wwPDB EM Validation Summary Report

Dec 19, 2022 – 12:54 pm GMT

PDB ID	:	7NP7
EMDB ID	:	EMD-12514
Title	:	Structure of an intact ESX-5 inner membrane complex, Composite C1 model
Authors	:	Fahrenkamp, D.; Bunduc, C.M.; Wald, J.; Ummels, R.; Bitter, W.; Houben, E.N.G.; Marlovits, T.C.
Deposited on	:	2021-02-26
Resolution	:	4.03 Å(reported)

This is a wwPDB EM 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/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:

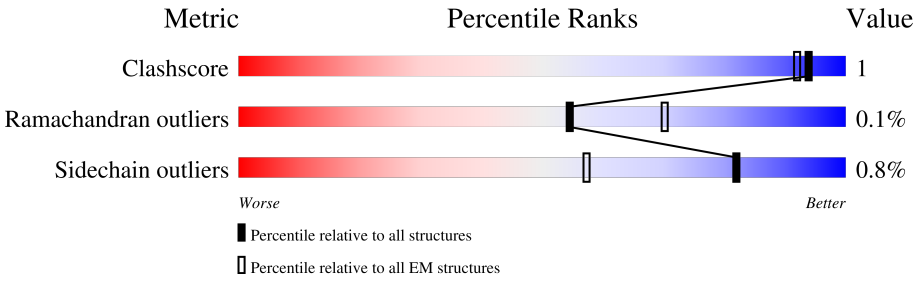
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 4.03 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B1	506	8% 91% · 6%
1	B2	506	8% 89% 6% 6%
1	B3	506	9% 89% 5% 6%
1	B4	506	· 89% 6% 5%
1	B5	506	· 91% · 5%
1	B6	506	· 89% 5% 5%
2	C1	1391	6% 28% · 71%
2	C2	1391	9% 28% · 71%

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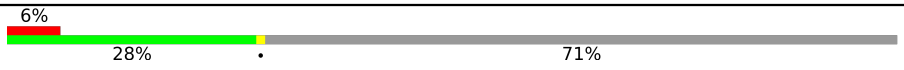
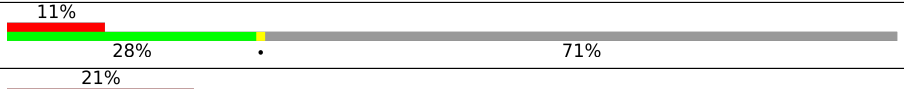
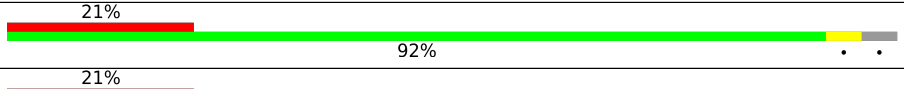
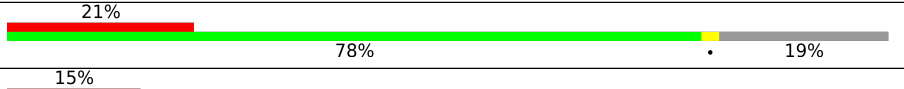
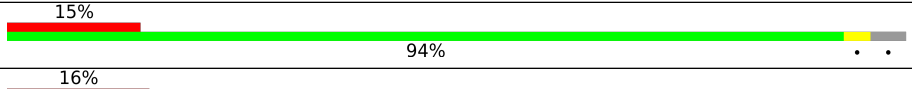
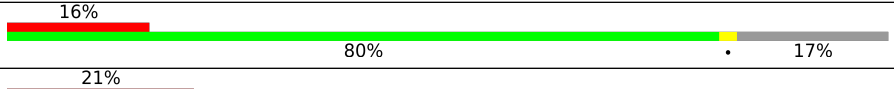
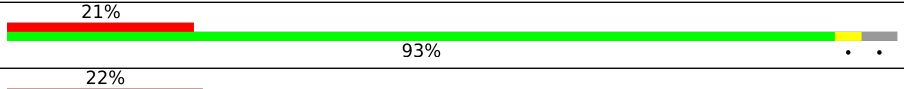
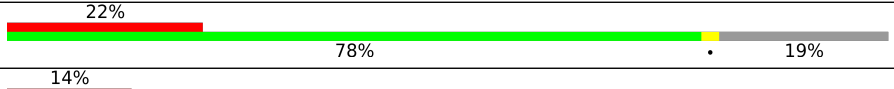
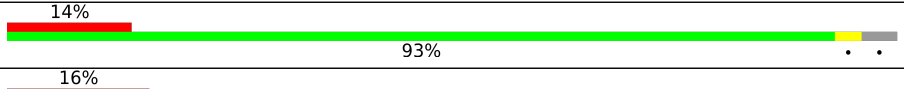
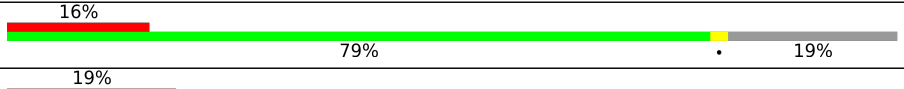
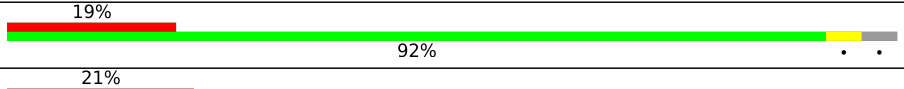
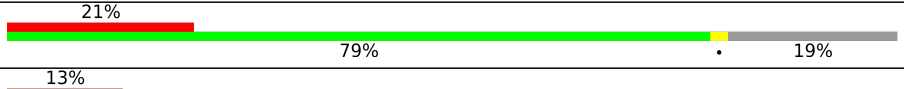
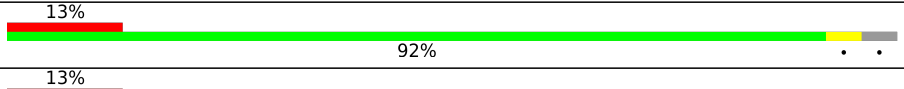
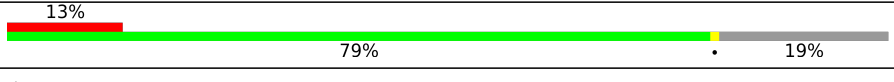
Mol	Chain	Length	Quality of chain
2	C3	1391	
2	C4	1391	
2	C5	1391	
2	C6	1391	
3	D1	503	
3	D2	503	
3	D3	503	
3	D4	503	
3	D5	503	
3	D6	503	
3	D7	503	
3	D8	503	
3	D9	503	
3	DA	503	
3	DB	503	
3	DC	503	
4	P1	585	
4	P2	585	
4	P3	585	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 182470 atoms, of which 92300 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 ESX-5 secretion system ATPase EccB5.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B1	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B2	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B3	478	Total	C	H	N	O	S	0	0
			7218	2266	3631	639	671	11		
1	B4	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		
1	B5	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		
1	B6	480	Total	C	H	N	O	S	0	0
			7212	2262	3621	644	675	10		

- Molecule 2 is a protein called ESX-5 secretion system protein EccC5.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C1	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		
2	C2	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		
2	C3	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		
2	C4	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		
2	C5	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		
2	C6	406	Total	C	H	N	O	S	0	0
			6335	2052	3145	536	576	26		

- Molecule 3 is a protein called ESX-5 secretion system protein EccD5.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D1	485	Total	C	H	N	O	S	0	0
			7458	2353	3823	633	628	21		

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Mol	Chain	Residues	Atoms						AltConf	Trace
3	D2	405	Total	C	H	N	O	S	0	0
			6155	1919	3166	528	524	18		
3	D3	485	Total	C	H	N	O	S	0	0
			7459	2353	3824	633	628	21		
3	D4	415	Total	C	H	N	O	S	0	0
			6308	1969	3245	541	535	18		
3	D5	485	Total	C	H	N	O	S	0	0
			7459	2353	3824	633	628	21		
3	D6	405	Total	C	H	N	O	S	0	0
			6155	1919	3166	528	524	18		
3	D7	485	Total	C	H	N	O	S	0	0
			7459	2353	3824	633	628	21		
3	D8	405	Total	C	H	N	O	S	0	0
			6154	1919	3165	528	524	18		
3	D9	485	Total	C	H	N	O	S	0	0
			7459	2353	3824	633	628	21		
3	DA	405	Total	C	H	N	O	S	0	0
			6156	1919	3167	528	524	18		
3	DB	485	Total	C	H	N	O	S	0	0
			7459	2353	3824	633	628	21		
3	DC	405	Total	C	H	N	O	S	0	0
			6154	1919	3165	528	524	18		

- Molecule 4 is a protein called Mycosin-5.

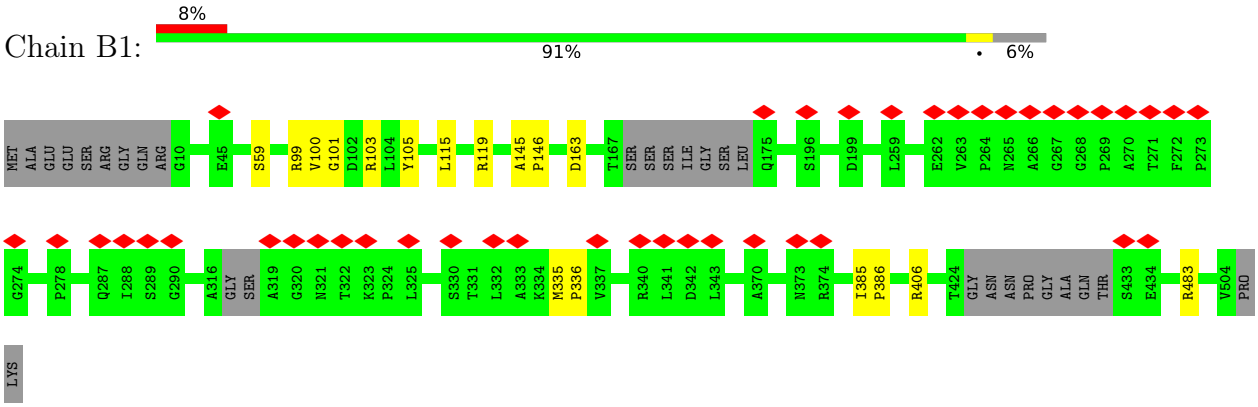
Mol	Chain	Residues	Atoms						AltConf	Trace
4	P1	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		
4	P2	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		
4	P3	444	Total	C	H	N	O	S	0	0
			6445	2046	3219	554	611	15		

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 and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

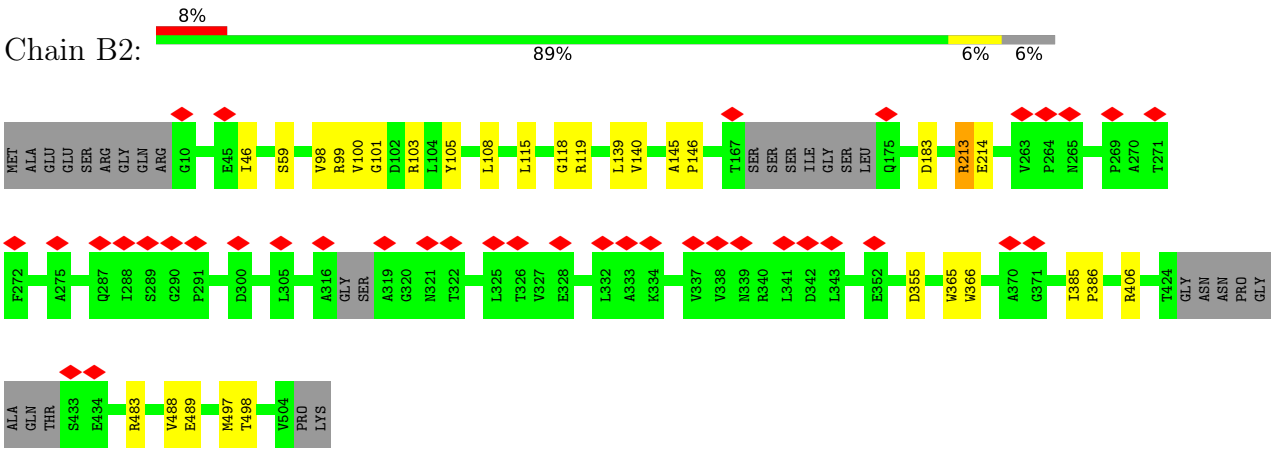
• Molecule 1: ESX-5 secretion system ATPase EccB5

Chain B1:



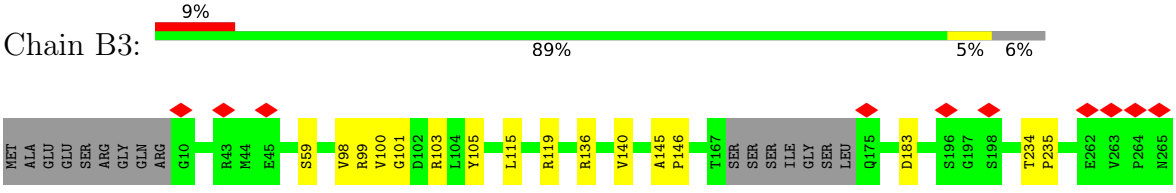
• Molecule 1: ESX-5 secretion system ATPase EccB5

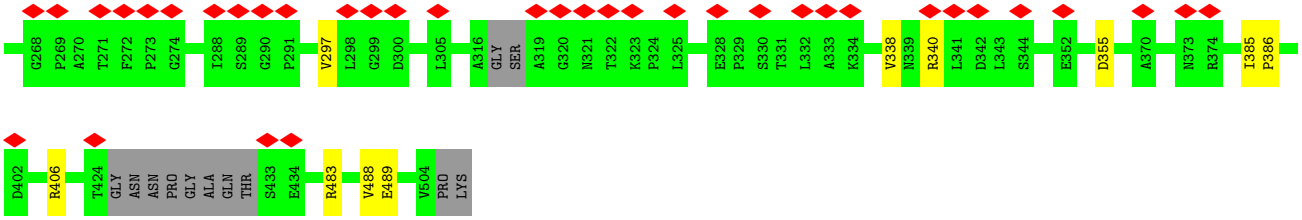
Chain B2:



• Molecule 1: ESX-5 secretion system ATPase EccB5

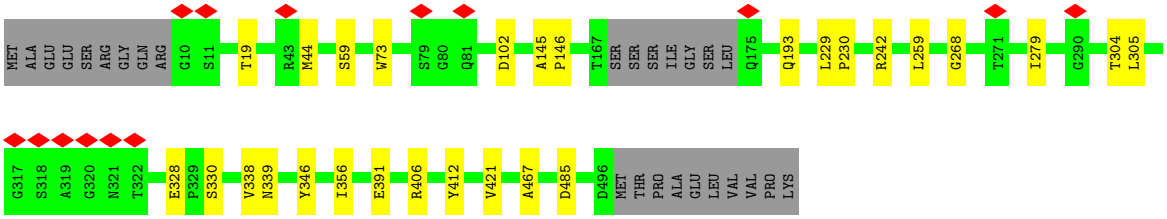
Chain B3:





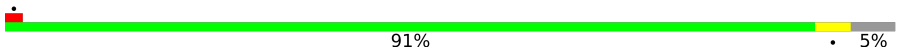
• Molecule 1: ESX-5 secretion system ATPase EccB5

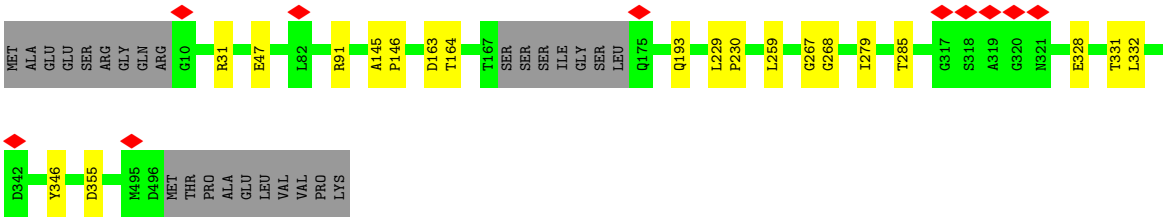
Chain B4:



• Molecule 1: ESX-5 secretion system ATPase EccB5

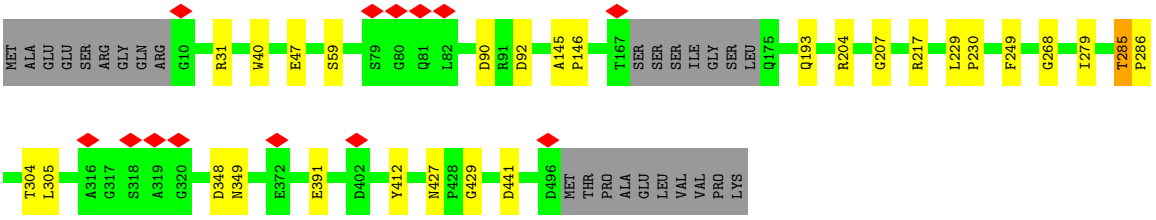
Chain B5:





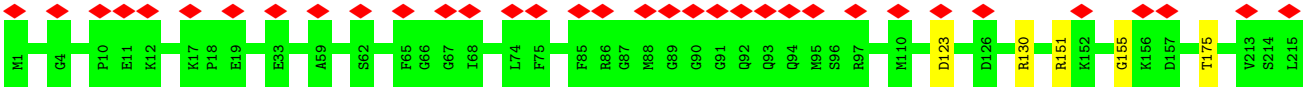
• Molecule 1: ESX-5 secretion system ATPase EccB5

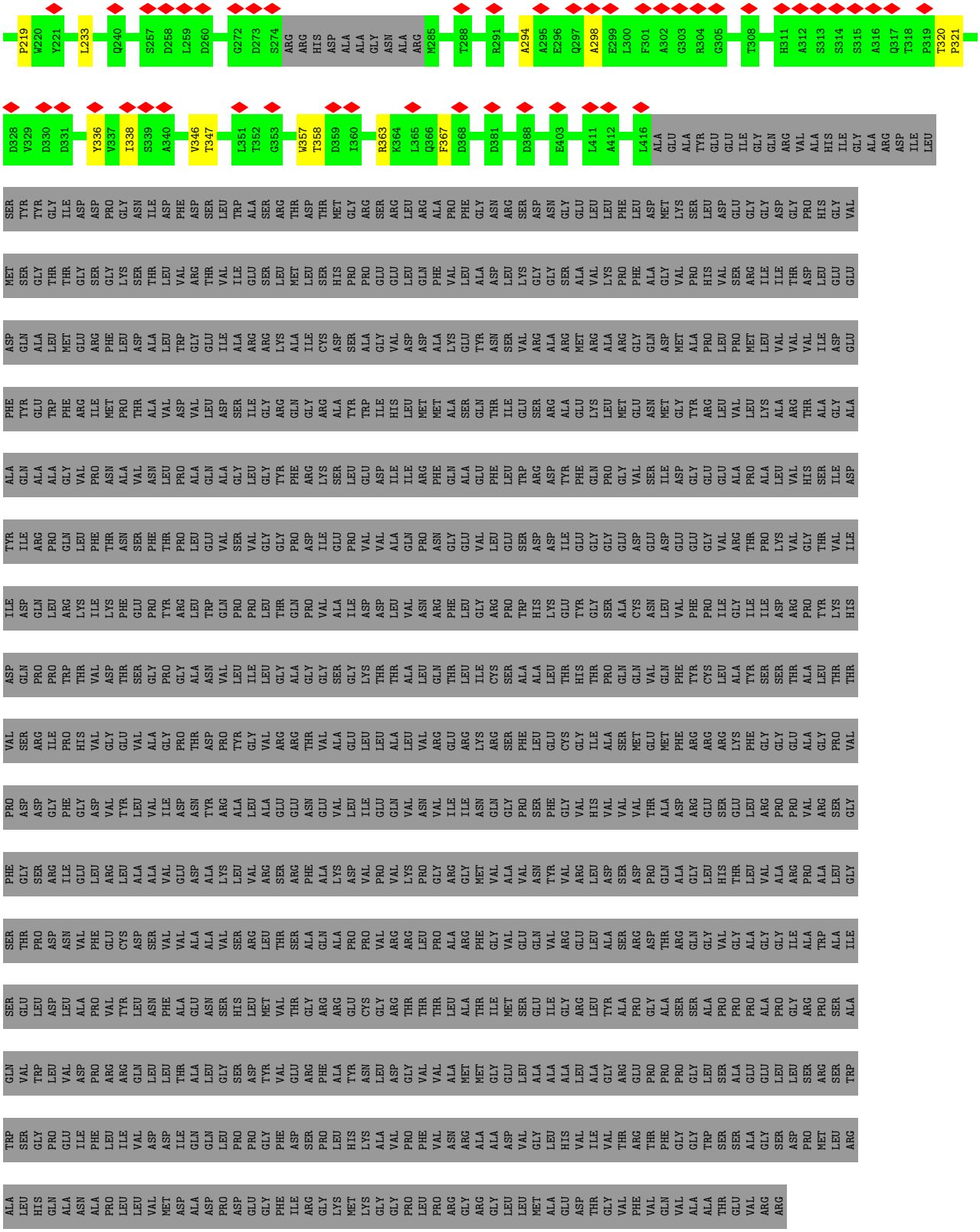
Chain B6:



• Molecule 2: ESX-5 secretion system protein EccC5

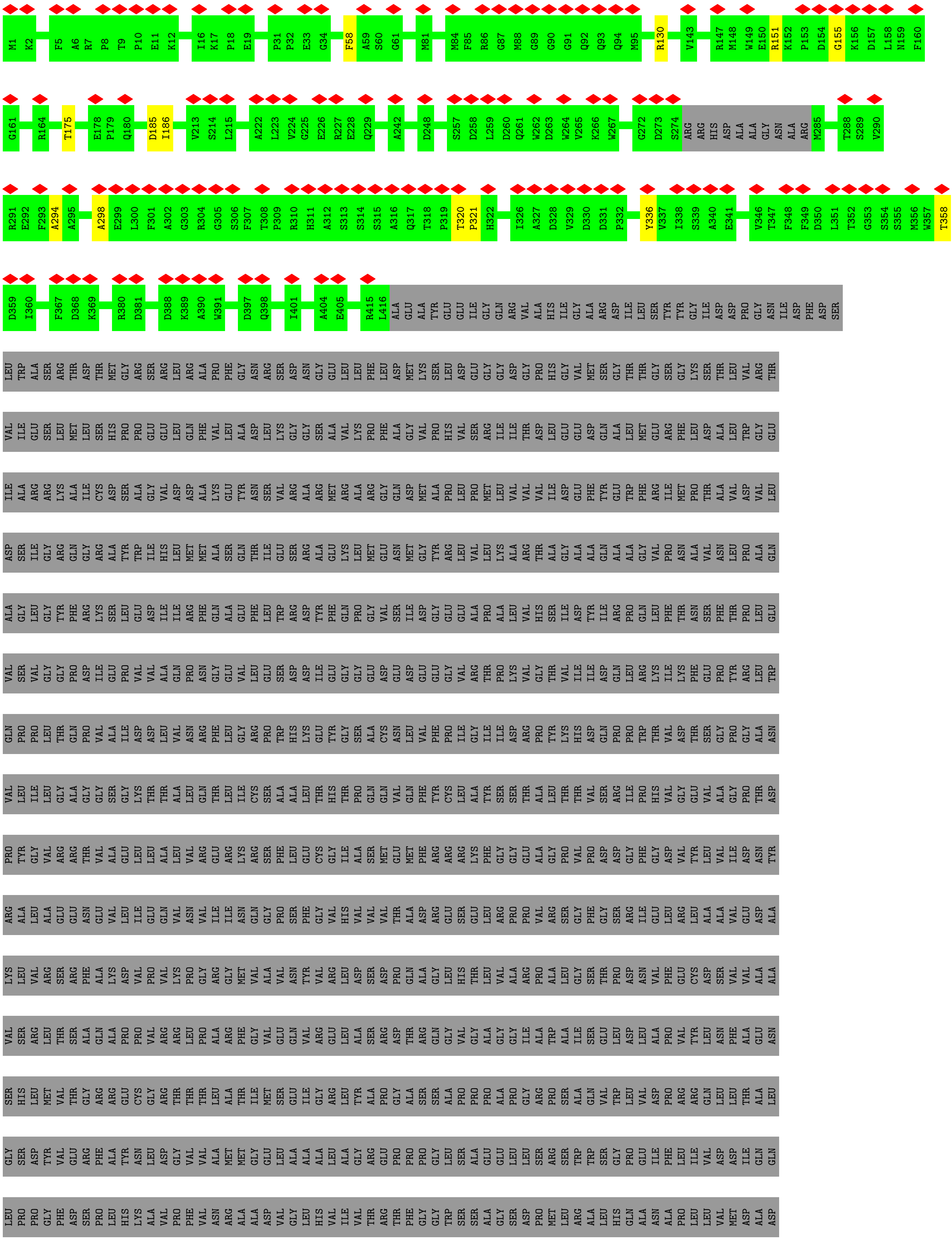
Chain C1:





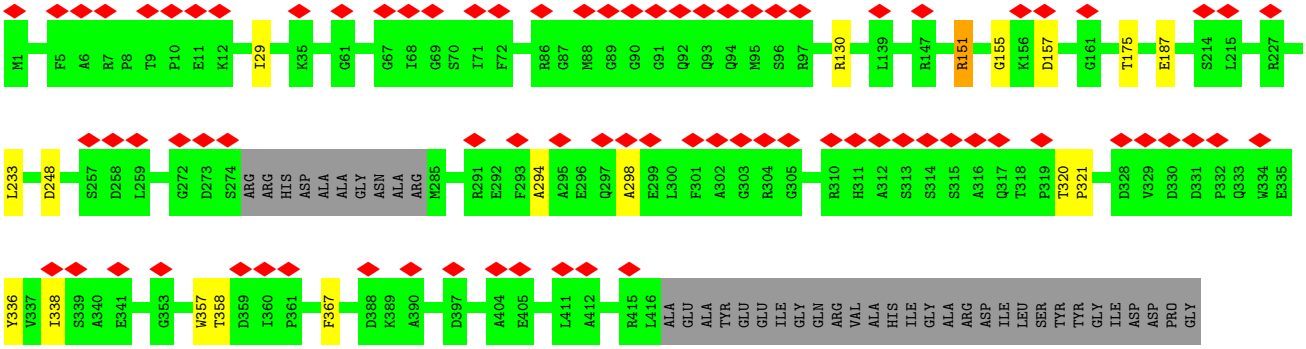
• Molecule 2: ESX-5 secretion system protein EccC5

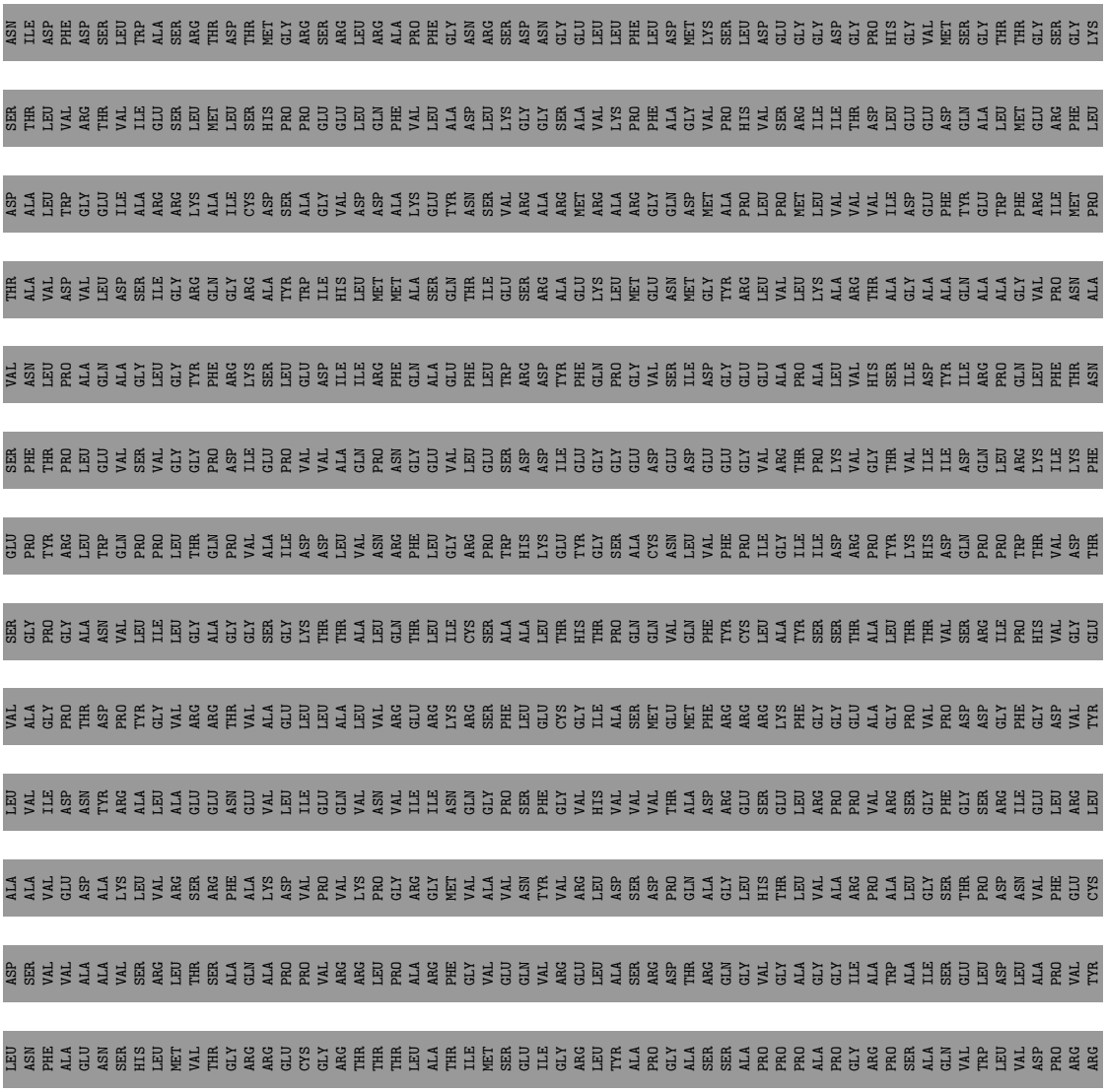
Chain C2:

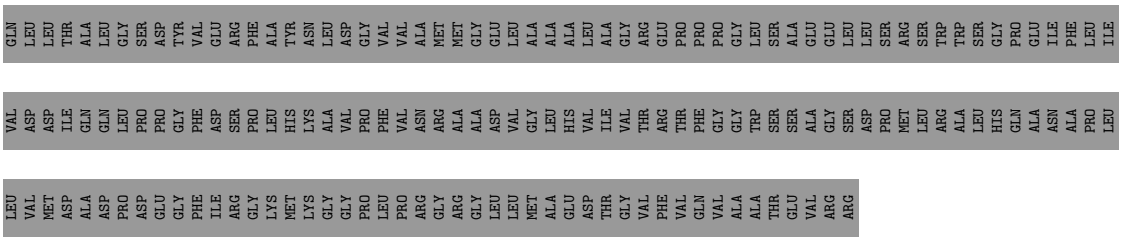

M1 K2 F5 A6 R7 P8 T9 P10 E11 K12 I16 K17 P18 E19 P31 P32 E33 G34 F58 A59 S60 G61 M81 M84 F85 R86 G87 M88 G89 G90 G91 Q92 Q93 Q94 M95 R130 V143 R147 M148 W149 E150 R151 K152 P153 D154 G155 K156 D157 L158 N159 F160
G161 R164 T175 E178 P179 Q180 D185 I186 V213 S214 L215 A222 L223 V224 G225 E226 R227 E228 Q229 A242 D248 S257 D258 L259 D260 Q261 W262 D263 W264 V265 K266 W267 G272 D273 S274 ARG ARG HIS ASP ALA ALA GLY ASN ALA ARG M285 T288 S289 V290
R291 E292 F293 A294 A295 A298 E299 L300 F301 A302 G303 R304 G305 S306 F307 T308 P309 R310 H311 A312 S313 S314 S315 A316 Q317 T318 P319 T320 P321 H322 I326 A327 D328 V329 D330 D331 P332 Y336 V337 I338 S339 A340 E341 V346 T347 F348 F349 D350 L351 T352 G353 S354 S355 M356 W357 T358
D359 I360 F367 D368 K369 R380 D381 D388 K389 A390 W391 D397 Q398 I401 A404 E405 R415 L416 ALA GLU ALA TYR GLU GLU ILE GLY GLN ARG VAL ALA HIS ILE GLY ALA ARG ASP ILE LEU SER TYR TYR GLY ILE ASP ASP PRO GLY ASN ILE ASP PHE ASP SER
LEU TRP ALA SER ARG THR ASP THR MET GLY ARG SER ARG LEU ARG ALA PRO PHE GLY ASN ARG SER ASP ASN GLY GLU LEU LEU PHE LEU ASP MET LYS SER LEU ASP GLU GLY GLY ASP GLY PRO HIS GLY VAL MET SER GLY THR THR GLY SER GLY LYS SER THR LEU VAL ARG THR
VAL ILE GLU SER LEU MET LEU SER HIS PRO PRO GLU GLU LEU GLN PHE VAL LEU ALA ASP LEU LYS GLY GLY SER ALA VAL LYS PRO PHE ALA GLY VAL PRO HIS VAL SER ARG ILE ILE THR ASP LEU GLU GLU ASP GLN ALA LEU MET GLU ARG PHE LEU ASP ALA LEU TRP GLY GLU
ILE ALA ARG ARG LYS ALA ILE CYS ASP SER ALA GLY VAL ASP ASP ALA LYS GLU TYR ASN SER VAL ARG ALA ARG MET ARG ALA ARG GLY GLN ASP MET ALA PRO LEU PRO MET LEU VAL VAL VAL ILE ASP GLU PHE TYR GLU TRP PHE ARG ILE MET PRO THR ALA VAL ASP VAL LEU
ASP SER ILE GLY ARG GLN GLY ARG ALA TYR TRP ILE HIS LEU MET MET ALA SER GLN THR ILE GLU SER ARG ALA GLU LYS LEU MET GLU ASN MET GLY TYR ARG LEU VAL LEU LYS ALA ARG THR ALA GLY ALA ALA GLN ALA ALA GLY VAL PRO ASN ALA VAL ASN LEU PRO ALA GLN
ALA GLY LEU GLY TYR PHE ARG LYS SER LEU GLU ASP ILE ILE ARG PHE GLN ALA GLU PHE LEU TRP ARG ASP TYR PHE GLN PRO GLY VAL SER ILE ASP GLY GLU GLU ALA PRO ALA LEU VAL HIS SER ILE ASP TYR ILE ARG PRO GLN LEU PHE THR ASN SER PHE THR PRO LEU GLU
VAL SER VAL GLY GLY PRO ASP ILE GLU PRO VAL VAL ALA GLN PRO ASN GLY GLU VAL LEU GLU SER ASP ASP ILE GLU GLY GLY GLU ASP GLU ASP GLU GLU GLY VAL ARG THR PRO LYS VAL GLY THR VAL ILE ILE ASP GLN LEU ARG LYS ILE LYS PHE GLU PRO TYR ARG LEU TRP
GLN PRO PRO LEU THR GLN PRO VAL ALA ILE ASP ASP LEU VAL ASN ARG PHE LEU GLY ARG PRO TRP HIS LYS GLU TYR GLY SER ALA CYS ASN LEU VAL PHE PRO ILE GLY ILE ILE ASP ARG PRO TYR LYS HIS ASP GLN PRO PRO TRP THR VAL ASP THR SER GLY PRO GLY ALA ASN
VAL LEU ILE LEU GLY ALA GLY GLY SER GLY LYS THR THR ALA LEU GLN THR LEU ILE CYS SER ALA ALA LEU THR HIS THR PRO GLN GLN VAL GLN PHE TYR CYS LEU ALA TYR SER SER THR ALA LEU THR THR VAL SER ARG ILE PRO HIS VAL GLY GLU VAL ALA GLY PRO THR ASP
PRO TYR GLY VAL ARG ARG THR VAL ALA GLU LEU LEU ALA LEU VAL ARG GLU ARG LYS ARG SER PHE LEU GLU CYS GLY ILE ALA SER MET GLU MET PHE ARG ARG ARG LYS PHE GLY GLY GLU ALA GLY PRO VAL PRO ASP ASP GLY PHE GLY ASP VAL TYR LEU VAL ILE ASP ASN TYR
ARG ALA LEU ALA GLU GLU ASN GLU VAL LEU ILE GLU GLN VAL ASN VAL ILE ILE ASN GLN GLY PRO SER PHE GLY VAL HIS VAL VAL VAL THR ALA ASP ARG GLU SER GLU LEU ARG PRO PRO VAL ARG SER GLY PHE GLY SER ARG ILE GLU LEU ARG LEU ALA ALA VAL GLU ASP ALA
LYS LEU VAL ARG SER ARG PHE ALA LYS ASP VAL PRO VAL LYS PRO GLY ARG GLY MET VAL ALA VAL ASN TYR VAL ARG LEU ASP SER ASP PRO GLN ALA GLY LEU HIS THR LEU VAL ALA ARG PRO ALA LEU GLY SER THR PRO ASP ASN VAL PHE GLU CYS ASP SER VAL VAL ALA ALA
VAL SER ARG LEU THR SER ALA GLN ALA PRO PRO VAL ARG ARG LEU PRO ALA ARG PHE GLY VAL GLU GLN VAL ARG GLU LEU ALA SER ARG ASP THR ARG GLN GLY VAL GLY ALA GLY GLY ILE ALA TRP ALA ILE SER GLU LEU ASP LEU ALA PRO VAL TYR LEU ASN PHE ALA GLU ASN
SER HIS LEU MET VAL THR GLY ARG ARG GLU CYS GLY ARG THR THR THR LEU ALA THR ILE MET SER GLU ILE GLY ARG LEU TYR ALA PRO GLY ALA SER SER ALA PRO PRO PRO ALA PRO GLY ARG PRO SER ALA GLN VAL TRP LEU VAL ASP PRO ARG ARG GLN LEU LEU THR ALA LEU
GLY SER ASP TYR VAL GLU ARG PHE ALA TYR ASN LEU ASP GLY VAL VAL ALA MET MET GLY GLU LEU ALA ALA ALA LEU ALA GLY ARG GLU PRO PRO PRO GLY LEU SER ALA GLU GLU LEU LEU SER ARG SER TRP TRP SER GLY PRO GLU ILE PHE LEU ILE VAL ASP ASP ILE GLN GLN
LEU PRO PRO GLY PHE ASP SER PRO LEU HIS LYS ALA VAL PRO PHE VAL ASN ARG ALA ALA ASP VAL GLY LEU HIS VAL ILE VAL THR ARG THR PHE GLY GLY TRP SER SER ALA GLY SER ASP PRO MET LEU ARG ALA LEU HIS GLN ALA ASN ALA PRO LEU LEU VAL MET ASP ALA ASP

• Molecule 2: ESX-5 secretion system protein EccC5

Chain C3:

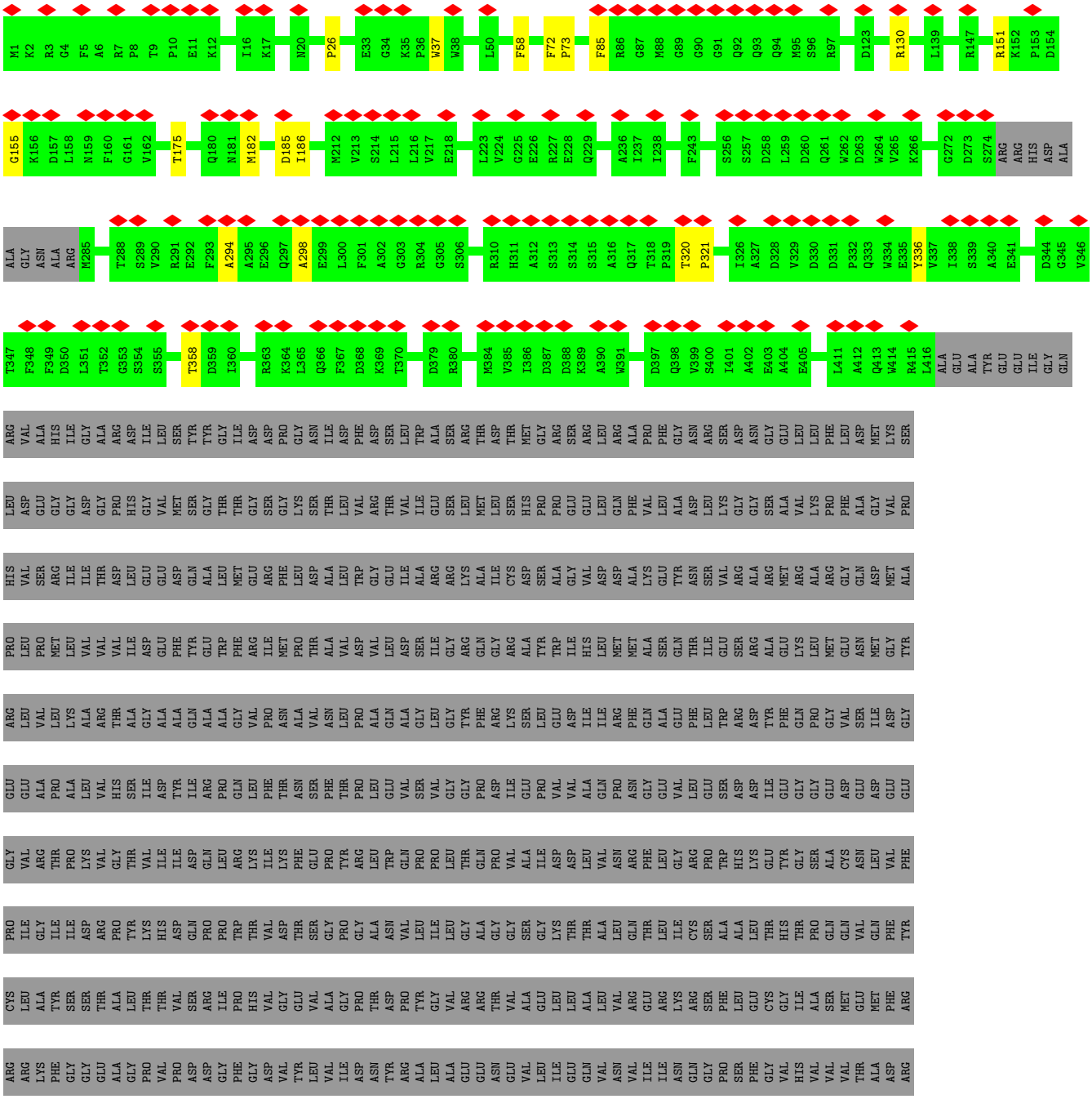






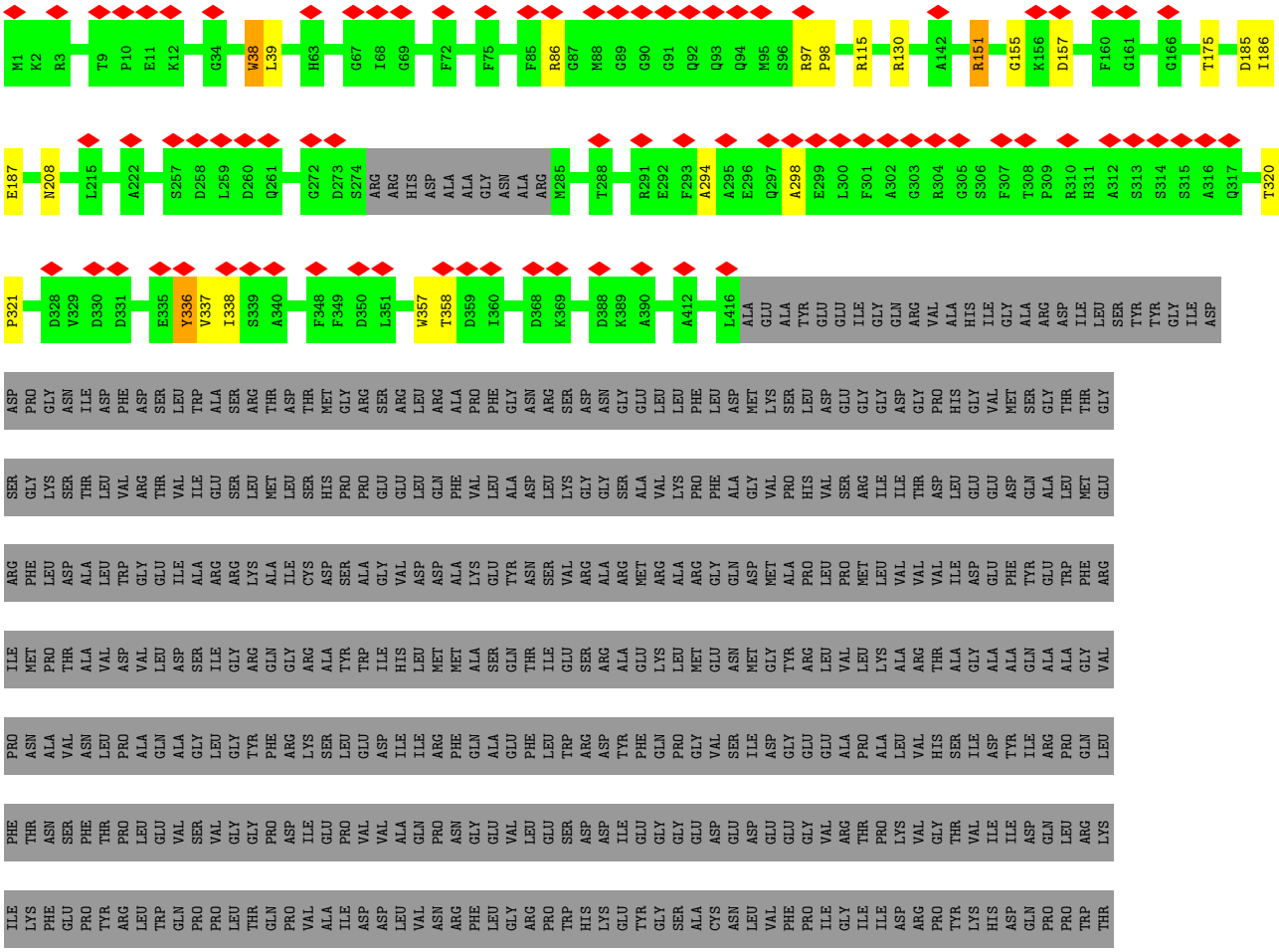
• Molecule 2: ESX-5 secretion system protein EccC5

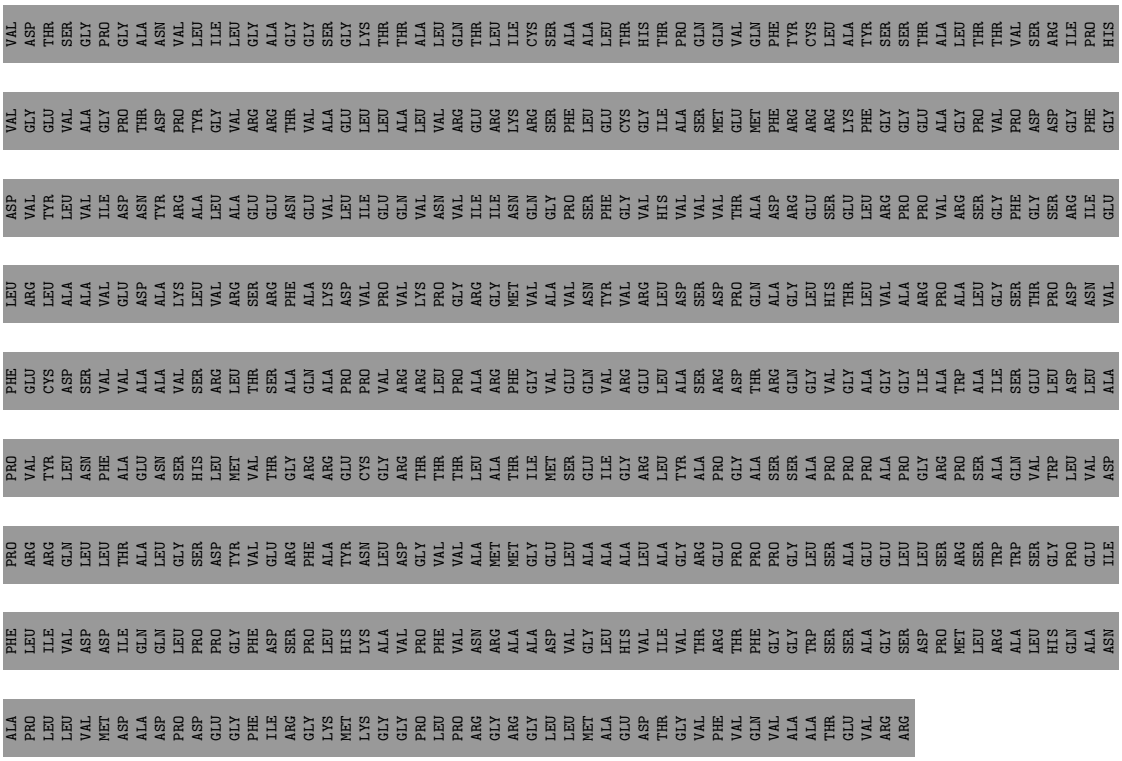
Chain C4:



• Molecule 2: ESX-5 secretion system protein EccC5

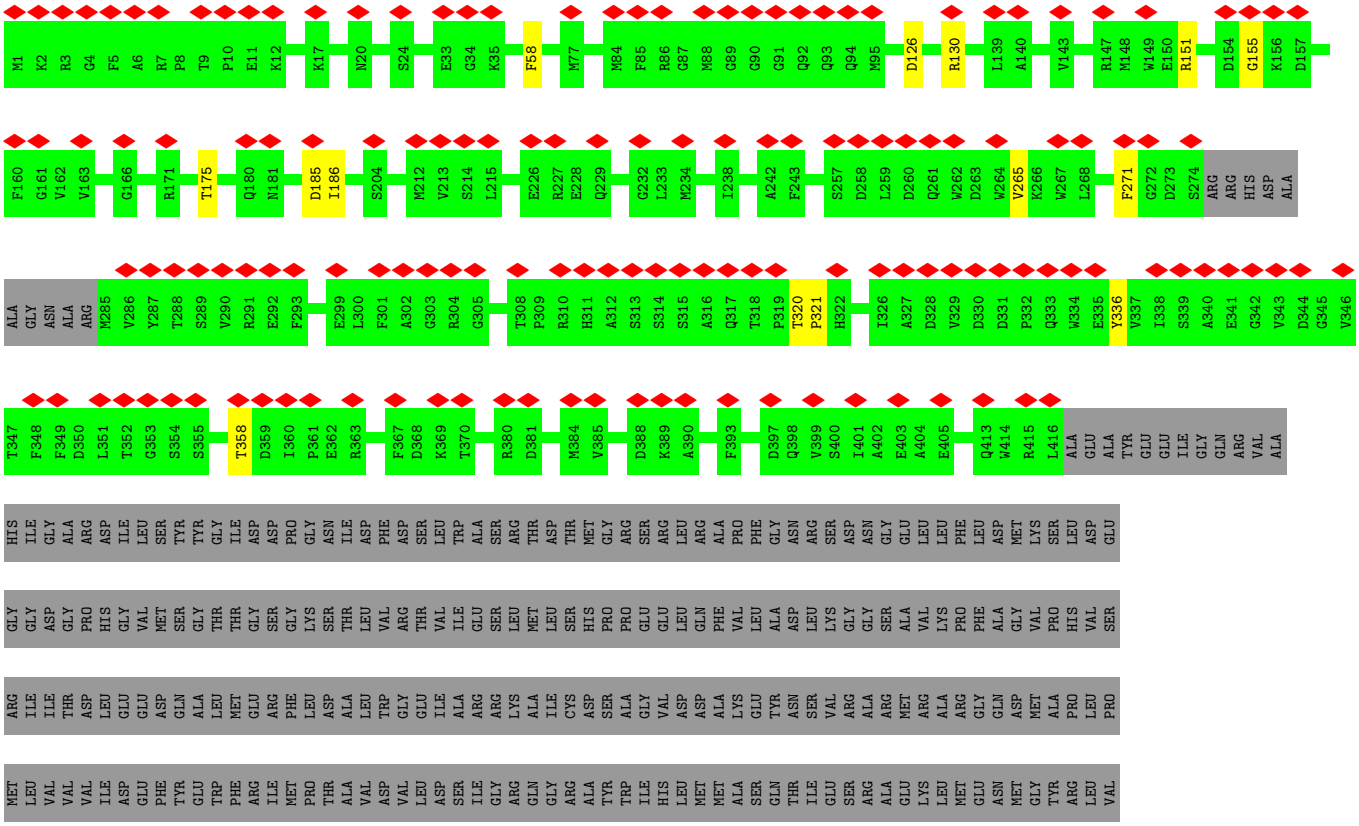
Chain C5:

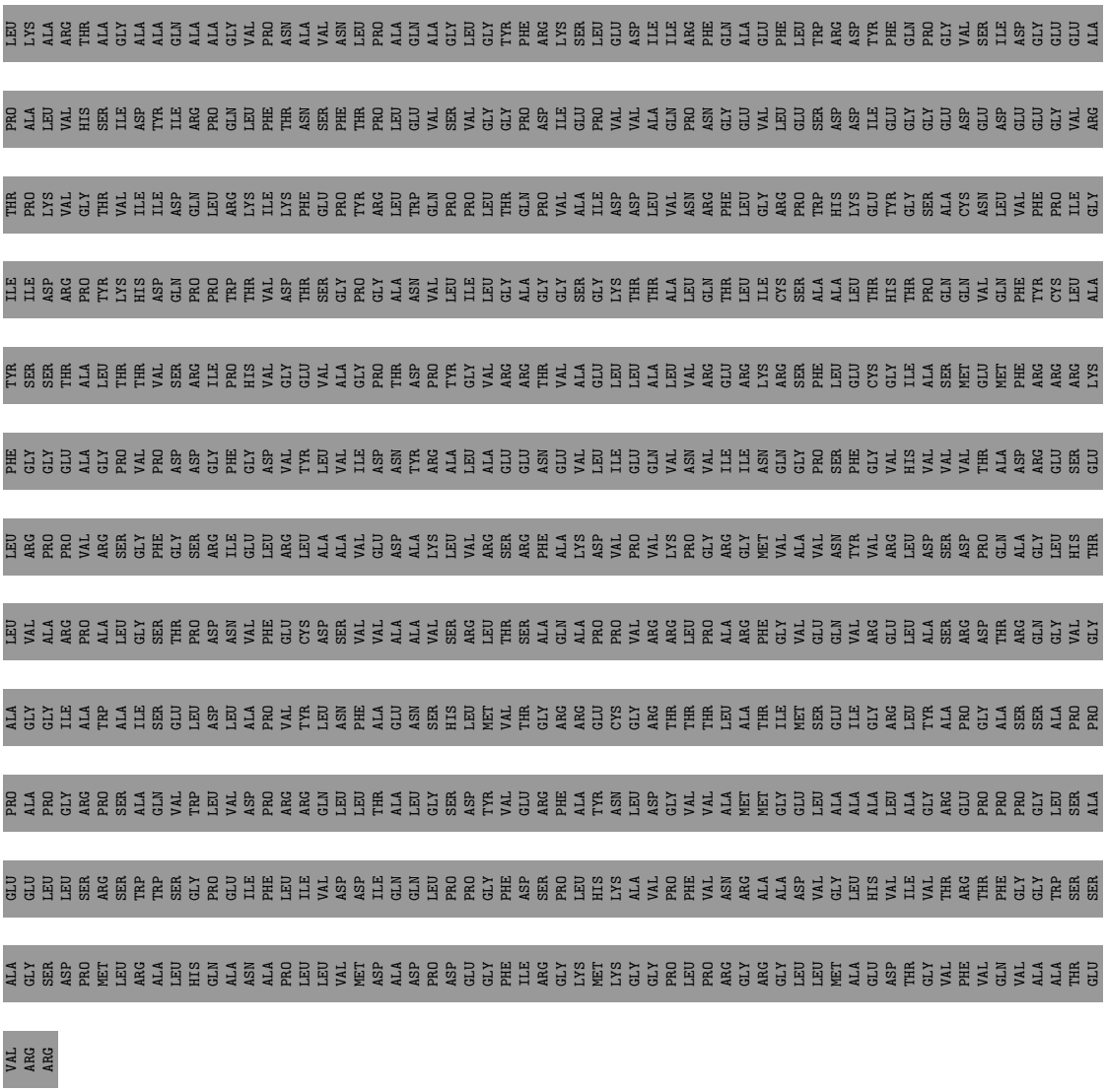




• Molecule 2: ESX-5 secretion system protein EccC5

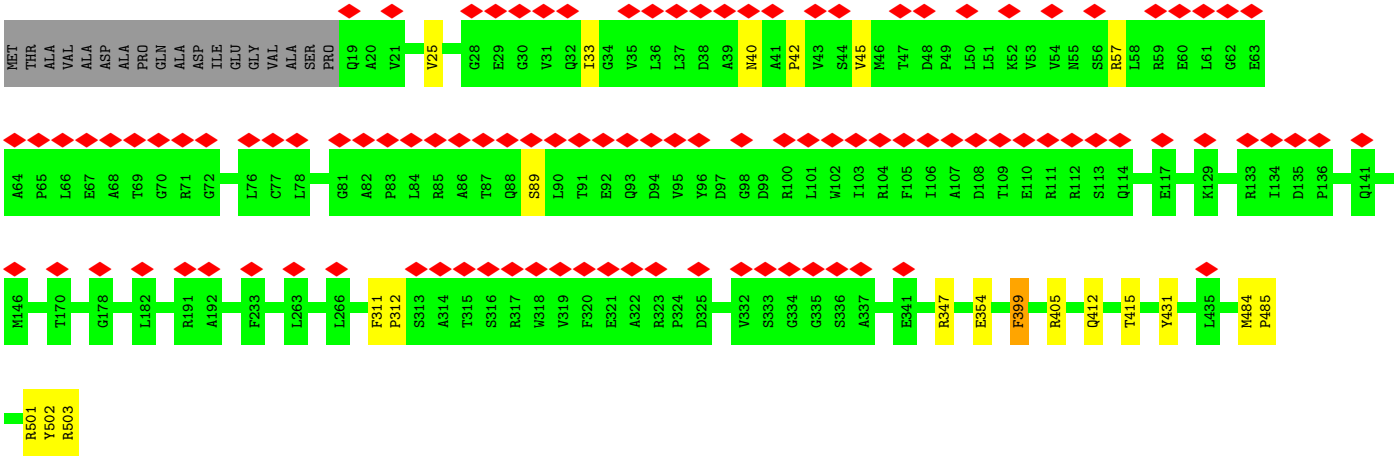
Chain C6:





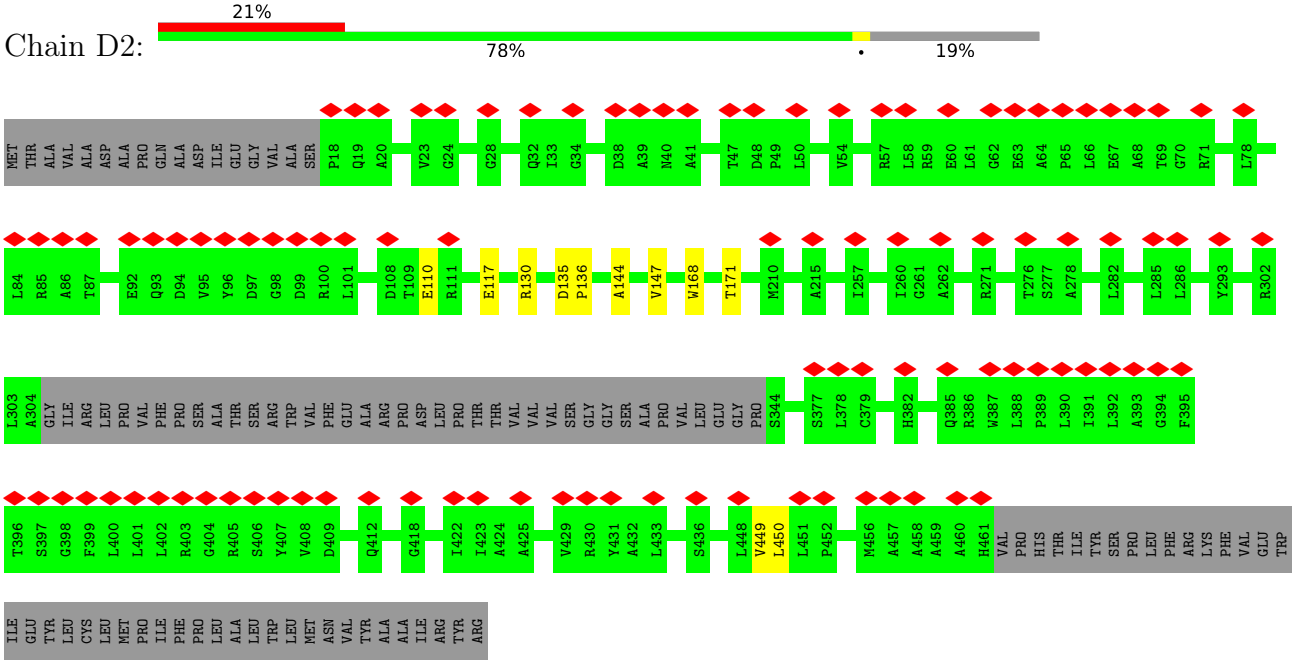
• Molecule 3: ESX-5 secretion system protein EccD5

Chain D1:



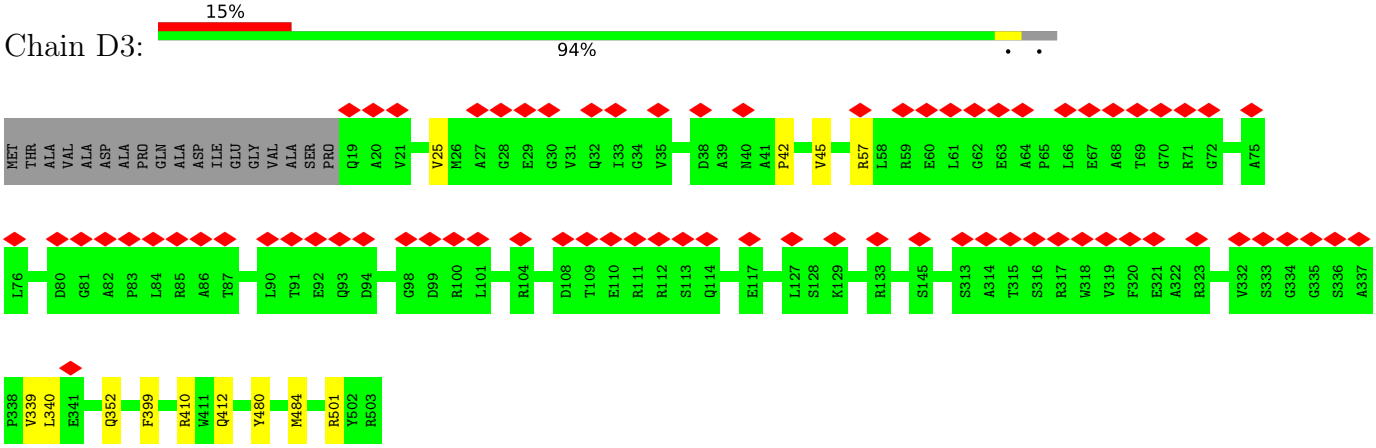
• Molecule 3: ESX-5 secretion system protein EccD5

Chain D2:



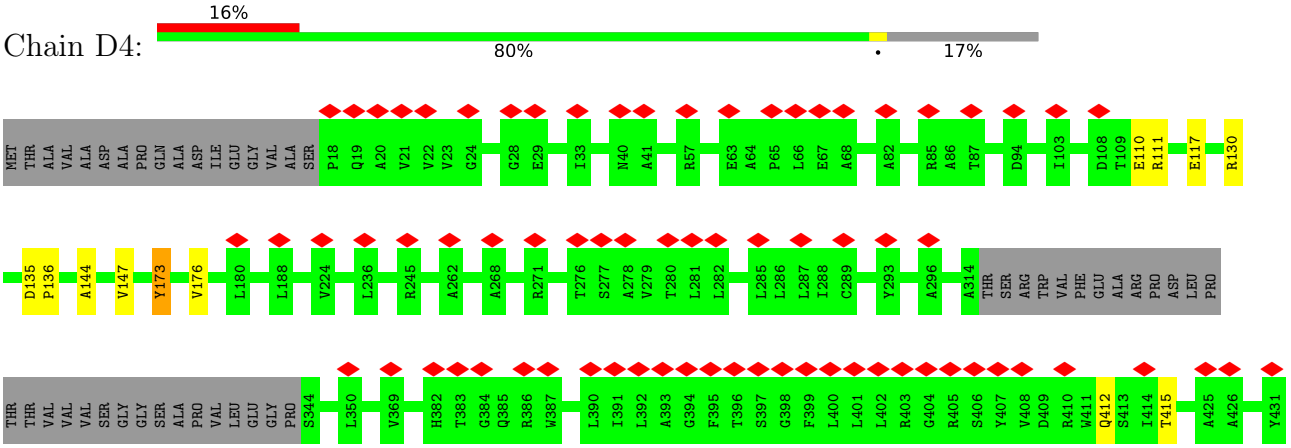
• Molecule 3: ESX-5 secretion system protein EccD5

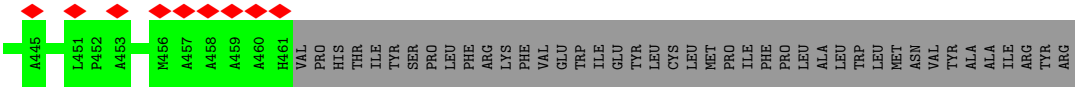
Chain D3:



• Molecule 3: ESX-5 secretion system protein EccD5

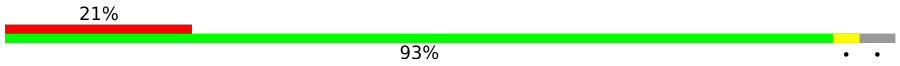
Chain D4:

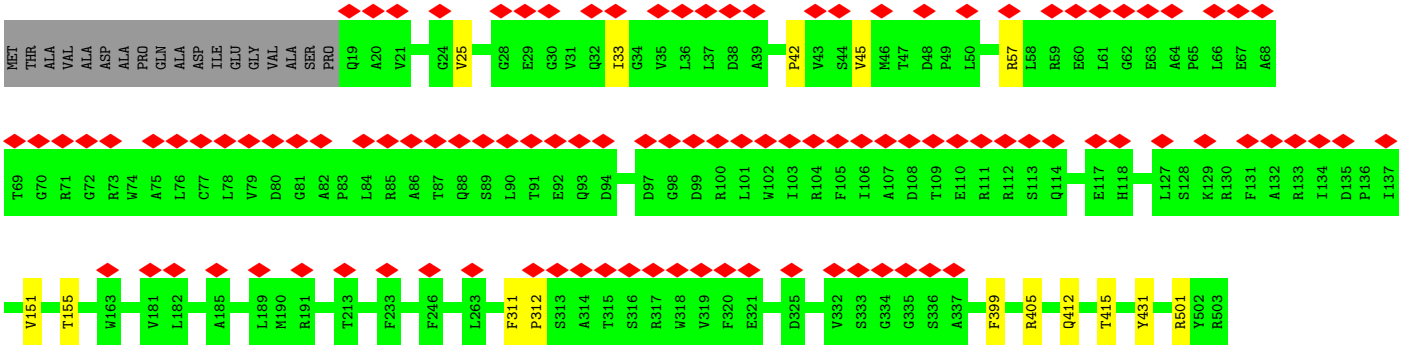




• Molecule 3: ESX-5 secretion system protein EccD5

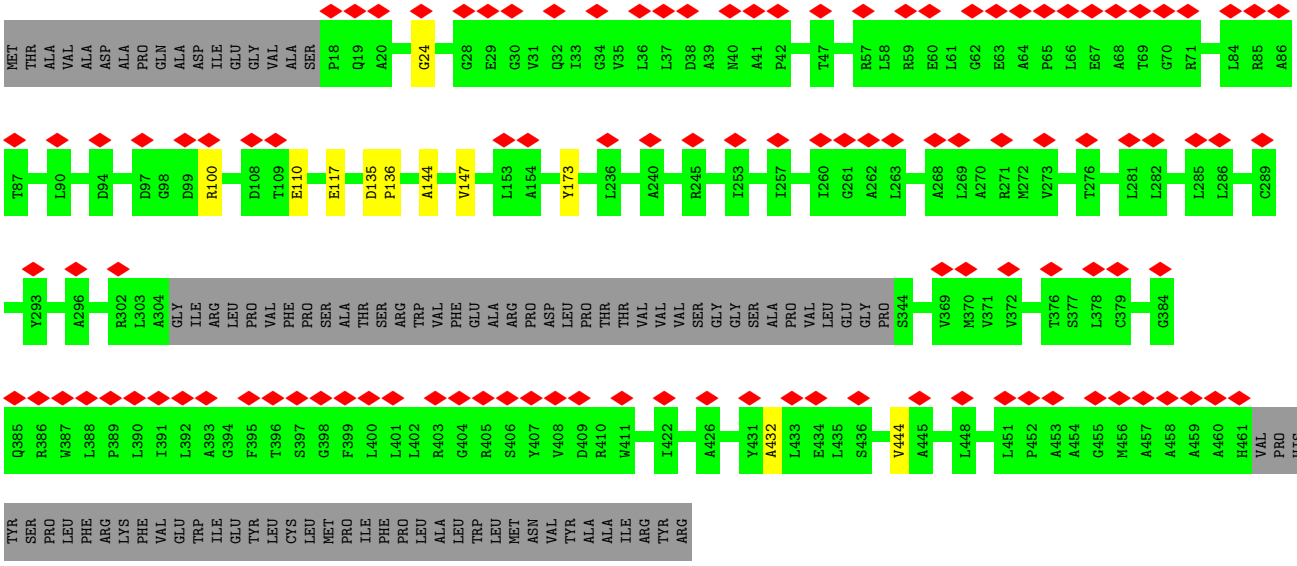
Chain D5:





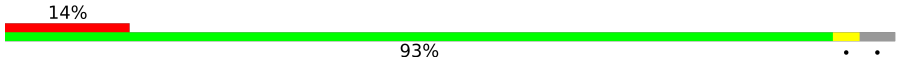
• Molecule 3: ESX-5 secretion system protein EccD5

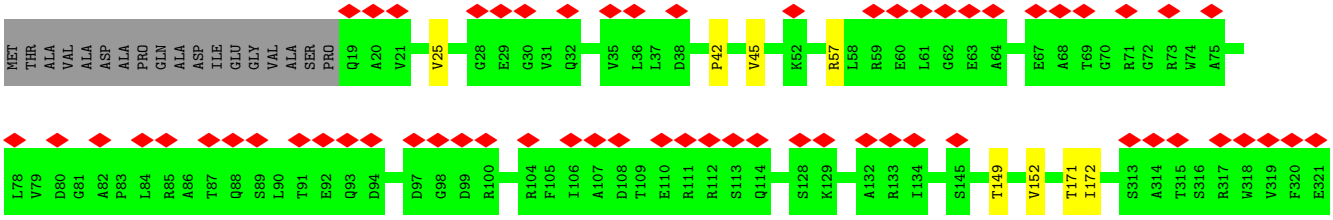
Chain D6:

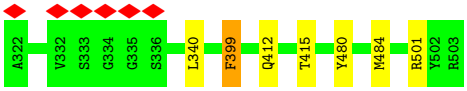


• Molecule 3: ESX-5 secretion system protein EccD5

Chain D7:

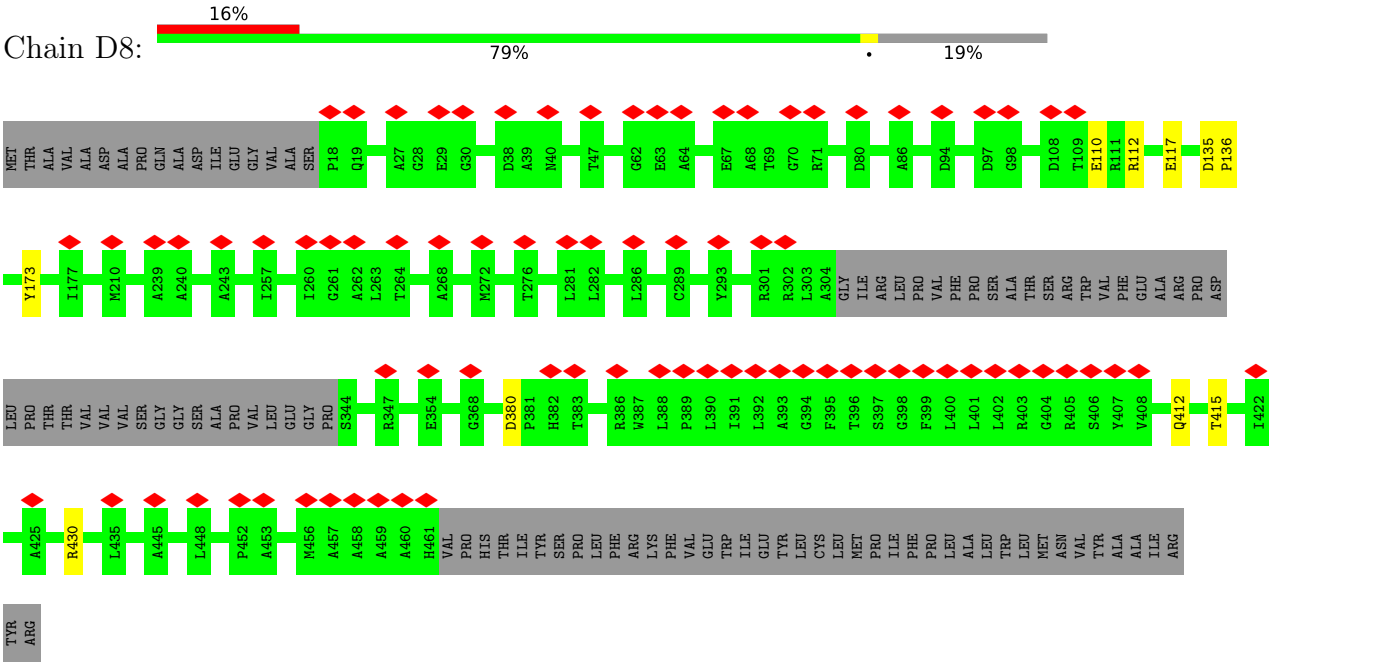






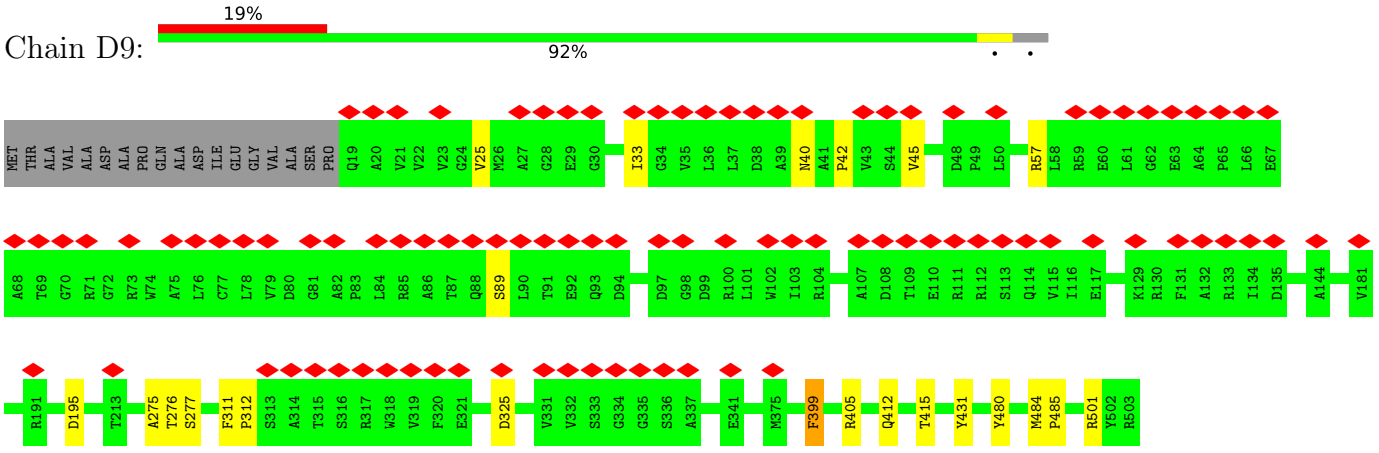
• Molecule 3: ESX-5 secretion system protein EccD5

Chain D8:



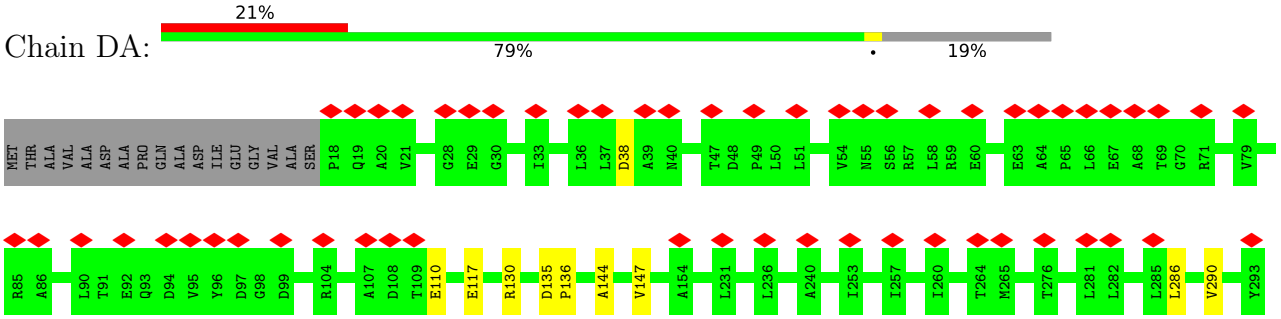
• Molecule 3: ESX-5 secretion system protein EccD5

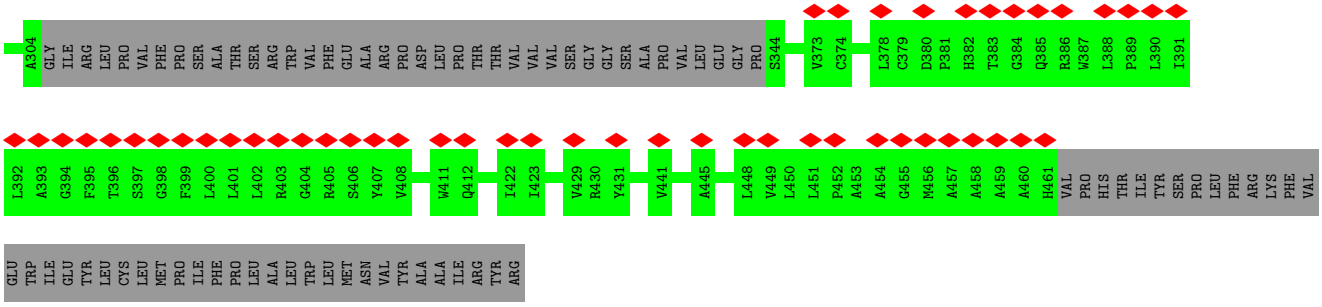
Chain D9:



• Molecule 3: ESX-5 secretion system protein EccD5

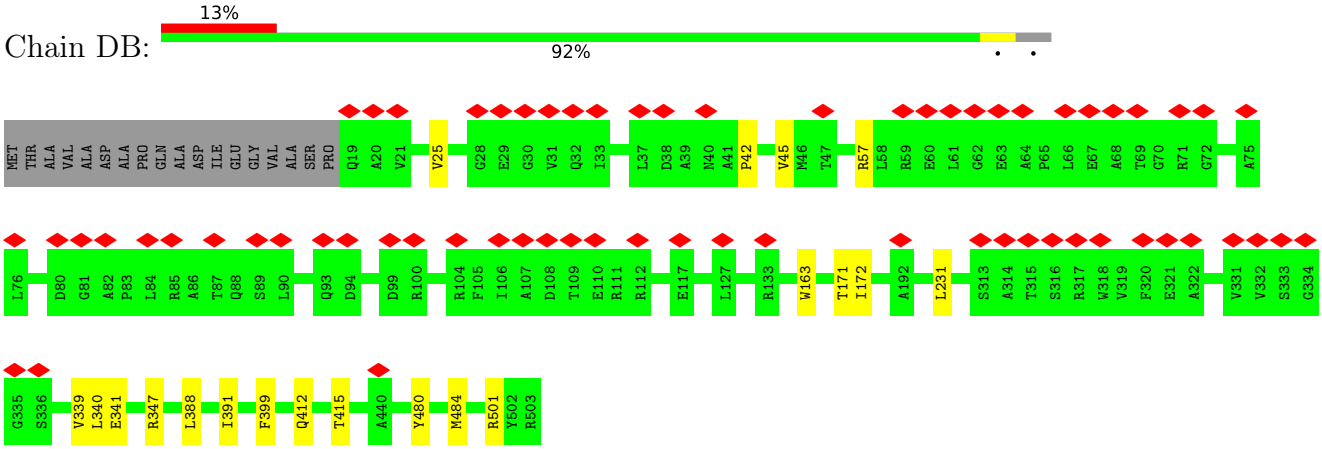
Chain DA:





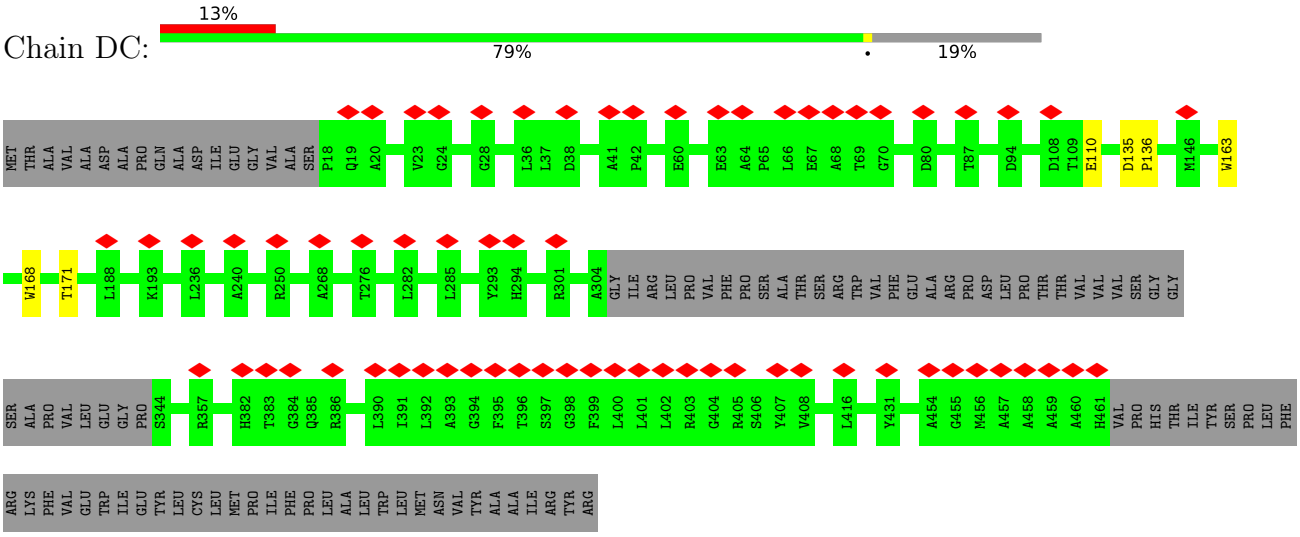
• Molecule 3: ESX-5 secretion system protein EccD5

Chain DB:



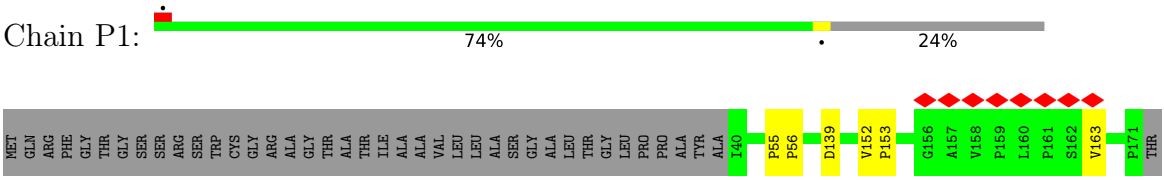
• Molecule 3: ESX-5 secretion system protein EccD5

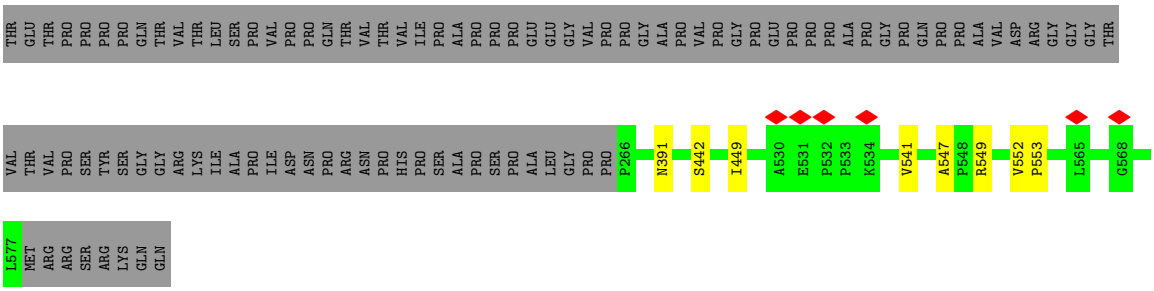
Chain DC:



• Molecule 4: Mycosin-5

Chain P1:



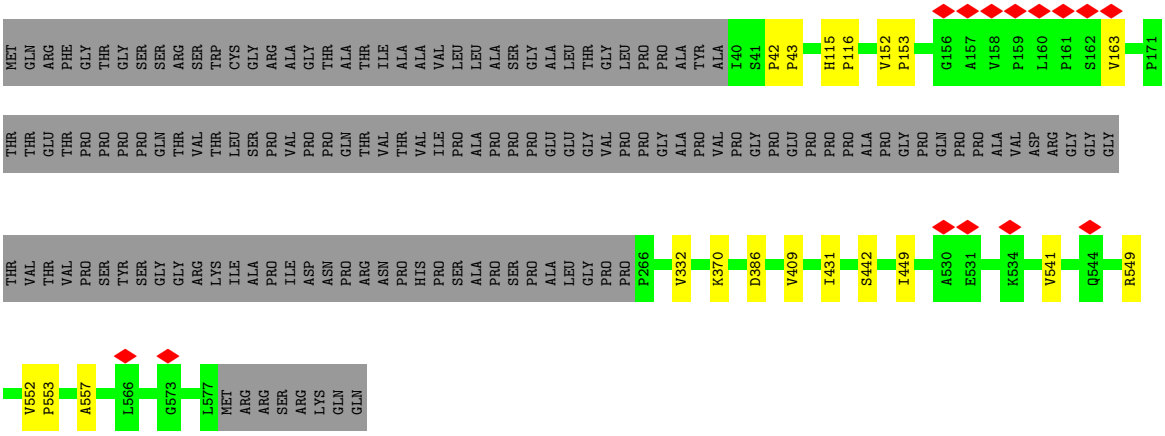


• Molecule 4: Mycosin-5

Chain P2:

• Molecule 4: Mycosin-5

Chain P3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154929	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	59.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	B1	0.71	13/3669 (0.4%)	0.79	11/5028 (0.2%)
1	B2	0.79	21/3669 (0.6%)	0.81	17/5028 (0.3%)
1	B3	0.77	20/3669 (0.5%)	0.80	11/5028 (0.2%)
1	B4	0.44	0/3675	0.64	0/5038
1	B5	0.43	0/3675	0.67	0/5038
1	B6	0.43	0/3675	0.65	0/5038
2	C1	0.34	0/3280	0.64	0/4459
2	C2	0.33	0/3280	0.63	0/4459
2	C3	0.35	0/3280	0.62	0/4459
2	C4	0.35	0/3280	0.61	0/4459
2	C5	0.35	0/3280	0.62	0/4459
2	C6	0.34	0/3280	0.62	0/4459
3	D1	0.37	0/3710	0.61	0/5078
3	D2	0.31	0/3038	0.57	0/4151
3	D3	0.40	0/3710	0.62	0/5078
3	D4	0.31	0/3115	0.58	0/4257
3	D5	0.38	0/3710	0.59	0/5078
3	D6	0.31	0/3038	0.58	0/4151
3	D7	0.40	0/3710	0.63	0/5078
3	D8	0.31	0/3038	0.60	0/4151
3	D9	0.37	0/3710	0.60	0/5078
3	DA	0.31	0/3038	0.57	0/4151
3	DB	0.40	0/3710	0.63	0/5078
3	DC	0.31	0/3038	0.60	0/4151
4	P1	0.57	5/3309 (0.2%)	0.72	4/4545 (0.1%)
4	P2	0.56	3/3309 (0.1%)	0.72	3/4545 (0.1%)
4	P3	0.57	4/3309 (0.1%)	0.73	4/4545 (0.1%)
All	All	0.45	66/92204 (0.1%)	0.65	50/126067 (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
4	P2	0	1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B2	483	ARG	CZ-NH1	-8.53	1.22	1.33
1	B2	483	ARG	CZ-NH2	-8.30	1.22	1.33
1	B1	483	ARG	CZ-NH1	-8.14	1.22	1.33
1	B1	103	ARG	CZ-NH1	-8.11	1.22	1.33
1	B1	103	ARG	CZ-NH2	-8.10	1.22	1.33

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B1	103	ARG	CA-CB-CG	7.17	129.18	113.40
4	P3	549	ARG	CD-NE-CZ	7.01	133.42	123.60
1	B2	103	ARG	CA-CB-CG	6.82	128.40	113.40
1	B2	105	TYR	CB-CG-CD2	6.60	124.96	121.00
1	B1	99	ARG	CD-NE-CZ	6.44	132.62	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	P2	444	ARG	Sidechain

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	B1	3587	3631	3626	6	0
1	B2	3587	3631	3626	11	0
1	B3	3587	3631	3626	9	0
1	B4	3591	3621	3618	16	0
1	B5	3591	3621	3618	9	0
1	B6	3591	3621	3618	15	0
2	C1	3190	3145	3142	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C2	3190	3145	3142	8	0
2	C3	3190	3145	3142	10	0
2	C4	3190	3145	3142	10	0
2	C5	3190	3145	3142	13	0
2	C6	3190	3145	3142	9	0
3	D1	3635	3823	3822	12	0
3	D2	2989	3166	3163	6	0
3	D3	3635	3824	3822	6	0
3	D4	3063	3245	3243	7	0
3	D5	3635	3824	3822	5	0
3	D6	2989	3166	3163	5	0
3	D7	3635	3824	3822	8	0
3	D8	2989	3165	3163	5	0
3	D9	3635	3824	3822	13	0
3	DA	2989	3167	3163	5	0
3	DB	3635	3824	3822	11	0
3	DC	2989	3165	3163	3	0
4	P1	3226	3219	3218	6	0
4	P2	3226	3219	3218	5	0
4	P3	3226	3219	3218	11	0
All	All	90170	92300	92228	217	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 1.

The worst 5 of 217 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)
2:C4:130:ARG:NH2	3:DA:110:GLU:OE2	2.22	0.72
2:C1:130:ARG:NH2	3:D8:110:GLU:OE2	2.22	0.72
2:C2:130:ARG:NH2	3:D6:110:GLU:OE2	2.25	0.70
2:C3:130:ARG:NH2	3:DC:110:GLU:OE2	2.26	0.69
4:P1:552:VAL:HG23	4:P1:553:PRO:HD3	1.75	0.69

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	B1	470/506 (93%)	457 (97%)	13 (3%)	0	100	100
1	B2	470/506 (93%)	464 (99%)	6 (1%)	0	100	100
1	B3	470/506 (93%)	456 (97%)	14 (3%)	0	100	100
1	B4	476/506 (94%)	469 (98%)	7 (2%)	0	100	100
1	B5	476/506 (94%)	468 (98%)	8 (2%)	0	100	100
1	B6	476/506 (94%)	467 (98%)	9 (2%)	0	100	100
2	C1	402/1391 (29%)	390 (97%)	11 (3%)	1 (0%)	47	80
2	C2	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	47	80
2	C3	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	47	80
2	C4	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	47	80
2	C5	402/1391 (29%)	391 (97%)	10 (2%)	1 (0%)	47	80
2	C6	402/1391 (29%)	392 (98%)	9 (2%)	1 (0%)	47	80
3	D1	483/503 (96%)	477 (99%)	6 (1%)	0	100	100
3	D2	401/503 (80%)	395 (98%)	6 (2%)	0	100	100
3	D3	483/503 (96%)	471 (98%)	12 (2%)	0	100	100
3	D4	411/503 (82%)	403 (98%)	8 (2%)	0	100	100
3	D5	483/503 (96%)	475 (98%)	8 (2%)	0	100	100
3	D6	401/503 (80%)	392 (98%)	9 (2%)	0	100	100
3	D7	483/503 (96%)	472 (98%)	11 (2%)	0	100	100
3	D8	401/503 (80%)	393 (98%)	8 (2%)	0	100	100
3	D9	483/503 (96%)	475 (98%)	8 (2%)	0	100	100
3	DA	401/503 (80%)	394 (98%)	7 (2%)	0	100	100
3	DB	483/503 (96%)	474 (98%)	9 (2%)	0	100	100
3	DC	401/503 (80%)	392 (98%)	9 (2%)	0	100	100
4	P1	440/585 (75%)	422 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	P2	440/585 (75%)	425 (97%)	15 (3%)	0	100 100
4	P3	440/585 (75%)	423 (96%)	17 (4%)	0	100 100
All	All	11884/19173 (62%)	11613 (98%)	265 (2%)	6 (0%)	54 84

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C2	155	GLY
2	C1	155	GLY
2	C3	155	GLY
2	C4	155	GLY
2	C5	155	GLY

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 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	B1	390/411 (95%)	389 (100%)	1 (0%)	92 95
1	B2	390/411 (95%)	388 (100%)	2 (0%)	88 93
1	B3	390/411 (95%)	389 (100%)	1 (0%)	92 95
1	B4	389/411 (95%)	384 (99%)	5 (1%)	69 82
1	B5	389/411 (95%)	385 (99%)	4 (1%)	76 86
1	B6	389/411 (95%)	387 (100%)	2 (0%)	88 93
2	C1	342/1137 (30%)	340 (99%)	2 (1%)	86 91
2	C2	342/1137 (30%)	339 (99%)	3 (1%)	78 88
2	C3	342/1137 (30%)	340 (99%)	2 (1%)	86 91
2	C4	342/1137 (30%)	338 (99%)	4 (1%)	71 84
2	C5	342/1137 (30%)	337 (98%)	5 (2%)	65 80
2	C6	342/1137 (30%)	339 (99%)	3 (1%)	78 88
3	D1	381/393 (97%)	376 (99%)	5 (1%)	69 82
3	D2	311/393 (79%)	310 (100%)	1 (0%)	92 95

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D3	381/393 (97%)	377 (99%)	4 (1%)	76 86
3	D4	319/393 (81%)	317 (99%)	2 (1%)	86 91
3	D5	381/393 (97%)	376 (99%)	5 (1%)	69 82
3	D6	311/393 (79%)	309 (99%)	2 (1%)	86 91
3	D7	381/393 (97%)	377 (99%)	4 (1%)	76 86
3	D8	311/393 (79%)	309 (99%)	2 (1%)	86 91
3	D9	381/393 (97%)	376 (99%)	5 (1%)	69 82
3	DA	311/393 (79%)	309 (99%)	2 (1%)	86 91
3	DB	381/393 (97%)	377 (99%)	4 (1%)	76 86
3	DC	311/393 (79%)	310 (100%)	1 (0%)	92 95
4	P1	343/453 (76%)	341 (99%)	2 (1%)	86 91
4	P2	343/453 (76%)	341 (99%)	2 (1%)	86 91
4	P3	343/453 (76%)	343 (100%)	0	100 100
All	All	9578/15363 (62%)	9503 (99%)	75 (1%)	82 89

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D8	117	GLU
4	P1	139	ASP
3	D9	57	ARG
3	DA	130	ARG
2	C4	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
3	DB	165	HIS
4	P1	391	ASN
3	DB	464	HIS
4	P2	283	GLN
3	D1	461	HIS

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.

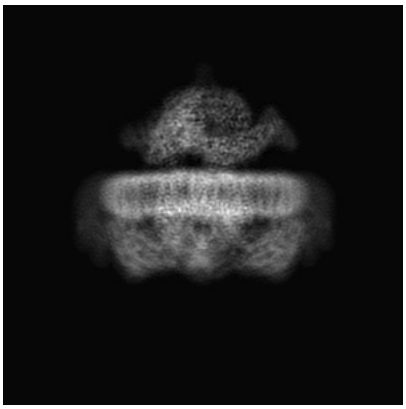
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12514. These allow visual inspection of the internal detail of the map and identification of artifacts.

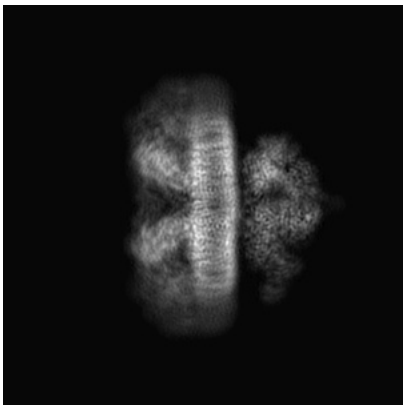
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

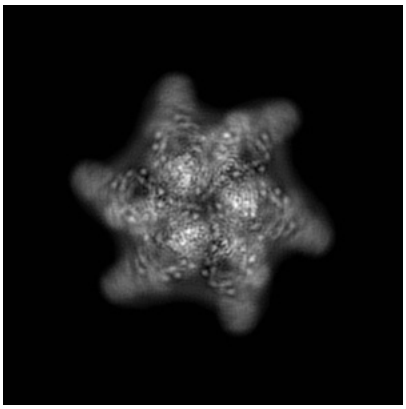
6.1.1 Primary map



X

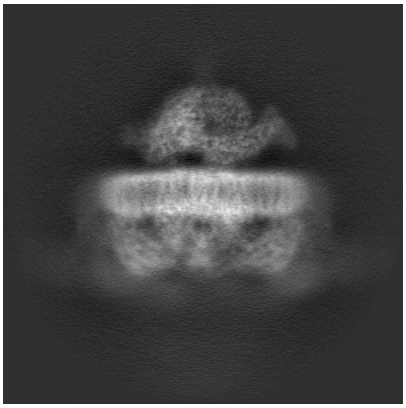


Y

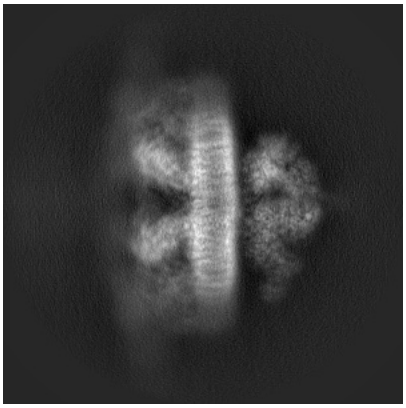


Z

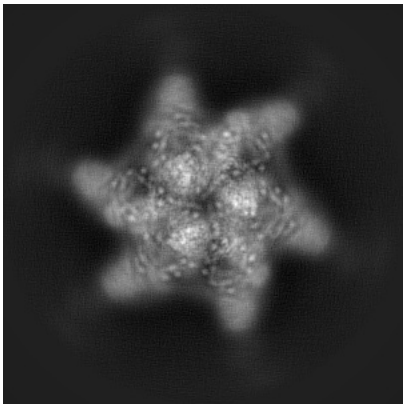
6.1.2 Raw map



X



Y



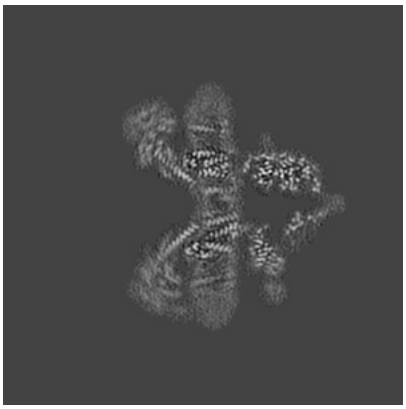
Z

The images above show the map projected in three orthogonal directions.

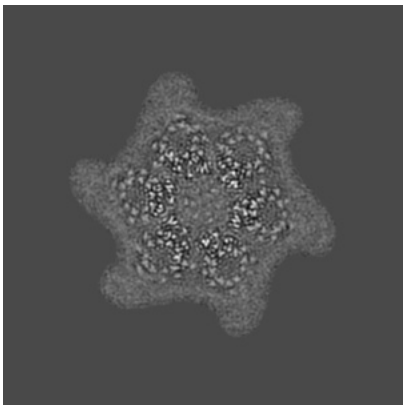
6.2 Central slices (i)

6.2.1 Primary map

X Index: 200

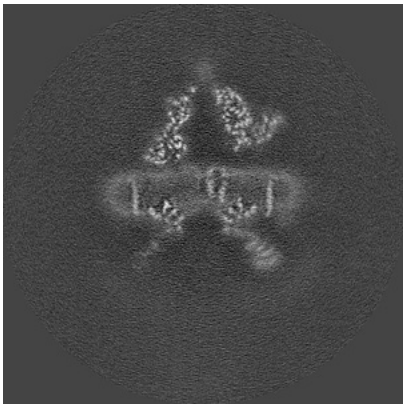


Y Index: 200

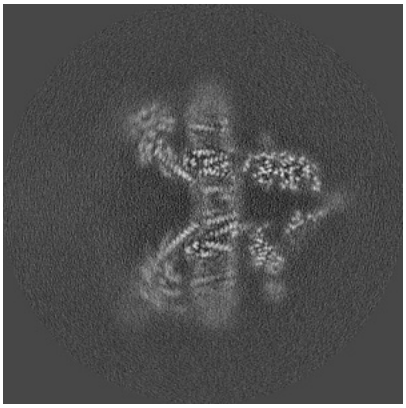


Z Index: 200

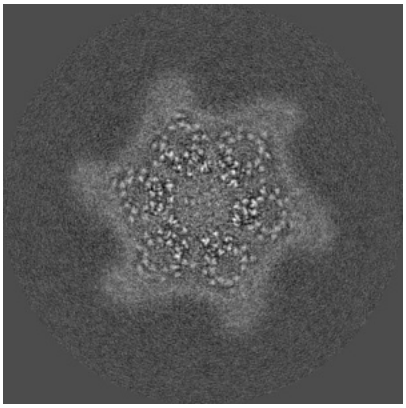
6.2.2 Raw map



X Index: 200



Y Index: 200

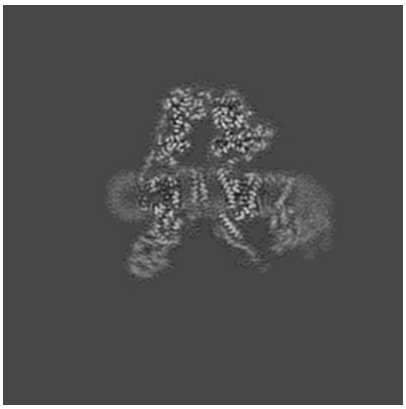


Z Index: 200

The images above show central slices of the map in three orthogonal directions.

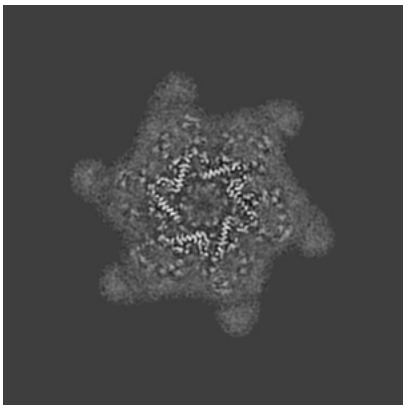
6.3 Largest variance slices (i)

6.3.1 Primary map



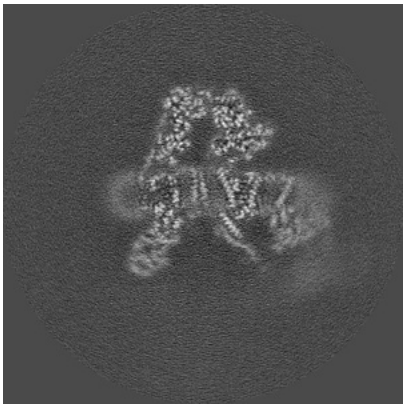
X Index: 184

Y Index: 199

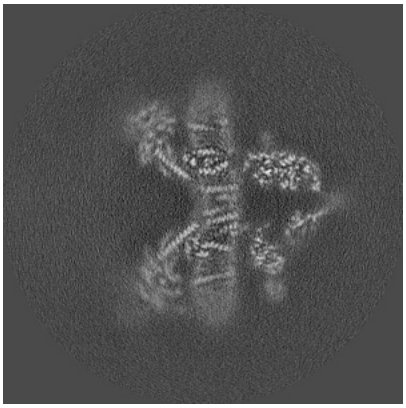


Z Index: 192

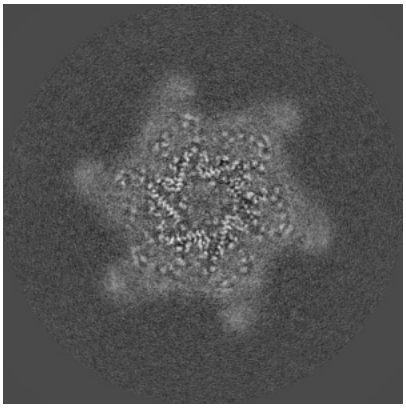
6.3.2 Raw map



X Index: 184



Y Index: 199



Z Index: 193

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

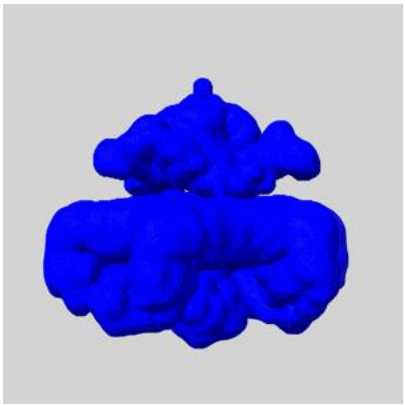
6.5 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

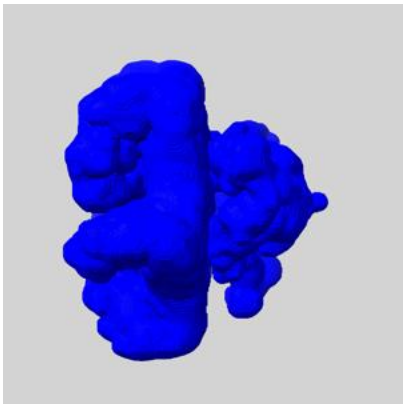
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

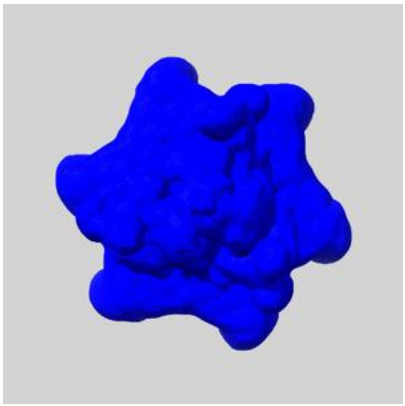
6.5.1 emd_12514_msk_1.map



X



Y

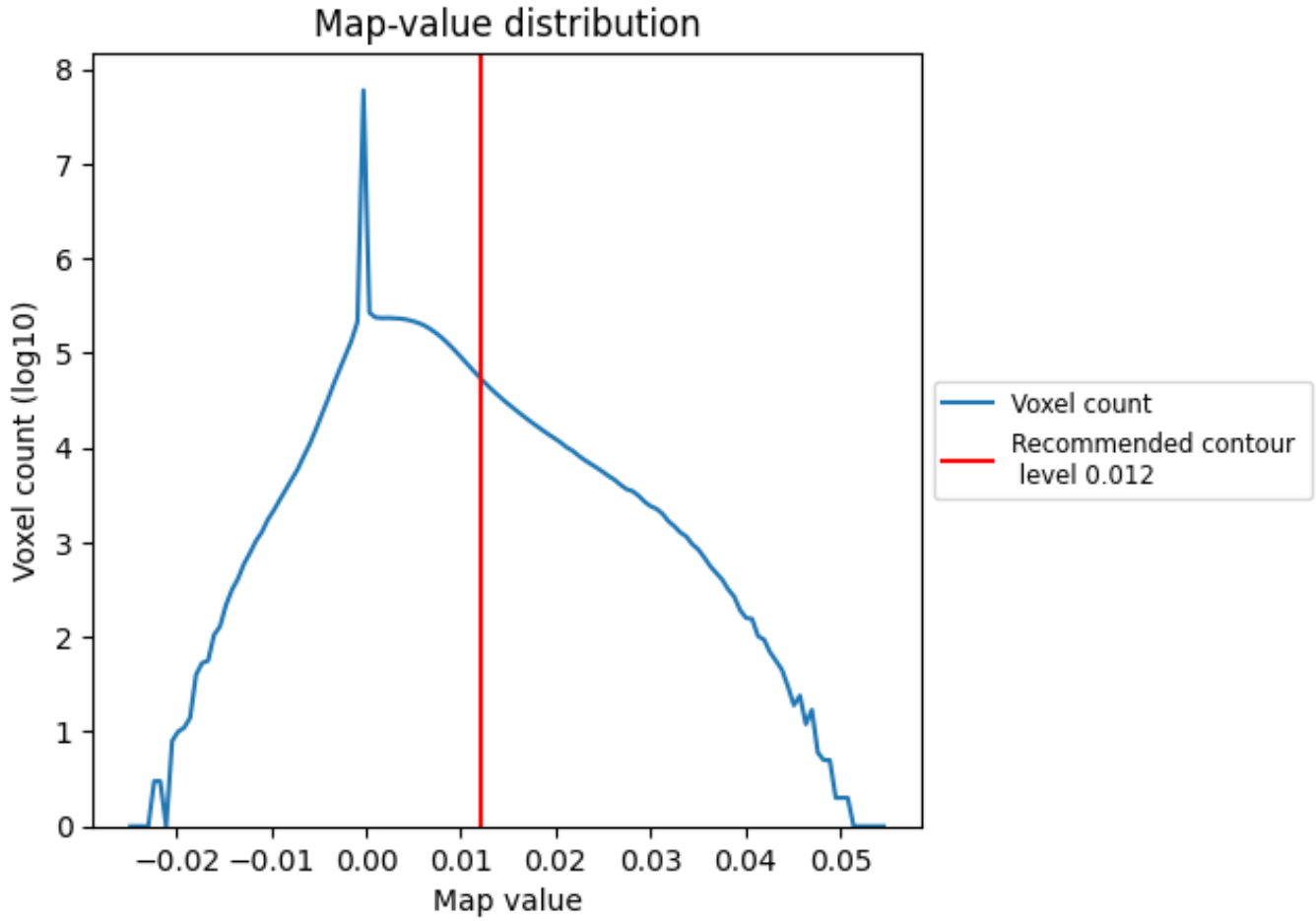


Z

7 Map analysis

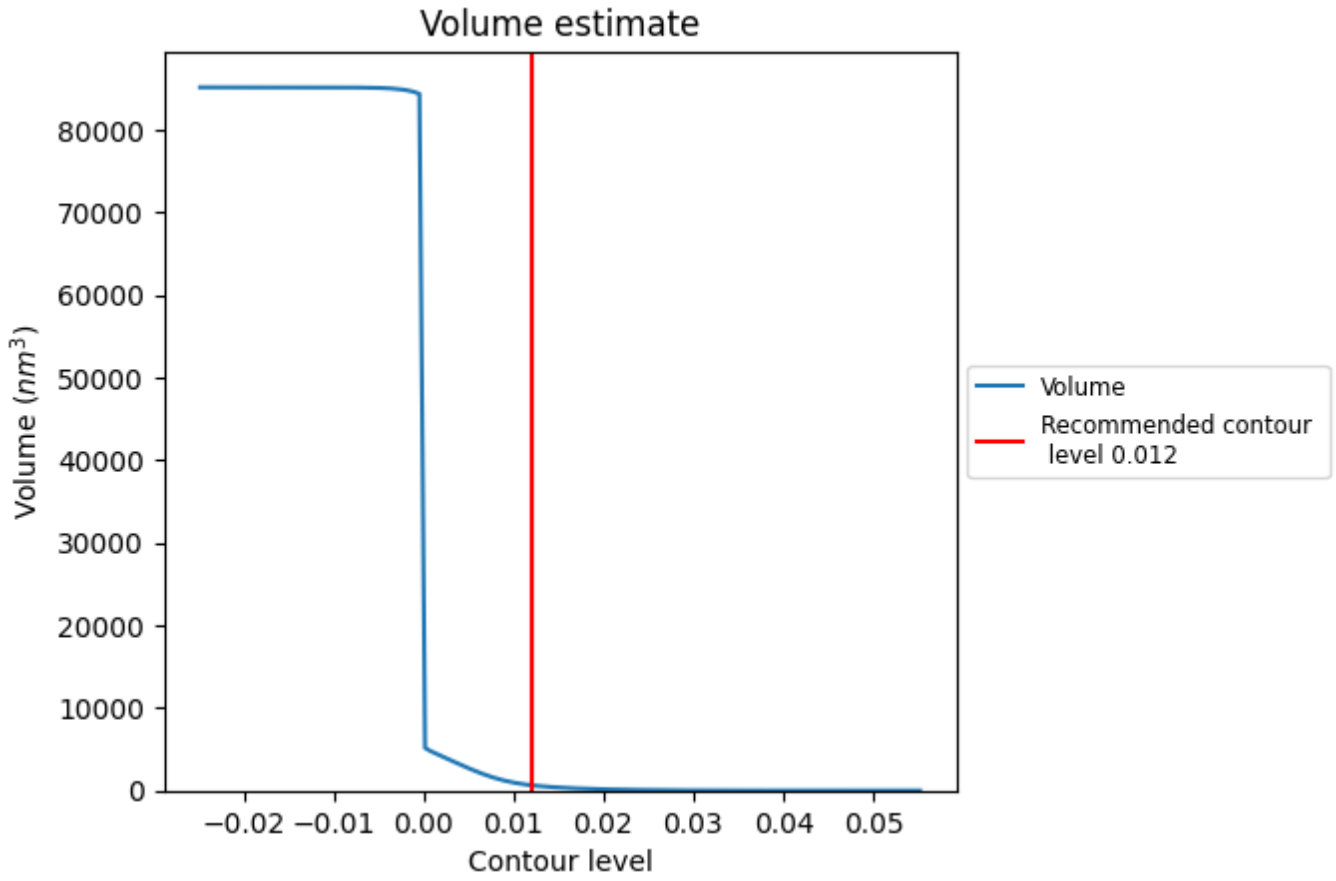
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

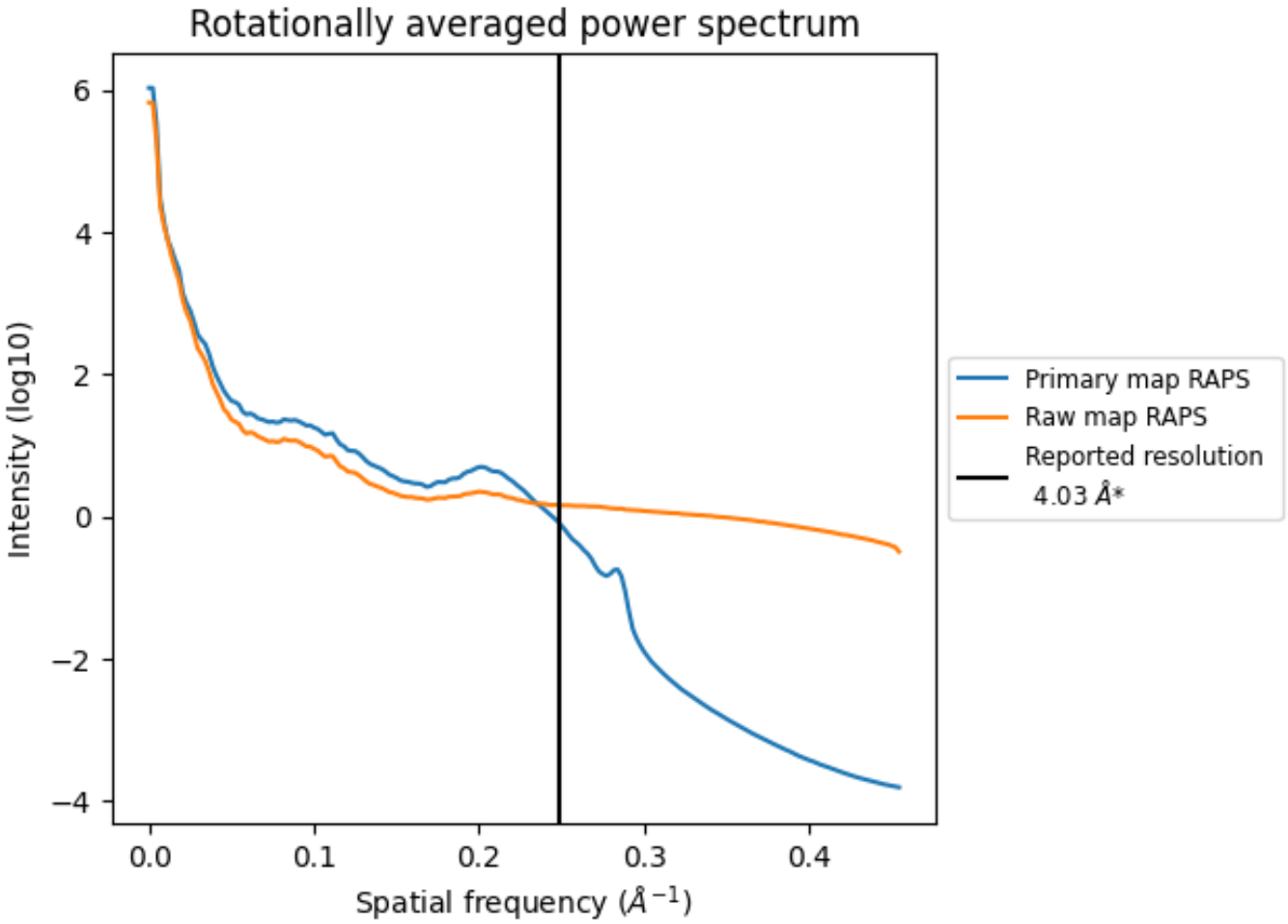
7.2 Volume estimate (i)



The volume at the recommended contour level is 643 nm^3; this corresponds to an approximate mass of 581 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

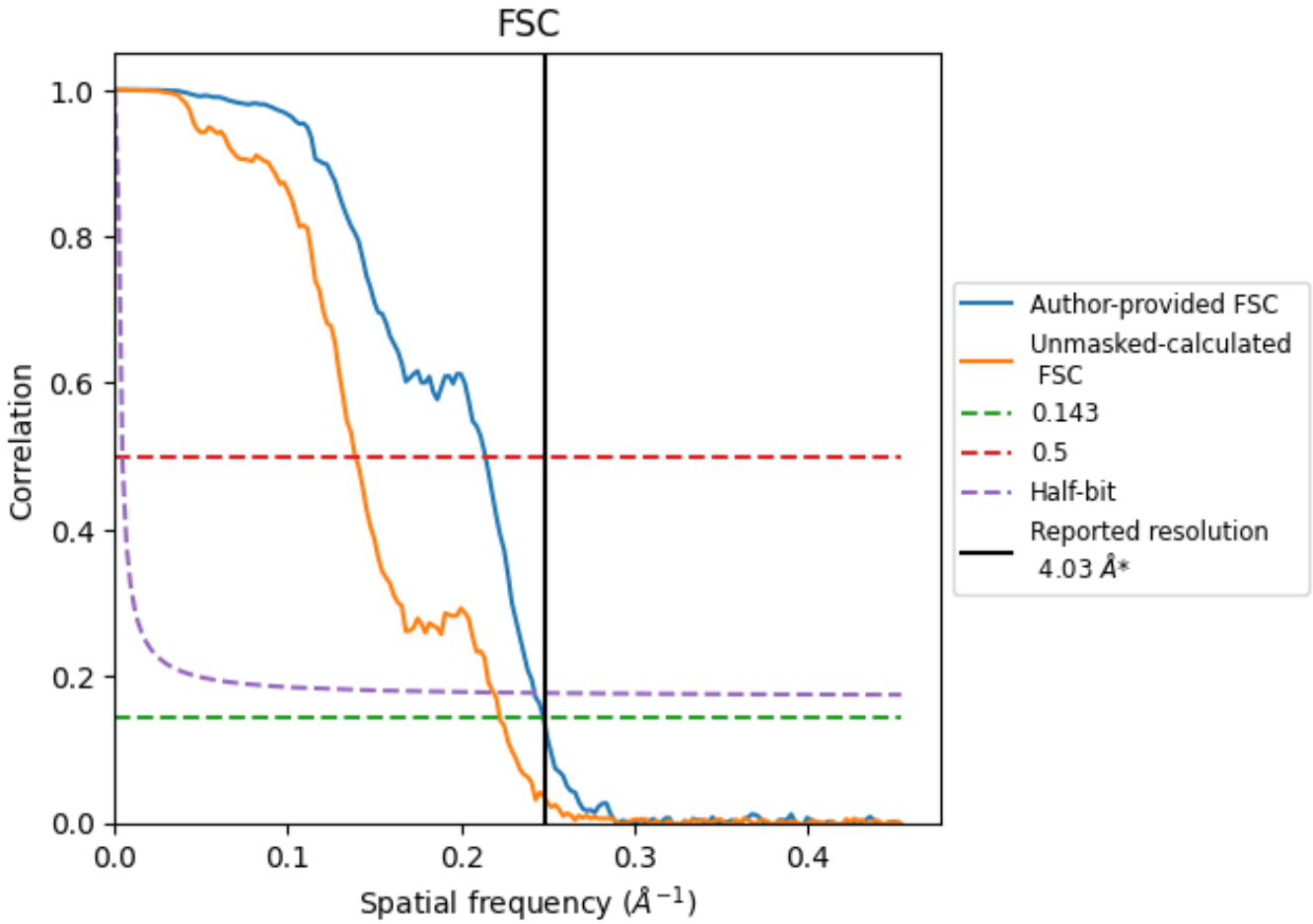


*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.248 Å^{-1}

8.2 Resolution estimates (i)

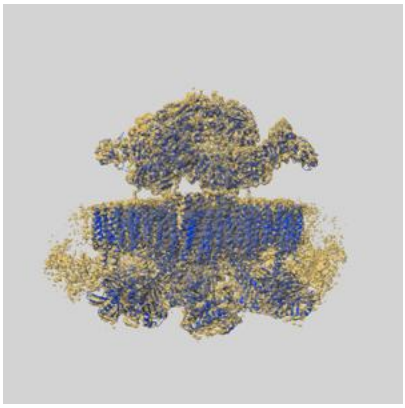
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.03	-	-
Author-provided FSC curve	4.04	4.67	4.12
Unmasked-calculated*	4.49	7.19	4.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.49 differs from the reported value 4.03 by more than 10 %

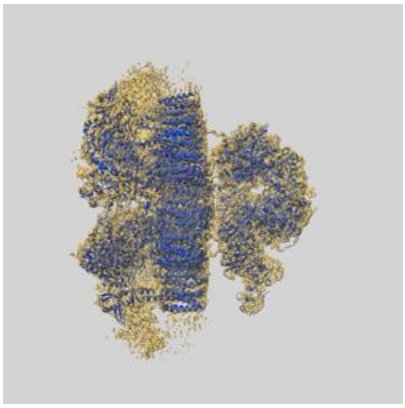
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12514 and PDB model 7NP7. Per-residue inclusion information can be found in section 3 on page 6.

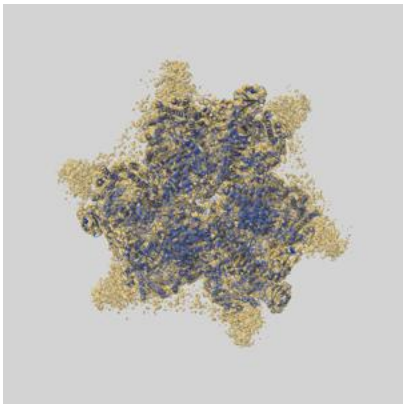
9.1 Map-model overlay



X



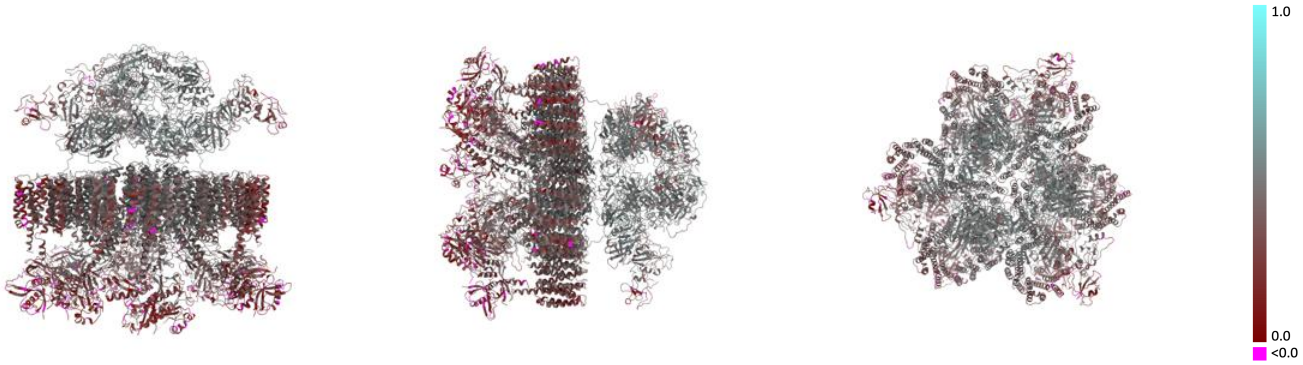
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

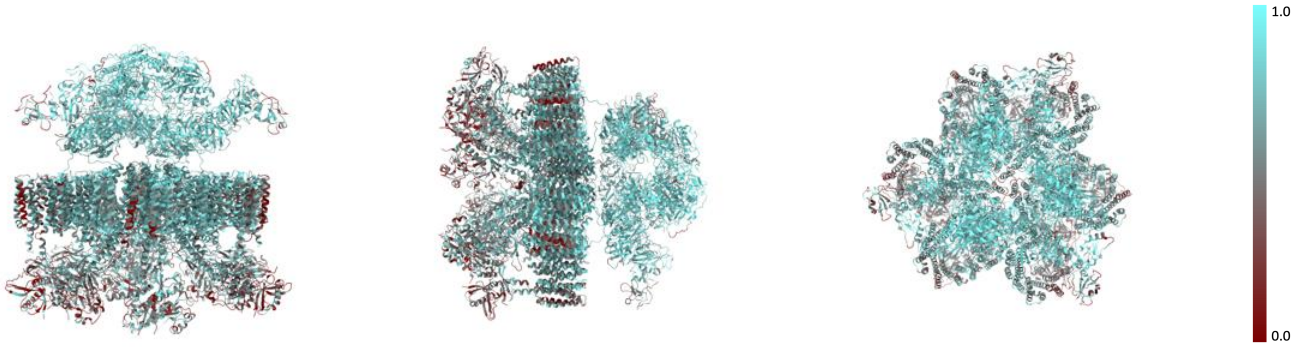
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

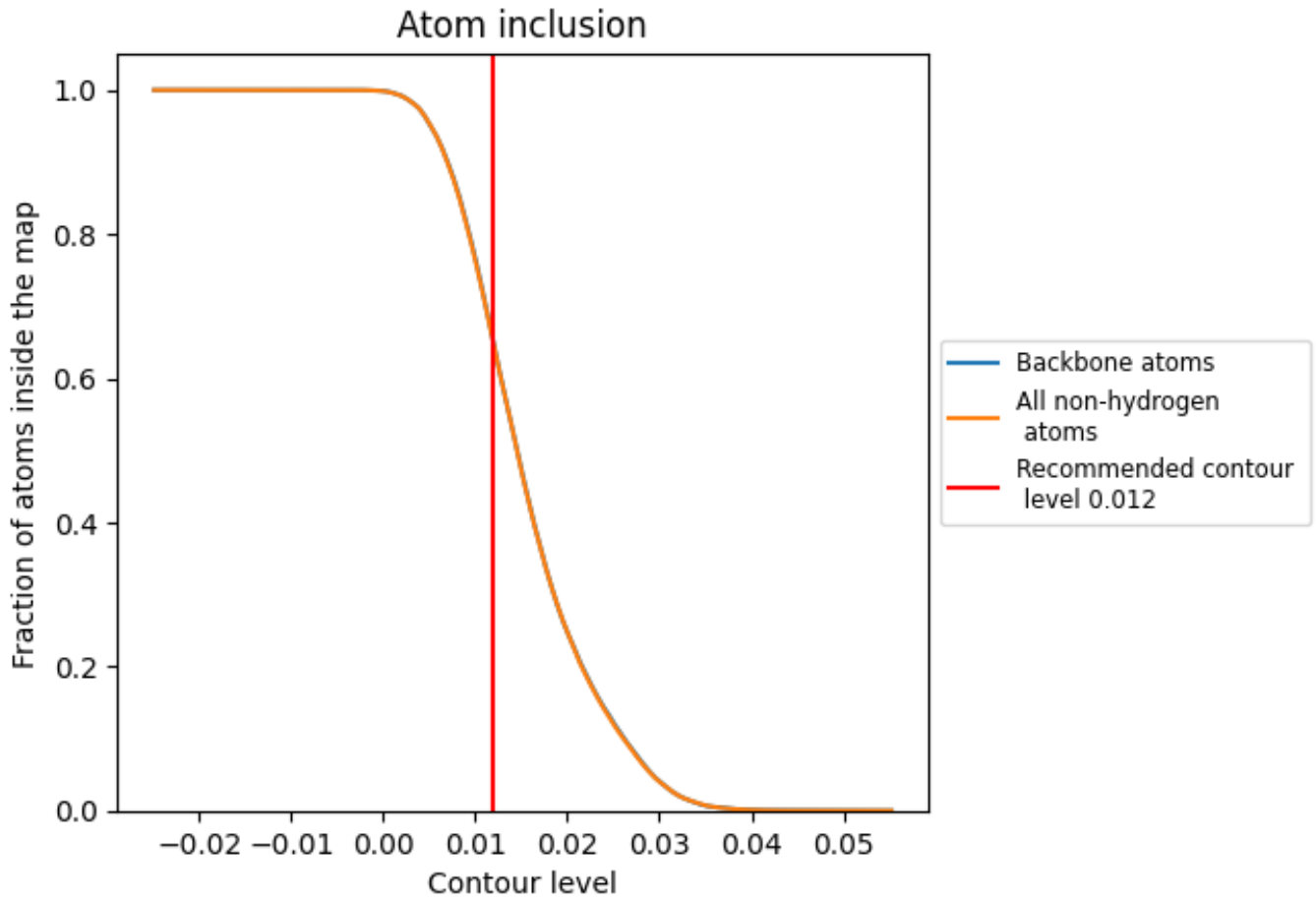
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6473	0.3830
B1	0.7562	0.4350
B2	0.7525	0.4340
B3	0.7459	0.4370
B4	0.8016	0.4640
B5	0.7987	0.4670
B6	0.8042	0.4690
C1	0.5940	0.3420
C2	0.5032	0.3010
C3	0.5959	0.3340
C4	0.4955	0.2960
C5	0.5969	0.3310
C6	0.4968	0.3000
D1	0.6134	0.3480
D2	0.5509	0.3160
D3	0.6817	0.4000
D4	0.5985	0.3450
D5	0.6089	0.3480
D6	0.5458	0.3110
D7	0.6817	0.3960
D8	0.5992	0.3530
D9	0.6064	0.3490
DA	0.5550	0.3150
DB	0.6843	0.4000
DC	0.5989	0.3430
P1	0.8189	0.4760
P2	0.8126	0.4760
P3	0.8142	0.4780