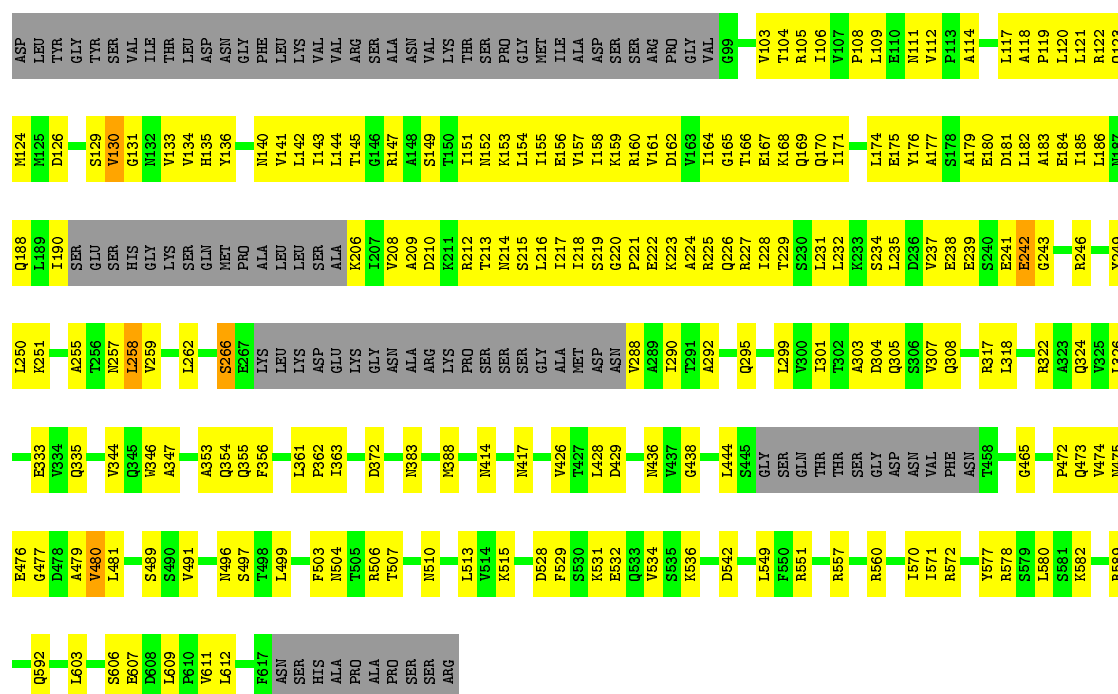


- Molecule 1: Putative type II secretion system protein D



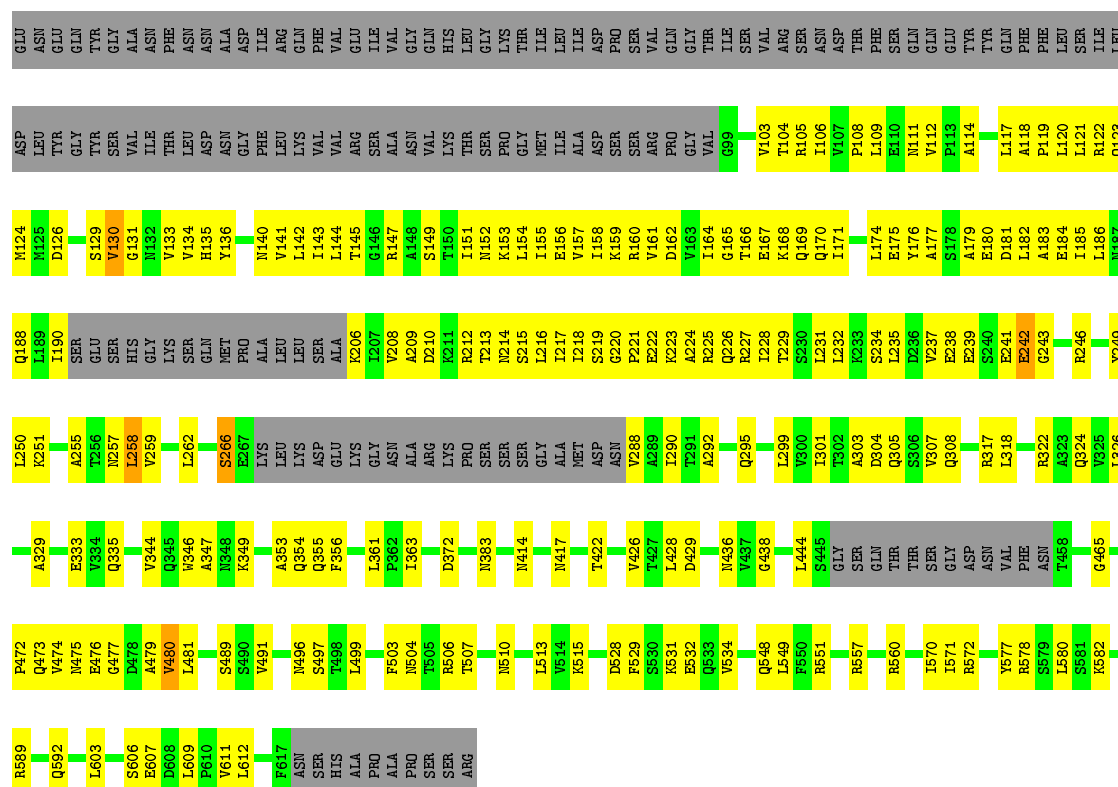
- Molecule 1: Putative type II secretion system protein D





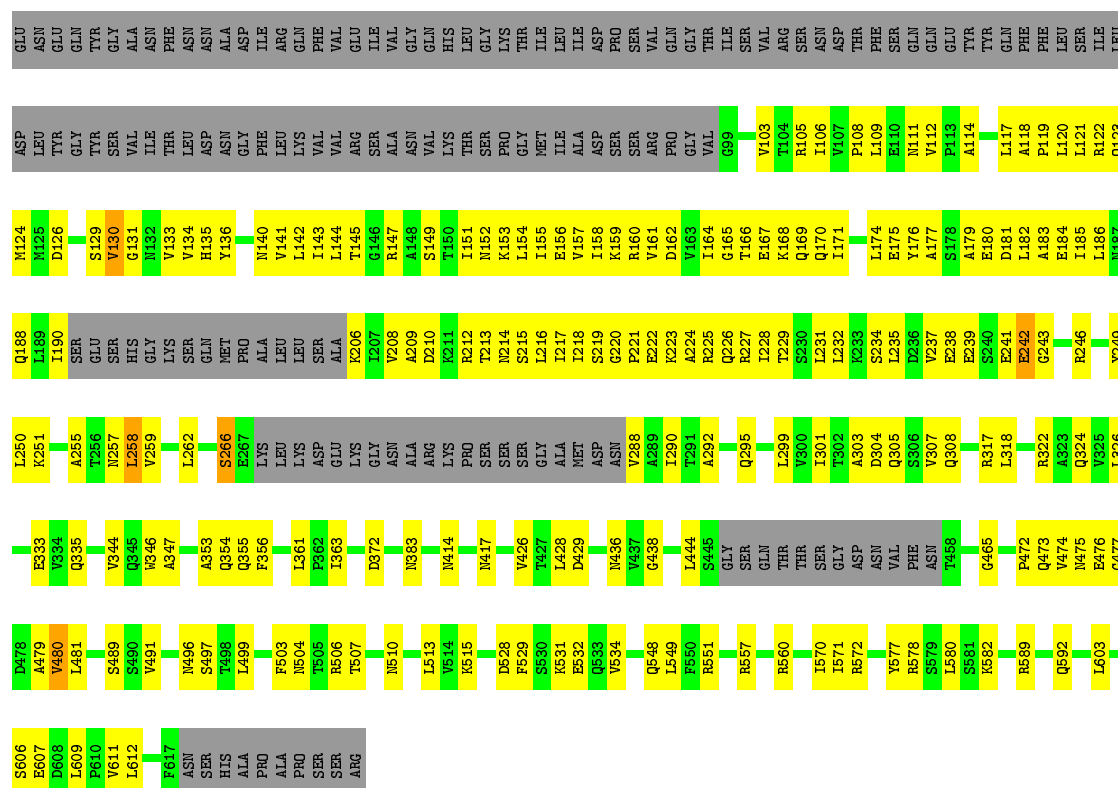
• Molecule 1: Putative type II secretion system protein D

Chain G: 44% 30% 25%



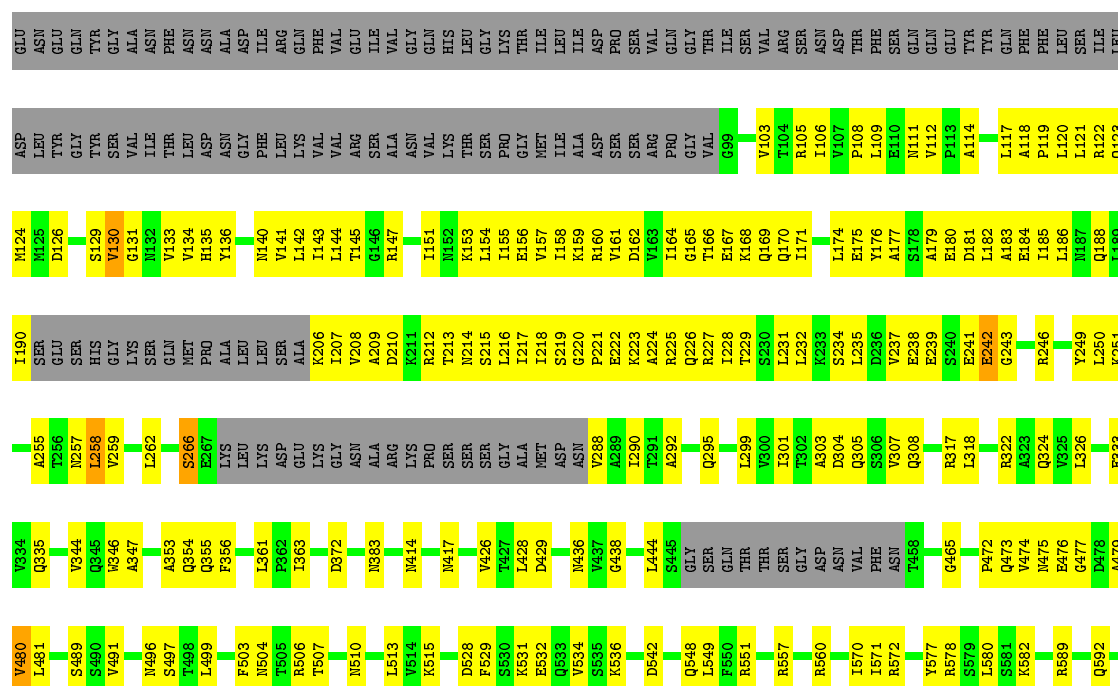
• Molecule 1: Putative type II secretion system protein D

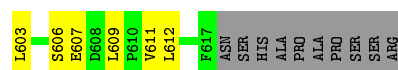
Chain H:



- Molecule 1: Putative type II secretion system protein D

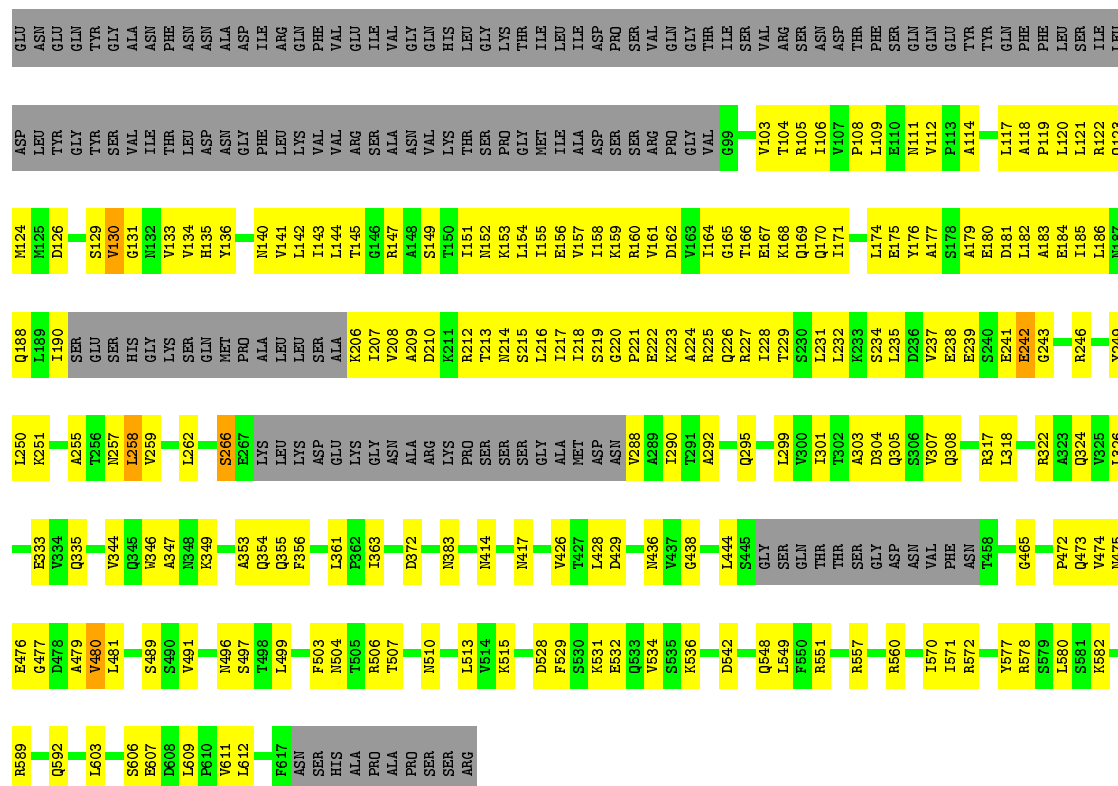
Chain I:





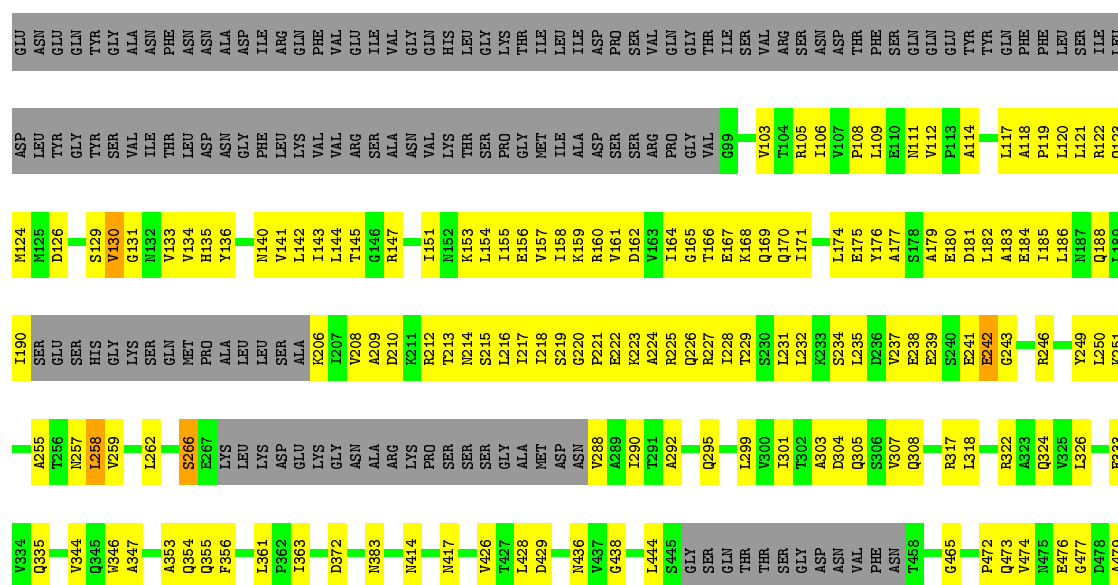
• Molecule 1: Putative type II secretion system protein D

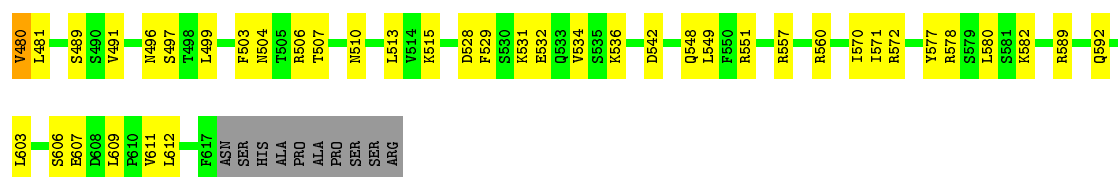
Chain J: 44% 31% 25%



• Molecule 1: Putative type II secretion system protein D

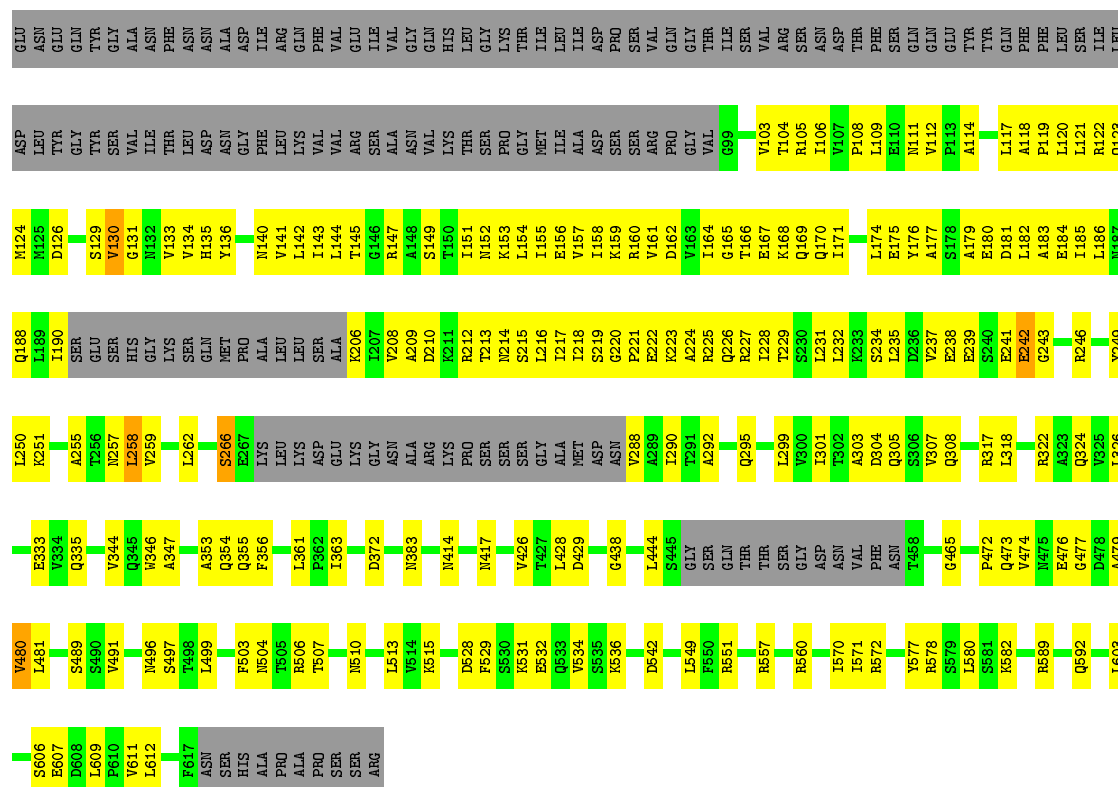
Chain K: 45% 30% 25%





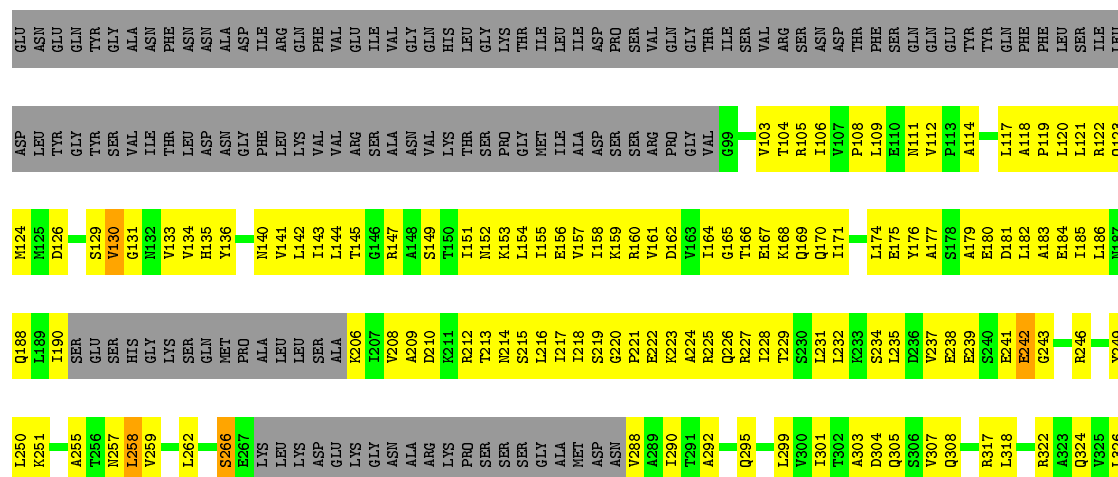
- Molecule 1: Putative type II secretion system protein D

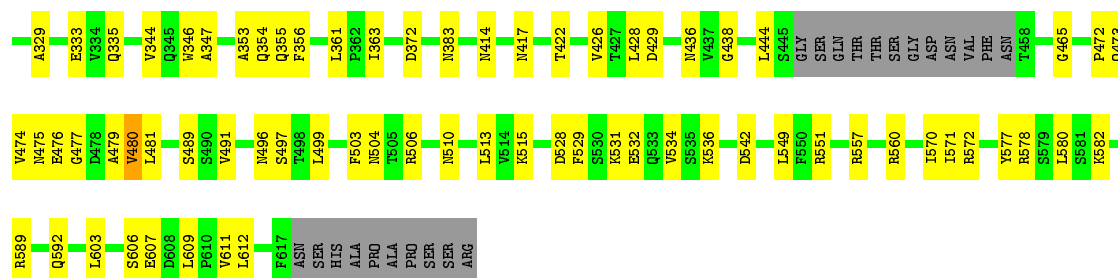
Chain L:  45% 30% 5% 20%



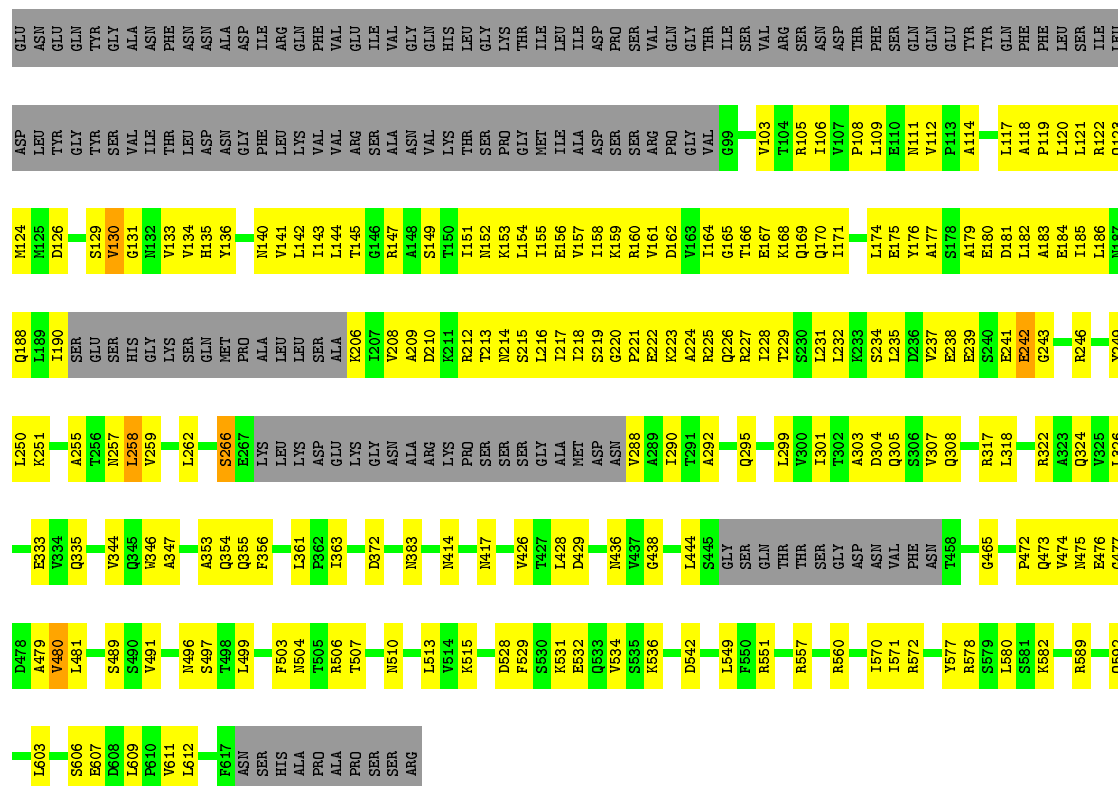
- Molecule 1: Putative type II secretion system protein D

Chain M:  44% 30% 1% 25%

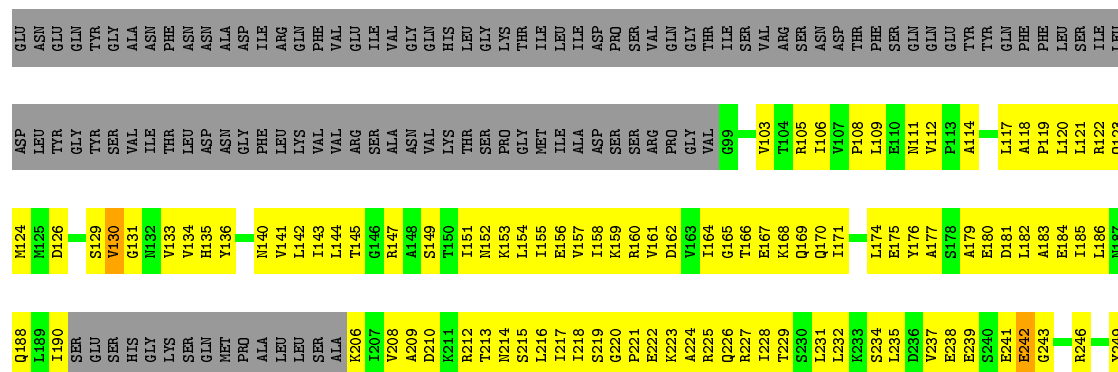




- Molecule 1: Putative type II secretion system protein D



- Molecule 1: Putative type II secretion system protein D



L250	E333	E476	R509
K251	V334	G477	Q592
A255	Q335	D478	L603
T256	V344	A479	S606
I257	Q345	V480	E607
L258	W346	L481	D608
V259	A347	S489	L609
L262	A353	S490	P610
S266	Q354	V491	V611
E267	Q355	S496	L612
LYS	F356	T498	F617
LEU	L361	L499	ASN
LYS	P362	L503	SER
ASP	I363	F503	HIS
GLU	D372	N504	ALA
LYS	N383	T505	PRO
GLY	M388	R506	ALA
ASN	N414	T507	PRO
ALA	N417	N510	SER
ARG	V426	L513	SER
LYS	T427	V514	ARG
PRO	L428	R515	
SER	D429	D528	
SER	N436	F529	
GLY	V437	S530	
ALA	G438	R531	
MET	L444	E532	
ASP	S445	Q533	
ASN	GLY	V534	
V288	GLN	S535	
A289	SER	R536	
I290	THR	D542	
T291	THR	Q548	
A292	THR	L549	
Q295	SER	F550	
L299	GLY	R551	
V300	THR	R557	
I301	GLY	R560	
T302	ASP	I570	
A303	ASN	L571	
D304	VAL	R572	
Q305	PHE	Y577	
S306	ASN	R578	
V307	T468	S579	
Q308	G465	L580	
R317	P472	S581	
L318	Q473	K582	
L322	V474		
A323	N475		
Q324			
V325			
L326			

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	30659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

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 >2	RMSZ	# Z >2
1	A	0.42	0/3673	0.59	1/4983 (0.0%)
1	B	0.42	0/3673	0.59	1/4983 (0.0%)
1	C	0.42	0/3673	0.59	1/4983 (0.0%)
1	D	0.42	0/3673	0.59	1/4983 (0.0%)
1	E	0.42	0/3673	0.59	1/4983 (0.0%)
1	F	0.42	0/3673	0.59	1/4983 (0.0%)
1	G	0.42	0/3673	0.59	1/4983 (0.0%)
1	H	0.42	0/3673	0.59	1/4983 (0.0%)
1	I	0.42	0/3673	0.59	1/4983 (0.0%)
1	J	0.42	0/3673	0.59	1/4983 (0.0%)
1	K	0.42	0/3673	0.59	1/4983 (0.0%)
1	L	0.42	0/3673	0.59	1/4983 (0.0%)
1	M	0.42	0/3673	0.59	1/4983 (0.0%)
1	N	0.42	0/3673	0.59	1/4983 (0.0%)
1	O	0.42	0/3673	0.59	1/4983 (0.0%)
All	All	0.42	0/55095	0.59	15/74745 (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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
1	O	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	266	SER	CB-CA-C	-5.47	99.70	110.10
1	L	266	SER	CB-CA-C	-5.47	99.70	110.10
1	B	266	SER	CB-CA-C	-5.46	99.73	110.10
1	D	266	SER	CB-CA-C	-5.46	99.73	110.10
1	O	266	SER	CB-CA-C	-5.45	99.74	110.10

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	THR	Peptide
1	B	166	THR	Peptide
1	C	166	THR	Peptide
1	D	166	THR	Peptide
1	E	166	THR	Peptide

5.2 Too-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 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	3632	0	3702	225	0
1	B	3632	0	3702	226	0
1	C	3632	0	3702	227	0
1	D	3632	0	3702	226	0
1	E	3632	0	3702	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3632	0	3702	225	0
1	G	3632	0	3702	227	0
1	H	3632	0	3702	224	0
1	I	3632	0	3702	228	0
1	J	3632	0	3702	233	0
1	K	3632	0	3702	224	0
1	L	3632	0	3702	223	0
1	M	3632	0	3702	227	0
1	N	3632	0	3702	227	0
1	O	3632	0	3702	227	0
All	All	54480	0	55530	2956	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 27.

The worst 5 of 2956 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:B:210:ASP:O	1:B:214:ASN:HA	1.50	1.11
1:E:210:ASP:O	1:E:214:ASN:HA	1.50	1.11
1:H:210:ASP:O	1:H:214:ASN:HA	1.50	1.11
1:I:210:ASP:O	1:I:214:ASN:HA	1.50	1.11
1:A:210:ASP:O	1:A:214:ASN:HA	1.50	1.11

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	A	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30 70
1	B	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	D	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	E	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	F	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	G	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	H	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	I	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	J	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	K	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	L	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	M	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	N	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
1	O	464/627 (74%)	442 (95%)	19 (4%)	3 (1%)	30	70
All	All	6960/9405 (74%)	6630 (95%)	285 (4%)	45 (1%)	34	70

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	VAL
1	B	480	VAL
1	C	480	VAL
1	D	480	VAL
1	E	480	VAL

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	A	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	B	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	C	405/537 (75%)	404 (100%)	1 (0%)	95	99

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	E	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	F	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	G	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	H	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	I	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	J	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	K	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	L	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	M	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	N	405/537 (75%)	404 (100%)	1 (0%)	95	99
1	O	405/537 (75%)	404 (100%)	1 (0%)	95	99
All	All	6075/8055 (75%)	6060 (100%)	15 (0%)	95	99

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	258	LEU
1	H	258	LEU
1	M	258	LEU
1	F	258	LEU
1	L	258	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 165 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	368	GLN
1	I	305	GLN
1	N	473	GLN
1	G	475	ASN
1	H	324	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 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.