



wwPDB EM Validation Summary Report ⓘ

Dec 19, 2022 – 12:55 pm GMT

PDB ID : 7NPR
EMDB ID : EMD-12517
Title : Structure of an intact ESX-5 inner membrane complex, Composite C3 model
Authors : Fahrenkamp, D.; Bunduc, C.M.; Wald, J.; Ummels, R.; Bitter, W.; Houben, E.N.G.; Marlovits, T.C.
Deposited on : 2021-02-28
Resolution : 3.82 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:

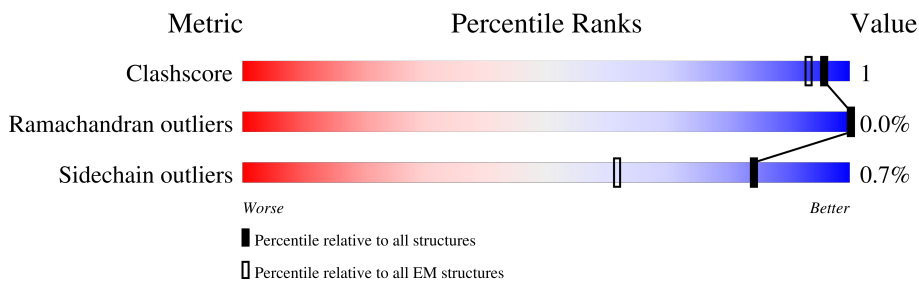
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 3.82 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.







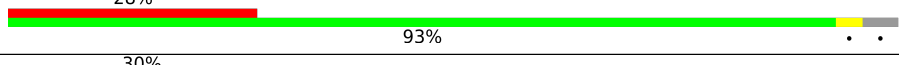
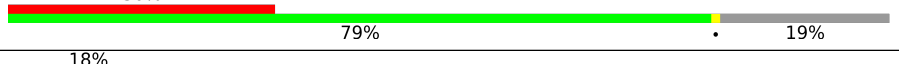
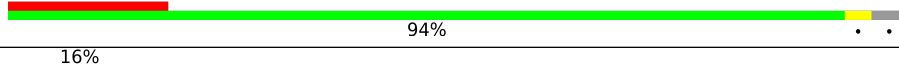

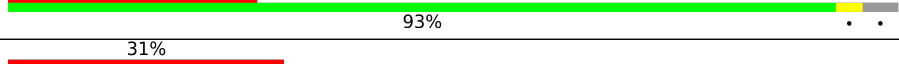

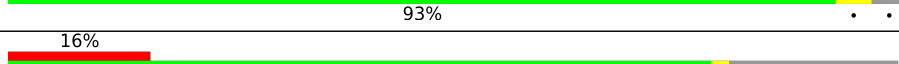
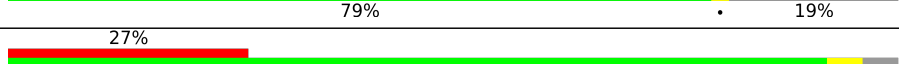
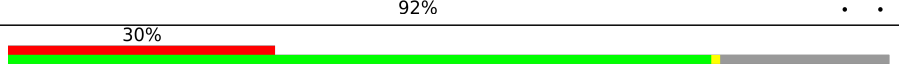
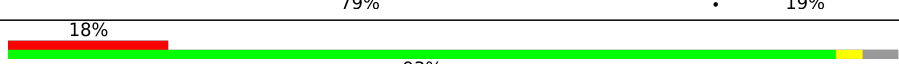
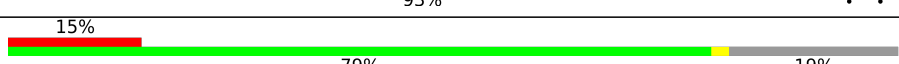
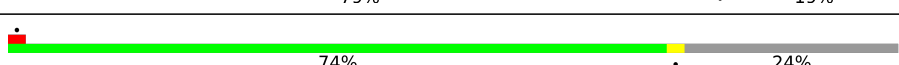
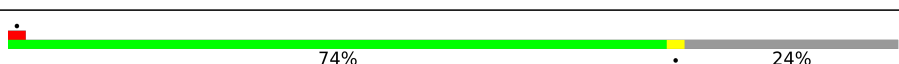
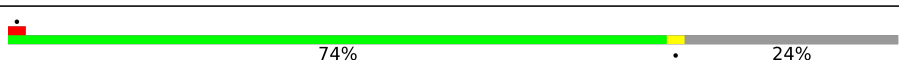

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$. 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	10% (red), 91% (green), 6% (grey)
1	B2	506	10% (red), 91% (green), 6% (grey)
1	B3	506	10% (red), 92% (green), 6% (grey)
1	B4	506	~1% (red), 92% (green), 5% (grey)
1	B5	506	~1% (red), 92% (green), 5% (grey)
1	B6	506	~1% (red), 93% (green), 5% (grey)
2	C1	1391	7% (red), 28% (green), 71% (grey)
2	C2	1391	12% (red), 28% (green), 71% (grey)

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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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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
			Total	C	H	N	O	S		
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		

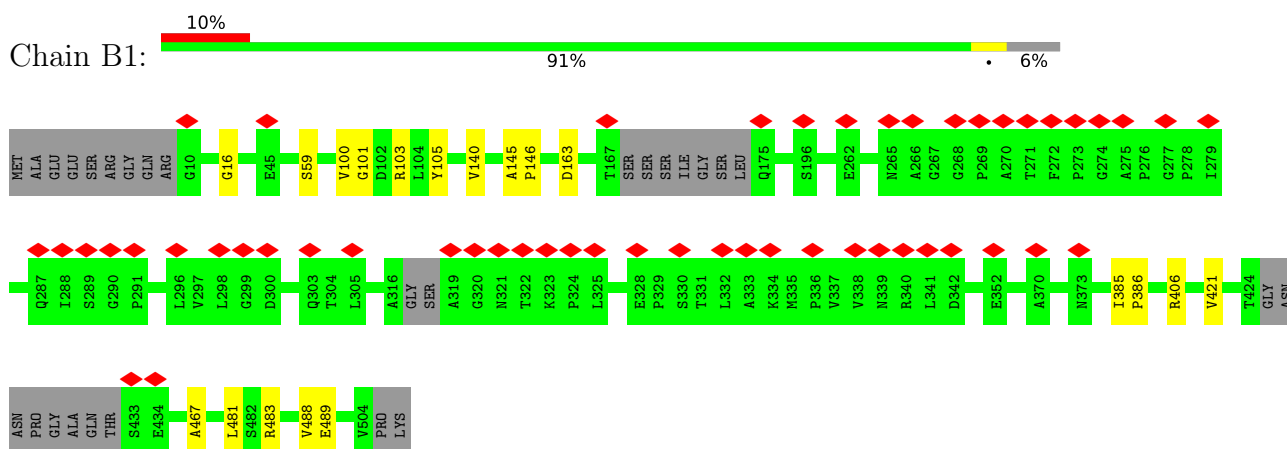
- Molecule 4 is a protein called Mycosin-5.

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		

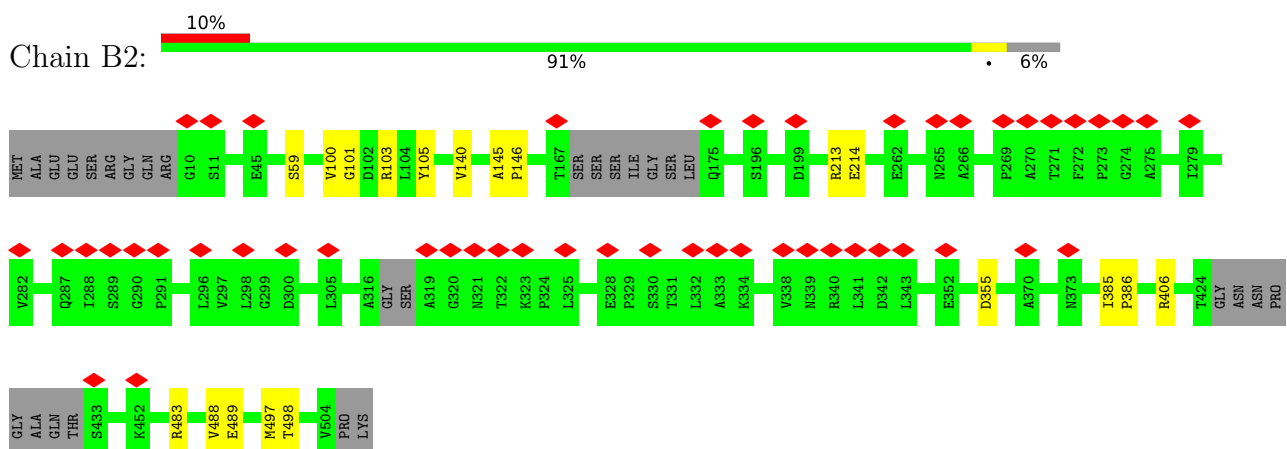
3 Residue-property plots [i](#)

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.

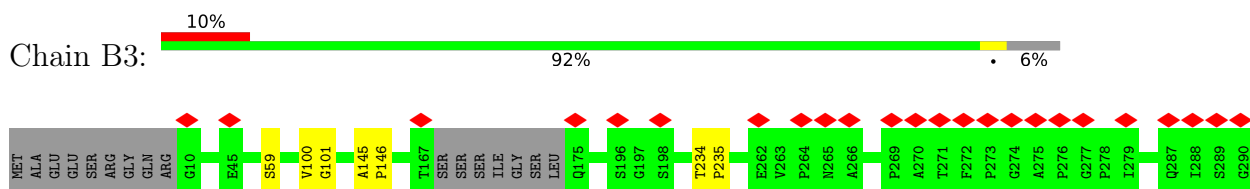
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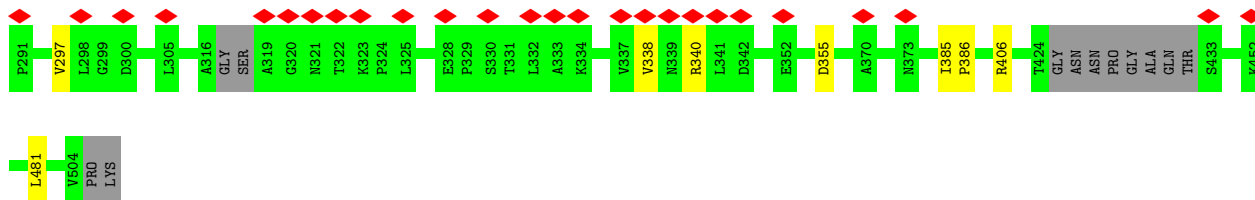


- Molecule 1: ESX-5 secretion system ATPase EccB5

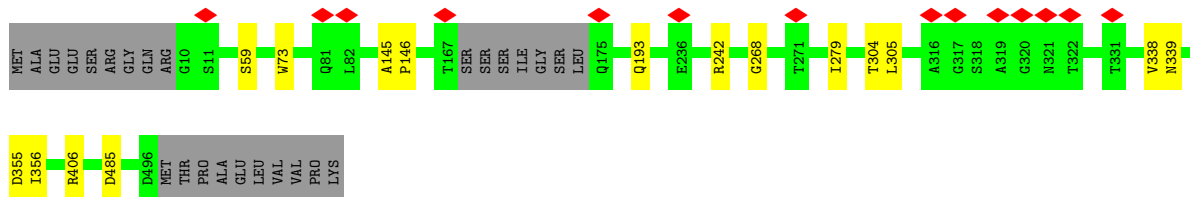


- Molecule 1: ESX-5 secretion system ATPase EccB5

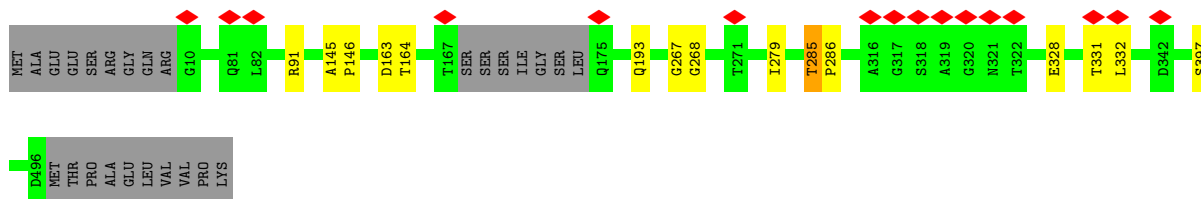




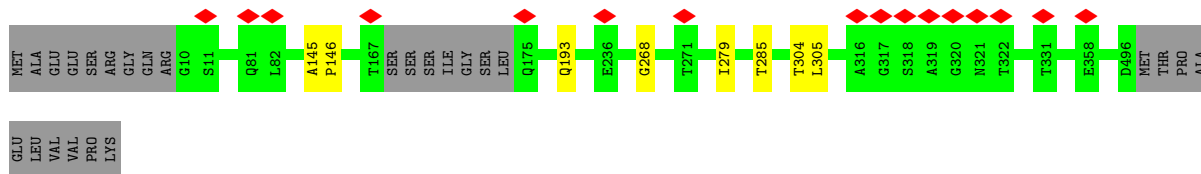
• Molecule 1: ESX-5 secretion system ATPase EccB5



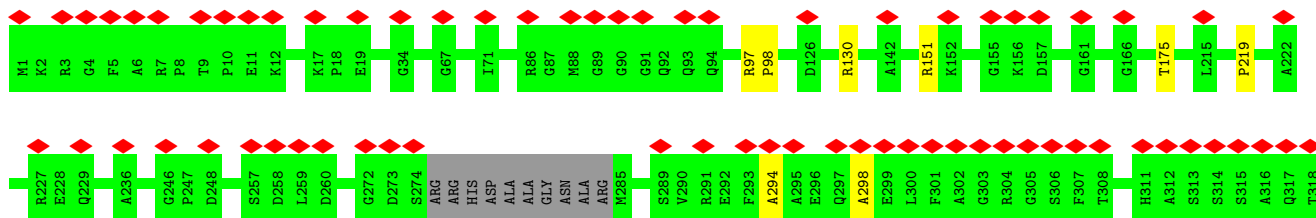
• Molecule 1: ESX-5 secretion system ATPase EccB5

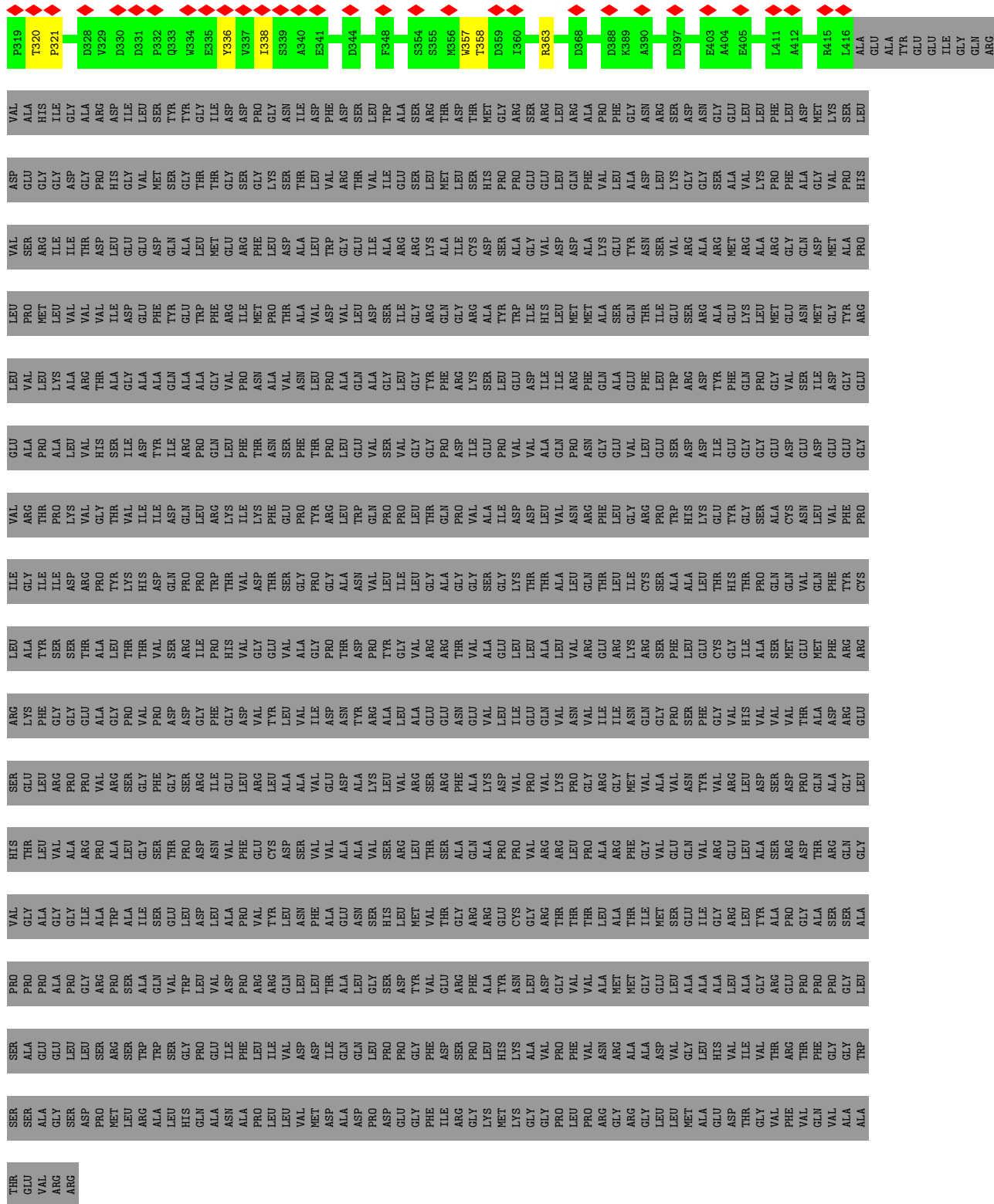


• Molecule 1: ESX-5 secretion system ATPase EccB5



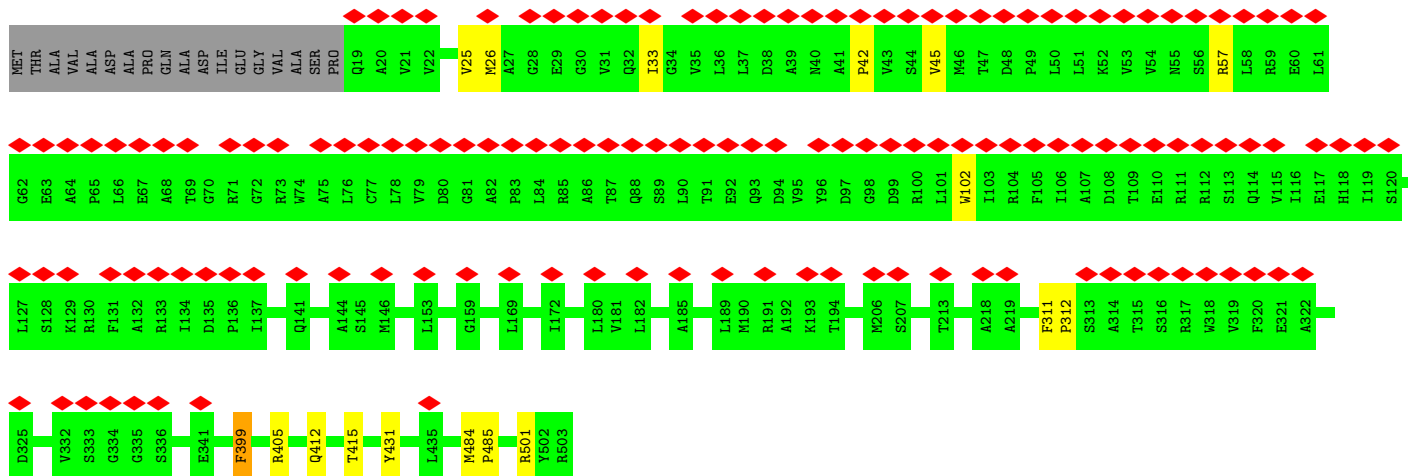
• Molecule 2: ESX-5 secretion system protein EccC5



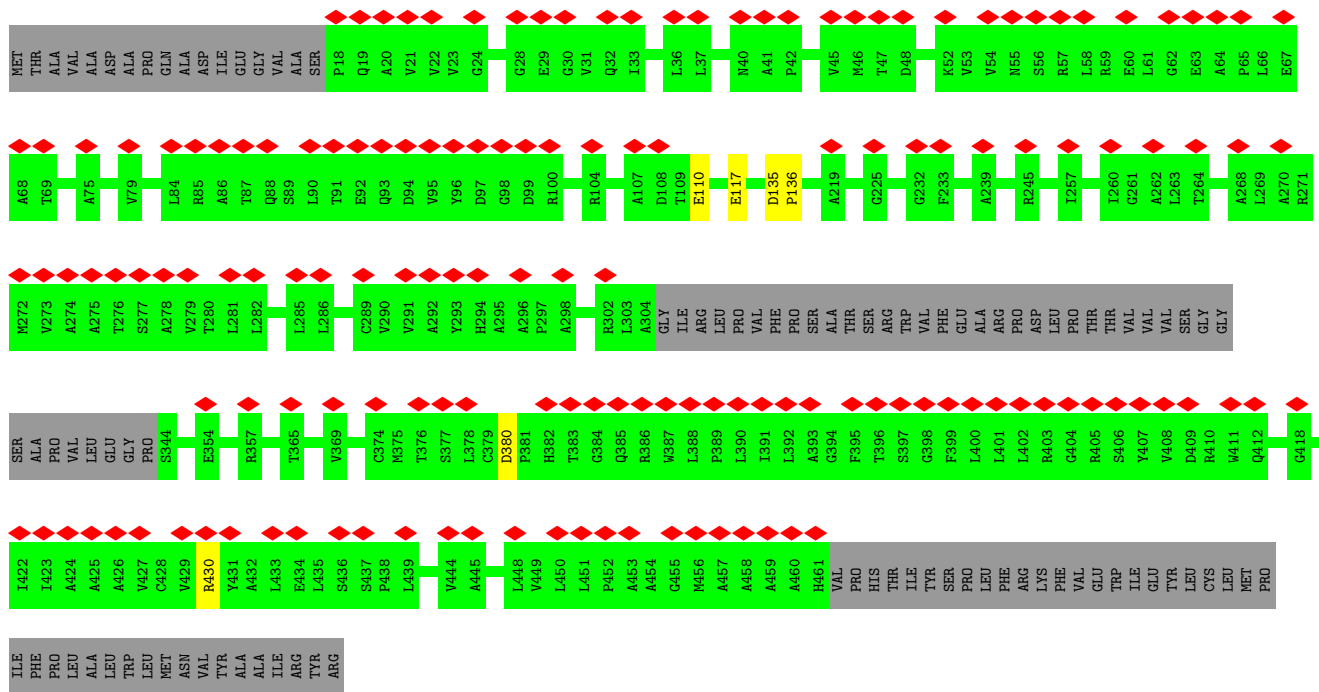
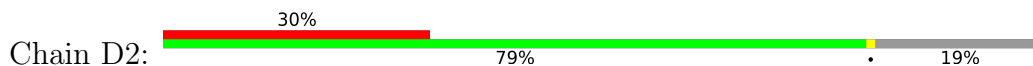


• Molecule 2: ESX-5 secretion system protein EccC5

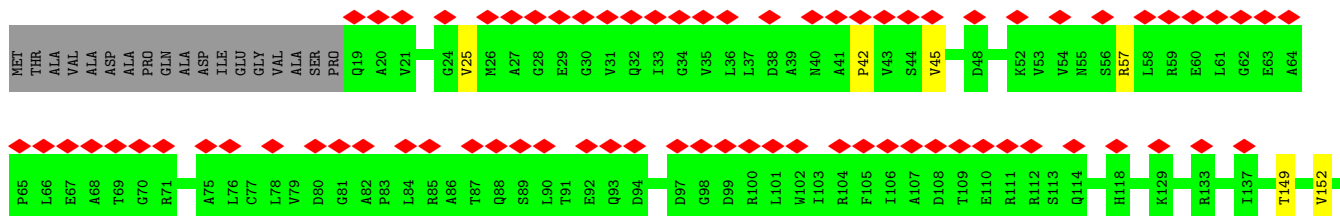


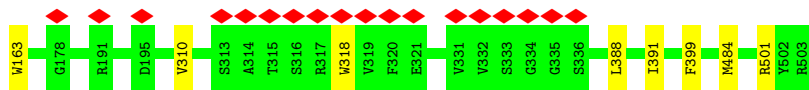


• Molecule 3: ESX-5 secretion system protein EccD5

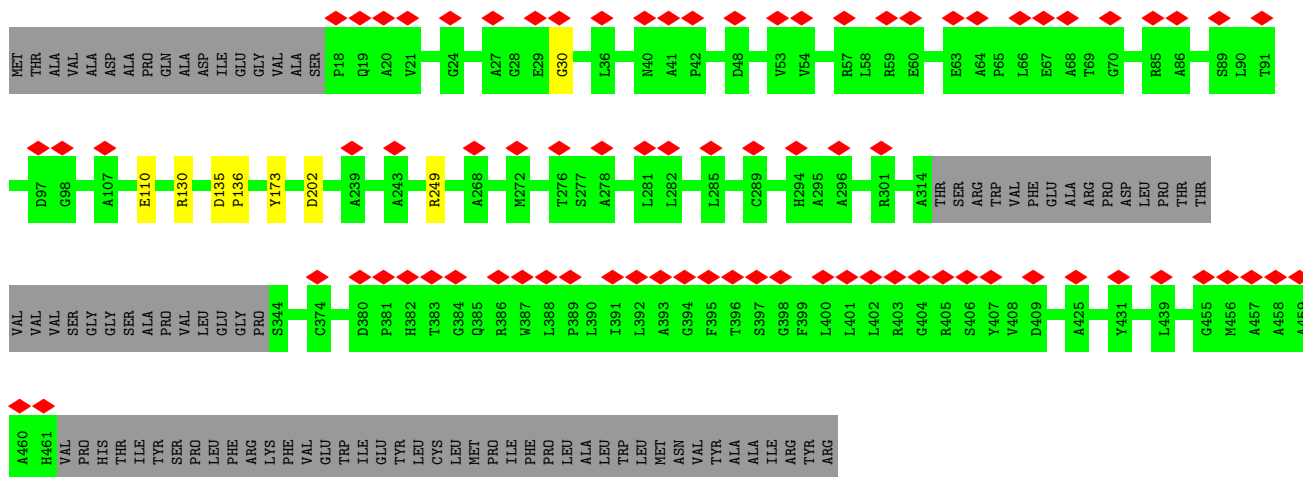
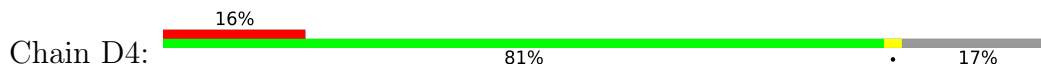


• Molecule 3: ESX-5 secretion system protein EccD5

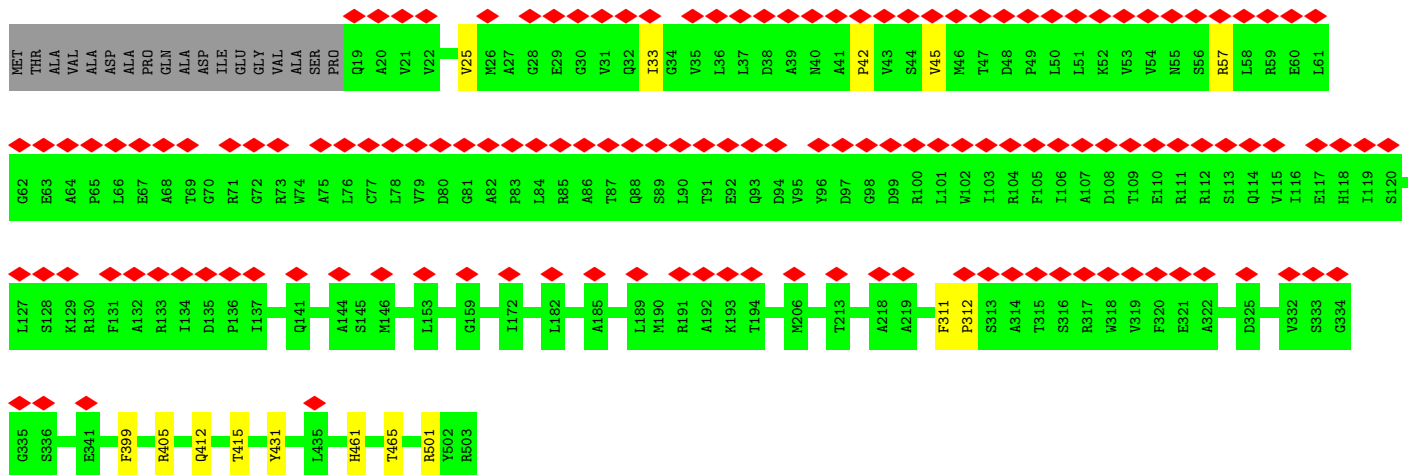




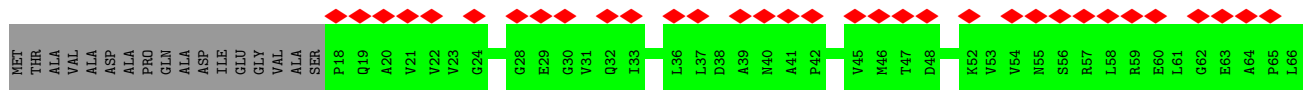
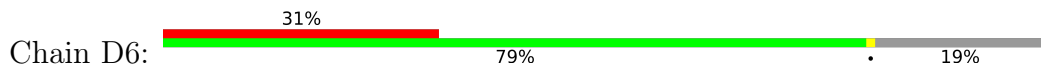
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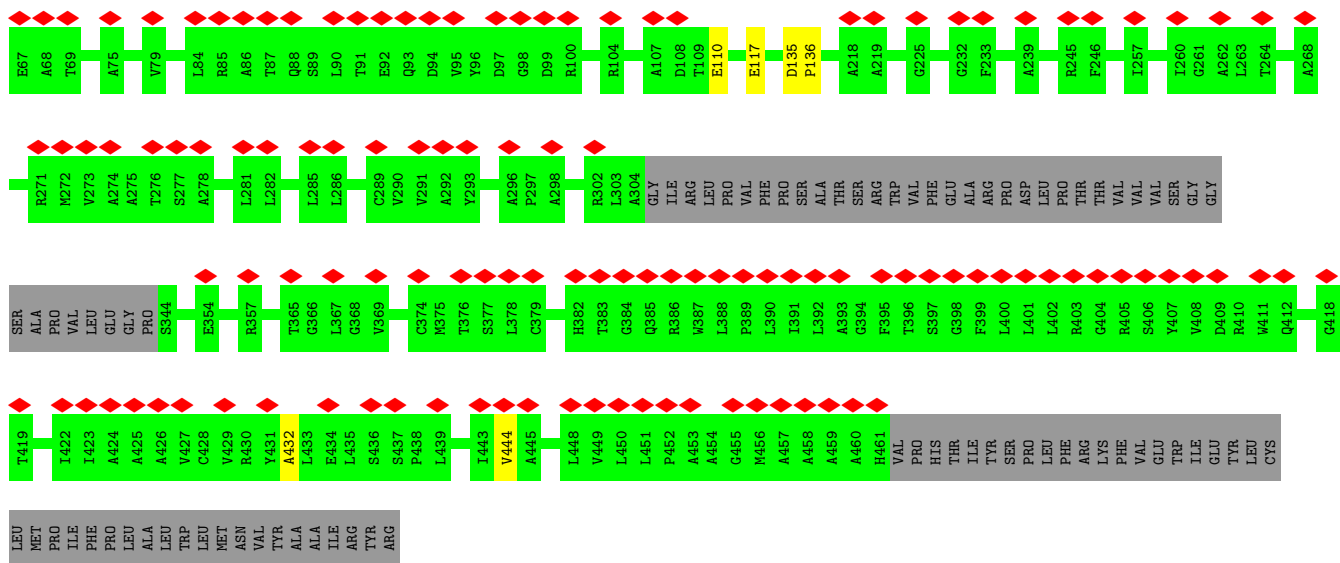


• Molecule 3: ESX-5 secretion system protein EccD5

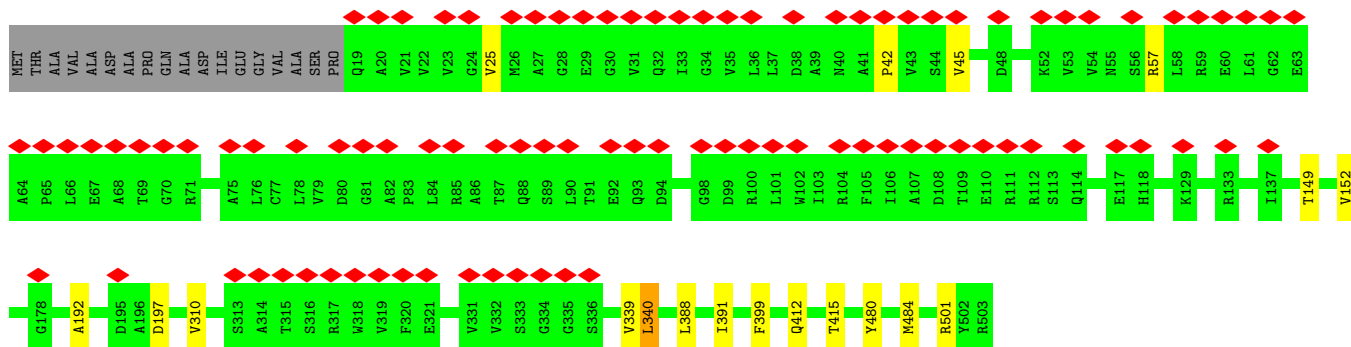


• Molecule 3: ESX-5 secretion system protein EccD5

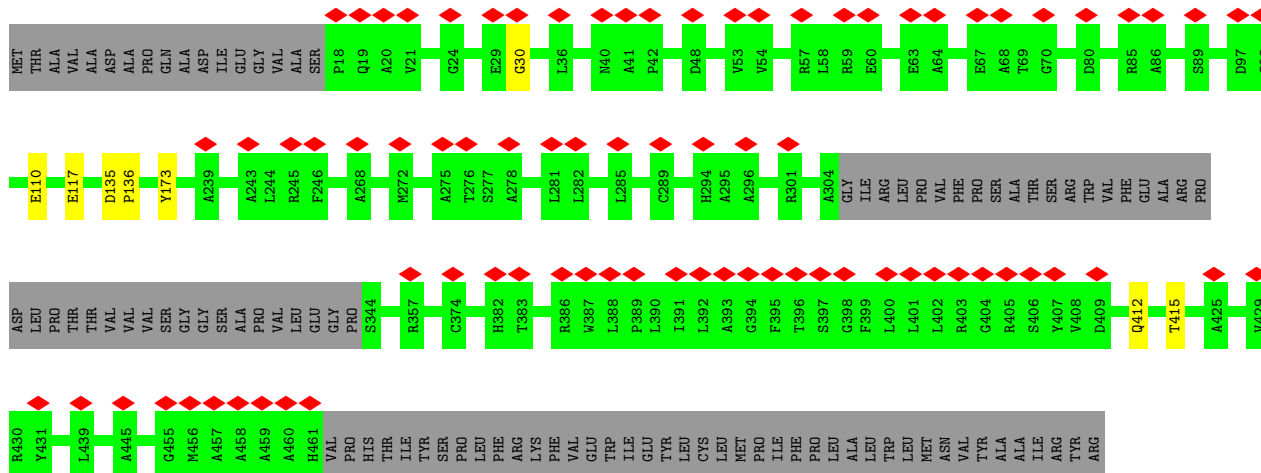
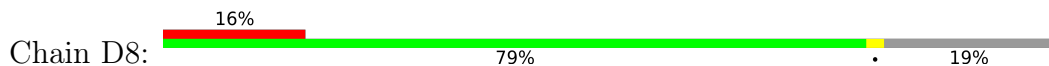




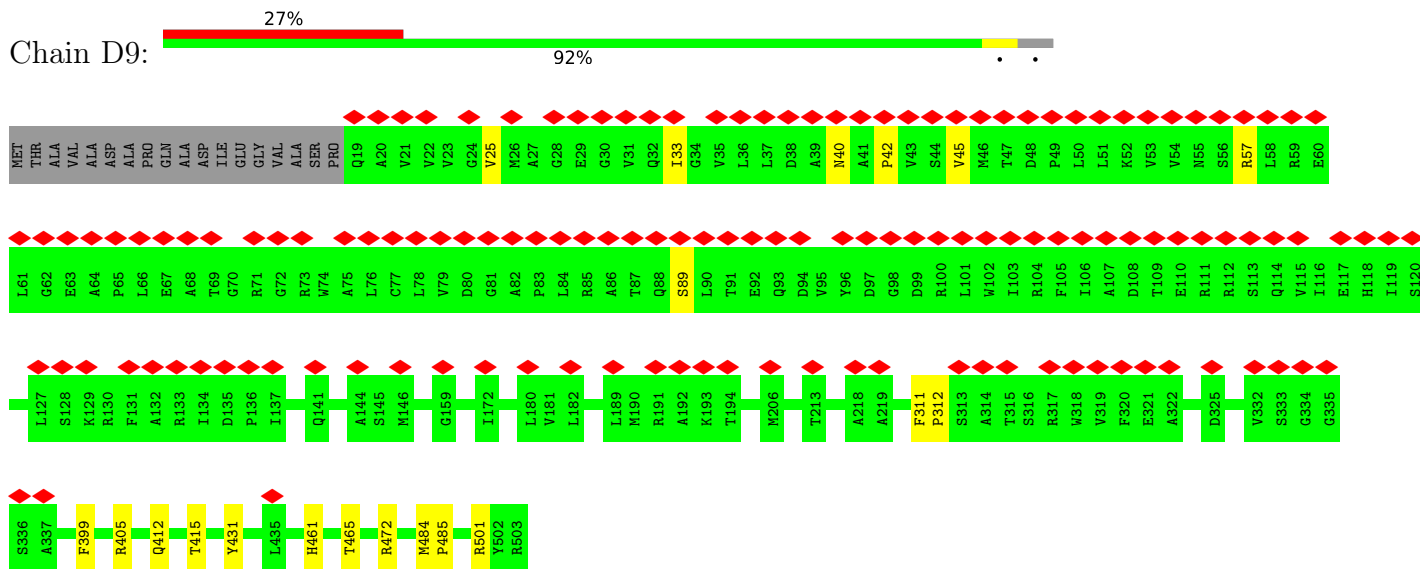
• Molecule 3: ESX-5 secretion system protein EccD5



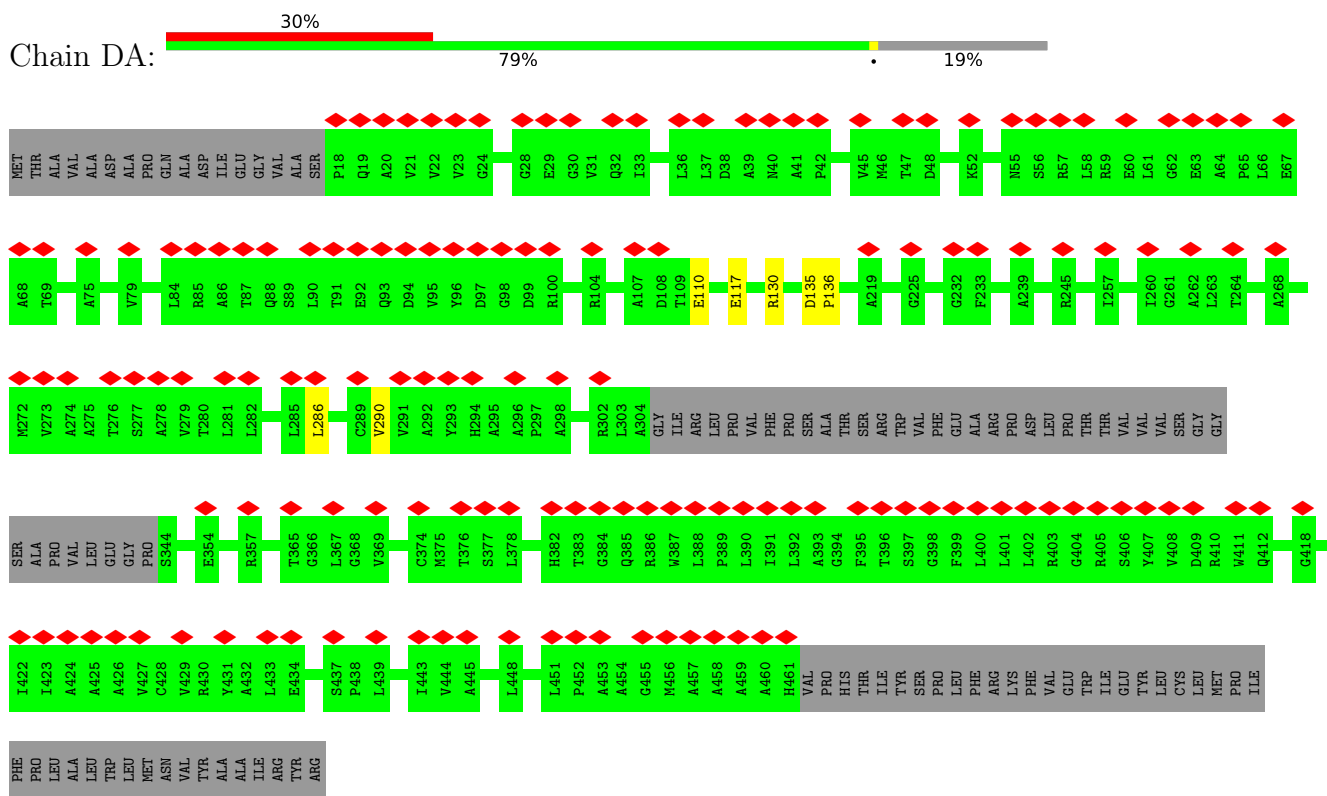
• Molecule 3: ESX-5 secretion system protein EccD5



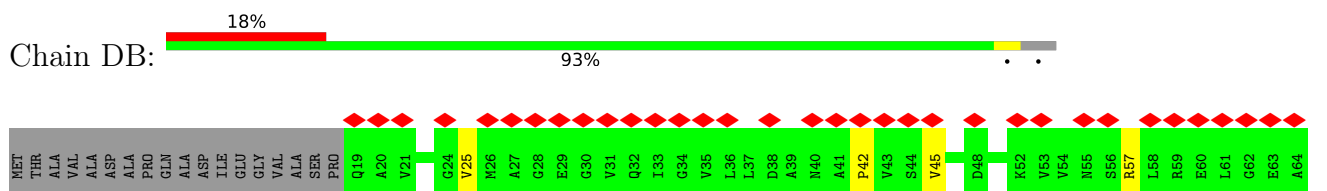
• Molecule 3: ESX-5 secretion system protein EccD5

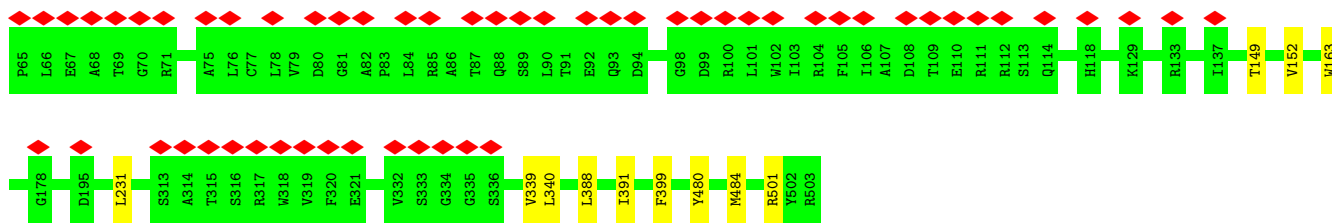


• Molecule 3: ESX-5 secretion system protein EccD5

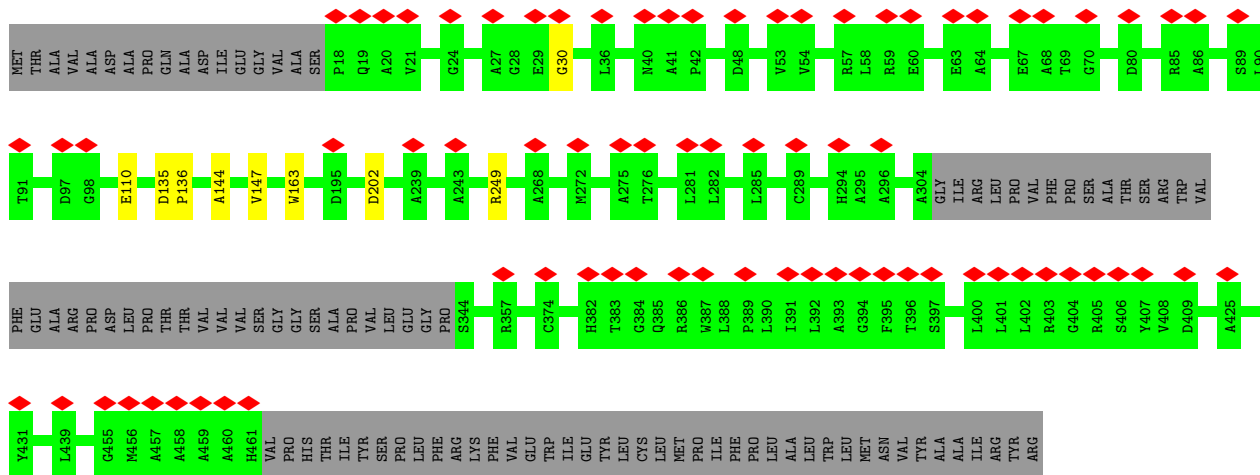
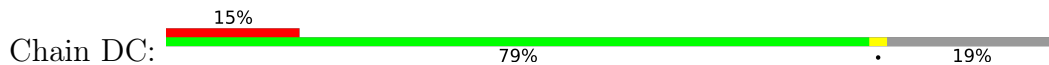


• Molecule 3: ESX-5 secretion system protein EccD5

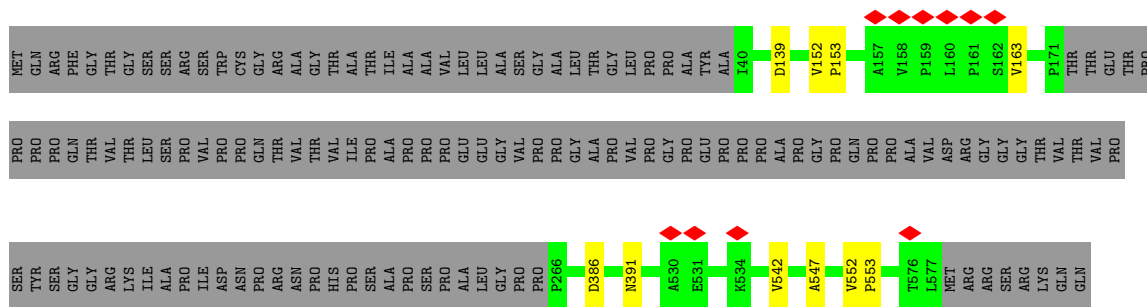
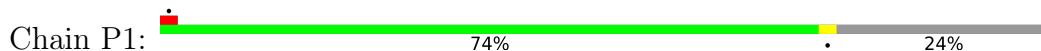




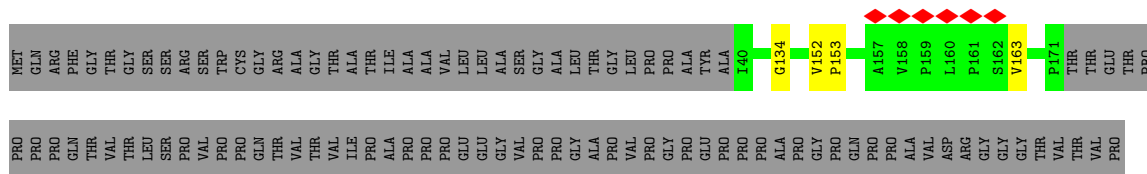
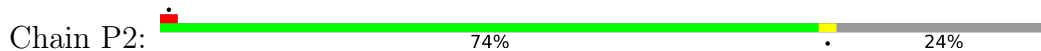
• Molecule 3: ESX-5 secretion system protein EccD5

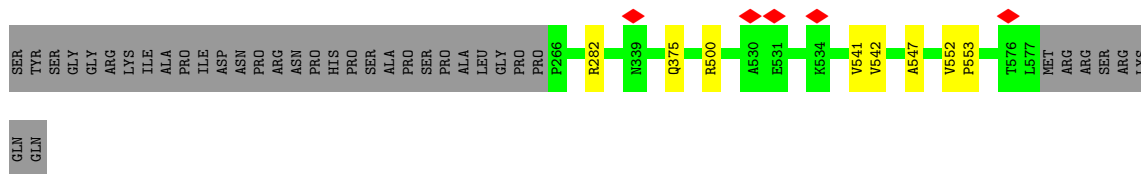


• Molecule 4: Mycosin-5

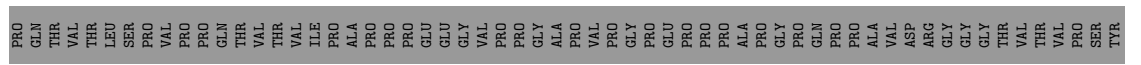
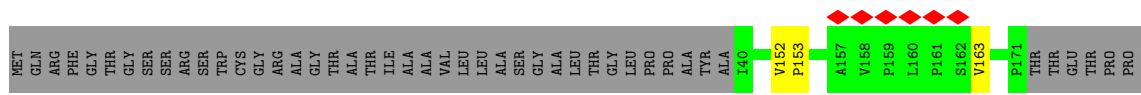
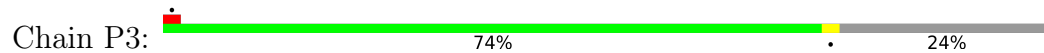


• Molecule 4: Mycosin-5





• Molecule 4: Mycosin-5



GLN

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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	0.136	Depositor
Minimum map value	-0.100	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.016	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	0.65	14/3669 (0.4%)	0.74	7/5028 (0.1%)
1	B2	0.65	14/3669 (0.4%)	0.74	6/5028 (0.1%)
1	B3	0.43	3/3669 (0.1%)	0.66	0/5028
1	B4	0.42	0/3675	0.65	0/5038
1	B5	0.43	1/3675 (0.0%)	0.67	0/5038
1	B6	0.42	0/3675	0.65	0/5038
2	C1	0.35	0/3280	0.64	0/4459
2	C2	0.34	0/3280	0.63	0/4459
2	C3	0.35	0/3280	0.64	0/4459
2	C4	0.34	0/3280	0.63	0/4459
2	C5	0.35	0/3280	0.63	0/4459
2	C6	0.34	0/3280	0.62	0/4459
3	D1	0.36	0/3710	0.62	0/5078
3	D2	0.31	0/3038	0.58	0/4151
3	D3	0.39	1/3710 (0.0%)	0.64	0/5078
3	D4	0.31	0/3115	0.59	1/4257 (0.0%)
3	D5	0.37	0/3710	0.61	0/5078
3	D6	0.32	0/3038	0.59	0/4151
3	D7	0.40	1/3710 (0.0%)	0.64	0/5078
3	D8	0.31	0/3038	0.60	1/4151 (0.0%)
3	D9	0.36	0/3710	0.62	0/5078
3	DA	0.31	0/3038	0.58	0/4151
3	DB	0.38	0/3710	0.64	0/5078
3	DC	0.31	0/3038	0.59	1/4151 (0.0%)
4	P1	0.55	3/3309 (0.1%)	0.71	0/4545
4	P2	0.55	6/3309 (0.2%)	0.70	0/4545
4	P3	0.56	4/3309 (0.1%)	0.72	0/4545
All	All	0.42	47/92204 (0.1%)	0.65	16/126067 (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
2	C3	0	1

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B1	483	ARG	CZ-NH1	-8.63	1.21	1.33
1	B1	483	ARG	CZ-NH2	-8.53	1.22	1.33
1	B2	483	ARG	CZ-NH1	-8.52	1.22	1.33
1	B2	483	ARG	CZ-NH2	-8.17	1.22	1.33
1	B2	103	ARG	CZ-NH2	-7.85	1.22	1.33

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B2	103	ARG	CA-CB-CG	6.89	128.57	113.40
1	B1	103	ARG	CA-CB-CG	6.88	128.53	113.40
1	B1	105	TYR	CB-CG-CD2	6.50	124.90	121.00
1	B2	105	TYR	CB-CG-CD2	6.38	124.83	121.00
1	B1	489	GLU	CA-CB-CG	6.03	126.67	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C3	86	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	7	0
1	B2	3587	3631	3626	6	0
1	B3	3587	3631	3626	8	0
1	B4	3591	3621	3618	7	0
1	B5	3591	3621	3618	6	0
1	B6	3591	3621	3618	4	0
2	C1	3190	3145	3142	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C2	3190	3145	3142	11	0
2	C3	3190	3145	3142	11	0
2	C4	3190	3145	3142	9	0
2	C5	3190	3145	3142	13	0
2	C6	3190	3145	3142	8	0
3	D1	3635	3823	3822	8	0
3	D2	2989	3166	3163	3	0
3	D3	3635	3824	3822	6	0
3	D4	3063	3245	3243	3	0
3	D5	3635	3824	3822	6	0
3	D6	2989	3166	3163	3	0
3	D7	3635	3824	3822	10	0
3	D8	2989	3165	3163	3	0
3	D9	3635	3824	3822	11	0
3	DA	2989	3167	3163	3	0
3	DB	3635	3824	3822	8	0
3	DC	2989	3165	3163	4	0
4	P1	3226	3219	3218	5	0
4	P2	3226	3219	3218	5	0
4	P3	3226	3219	3218	6	0
All	All	90170	92300	92228	171	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 171 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)
4:P1:552:VAL:HG23	4:P1:553:PRO:HD3	1.77	0.65
2:C5:185:ASP:OD1	2:C5:186:ILE:N	2.32	0.63
2:C4:130:ARG:NH2	3:DA:110:GLU:OE2	2.32	0.62
2:C6:130:ARG:NH2	3:D2:110:GLU:OE2	2.32	0.62
3:D6:432:ALA:HB2	3:D6:444:VAL:HG21	1.83	0.60

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 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%)	460 (98%)	10 (2%)	0	100	100
1	B2	470/506 (93%)	466 (99%)	4 (1%)	0	100	100
1	B3	470/506 (93%)	457 (97%)	13 (3%)	0	100	100
1	B4	476/506 (94%)	470 (99%)	6 (1%)	0	100	100
1	B5	476/506 (94%)	467 (98%)	9 (2%)	0	100	100
1	B6	476/506 (94%)	470 (99%)	6 (1%)	0	100	100
2	C1	402/1391 (29%)	391 (97%)	11 (3%)	0	100	100
2	C2	402/1391 (29%)	393 (98%)	8 (2%)	1 (0%)	47	78
2	C3	402/1391 (29%)	390 (97%)	12 (3%)	0	100	100
2	C4	402/1391 (29%)	389 (97%)	13 (3%)	0	100	100
2	C5	402/1391 (29%)	393 (98%)	9 (2%)	0	100	100
2	C6	402/1391 (29%)	389 (97%)	13 (3%)	0	100	100
3	D1	483/503 (96%)	476 (99%)	7 (1%)	0	100	100
3	D2	401/503 (80%)	392 (98%)	9 (2%)	0	100	100
3	D3	483/503 (96%)	473 (98%)	10 (2%)	0	100	100
3	D4	411/503 (82%)	404 (98%)	7 (2%)	0	100	100
3	D5	483/503 (96%)	473 (98%)	10 (2%)	0	100	100
3	D6	401/503 (80%)	394 (98%)	7 (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%)	393 (98%)	8 (2%)	0	100	100
3	DB	483/503 (96%)	472 (98%)	11 (2%)	0	100	100
3	DC	401/503 (80%)	393 (98%)	8 (2%)	0	100	100
4	P1	440/585 (75%)	419 (95%)	21 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P2	440/585 (75%)	424 (96%)	16 (4%)	0	100	100
4	P3	440/585 (75%)	422 (96%)	18 (4%)	0	100	100
All	All	11884/19173 (62%)	11610 (98%)	273 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C2	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	96
1	B2	390/411 (95%)	389 (100%)	1 (0%)	92	96
1	B3	390/411 (95%)	389 (100%)	1 (0%)	92	96
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	94
2	C1	342/1137 (30%)	340 (99%)	2 (1%)	86	92
2	C2	342/1137 (30%)	339 (99%)	3 (1%)	78	88
2	C3	342/1137 (30%)	340 (99%)	2 (1%)	86	92
2	C4	342/1137 (30%)	339 (99%)	3 (1%)	78	88
2	C5	342/1137 (30%)	338 (99%)	4 (1%)	71	84
2	C6	342/1137 (30%)	340 (99%)	2 (1%)	86	92
3	D1	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	D2	311/393 (79%)	310 (100%)	1 (0%)	92	96
3	D3	381/393 (97%)	377 (99%)	4 (1%)	76	86
3	D4	319/393 (81%)	317 (99%)	2 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D5	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	D6	311/393 (79%)	310 (100%)	1 (0%)	92	96
3	D7	381/393 (97%)	377 (99%)	4 (1%)	76	86
3	D8	311/393 (79%)	309 (99%)	2 (1%)	86	92
3	D9	381/393 (97%)	376 (99%)	5 (1%)	69	82
3	DA	311/393 (79%)	309 (99%)	2 (1%)	86	92
3	DB	381/393 (97%)	377 (99%)	4 (1%)	76	86
3	DC	311/393 (79%)	310 (100%)	1 (0%)	92	96
4	P1	343/453 (76%)	341 (99%)	2 (1%)	86	92
4	P2	343/453 (76%)	342 (100%)	1 (0%)	92	96
4	P3	343/453 (76%)	343 (100%)	0	100	100
All	All	9578/15363 (62%)	9509 (99%)	69 (1%)	84	91

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D9	431	TYR
3	DA	117	GLU
3	DC	163	TRP
2	C5	38	TRP
2	C4	151	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	D7	165	HIS
4	P1	391	ASN
4	P3	391	ASN
4	P2	283	GLN
4	P2	391	ASN

5.3.3 RNA ⓘ

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.

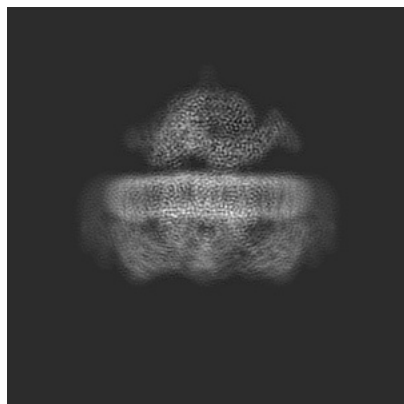
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12517. These allow visual inspection of the internal detail of the map and identification of artifacts.

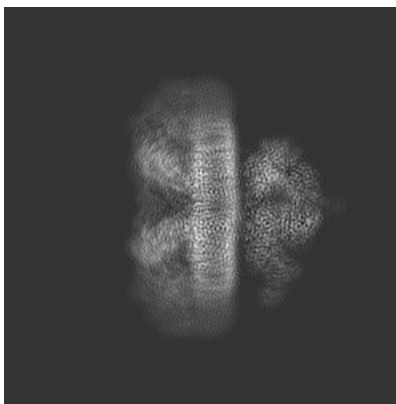
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

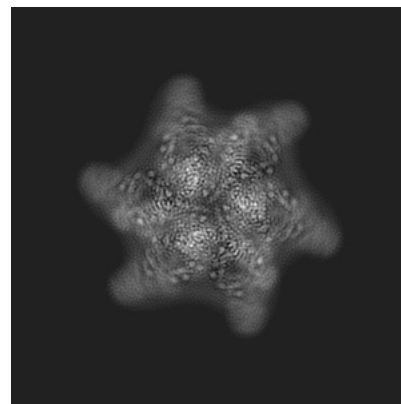
6.1.1 Primary map



X

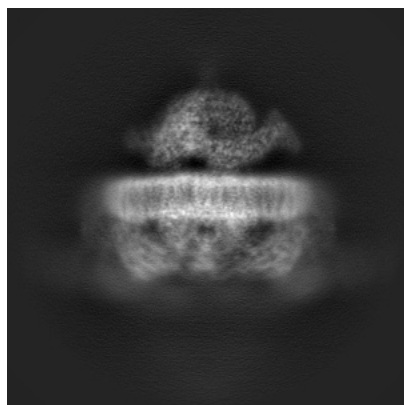


Y

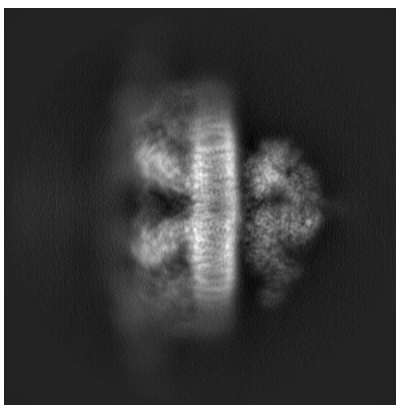


Z

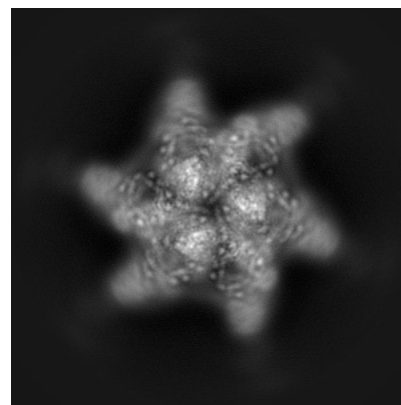
6.1.2 Raw map



X



Y

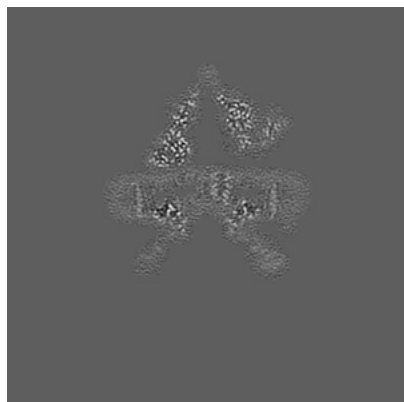


Z

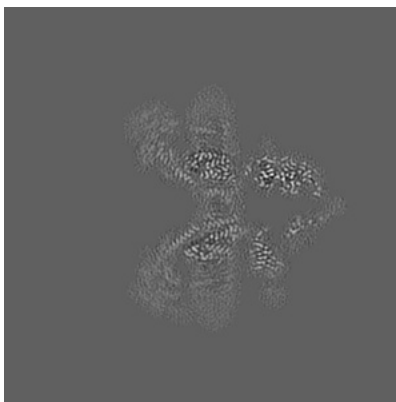
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

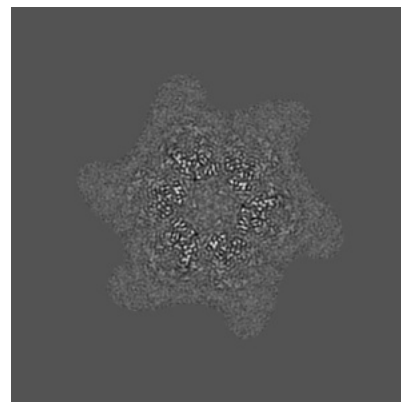
6.2.1 Primary map



X Index: 200

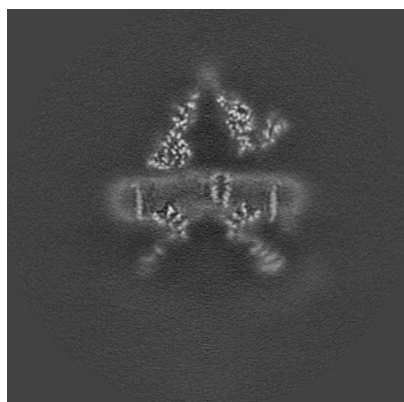


Y Index: 200

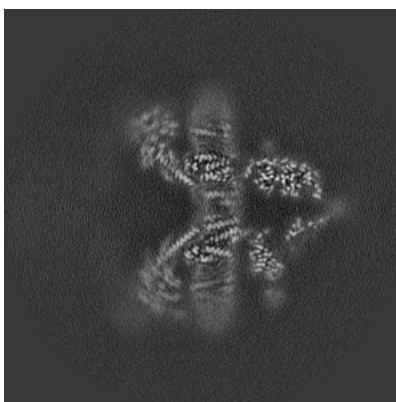


Z Index: 200

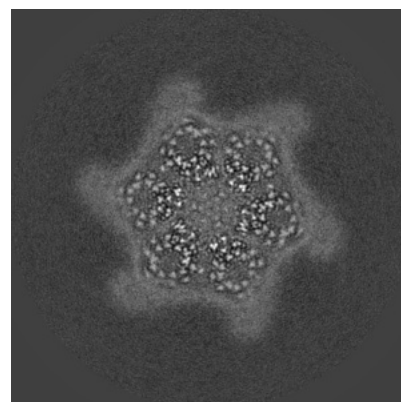
6.2.2 Raw map



X Index: 200



Y Index: 200

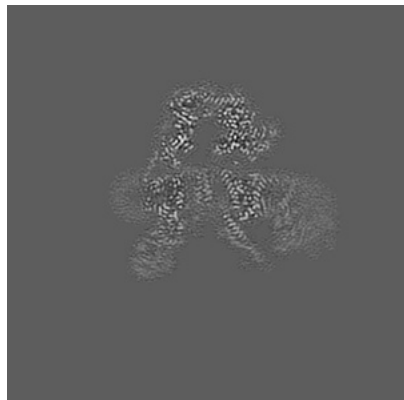


Z Index: 200

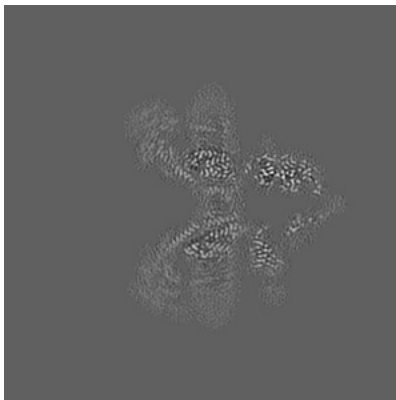
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

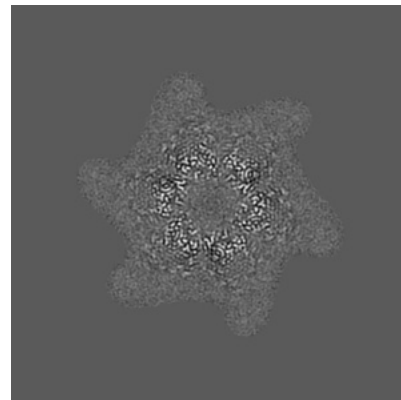
6.3.1 Primary map



X Index: 184

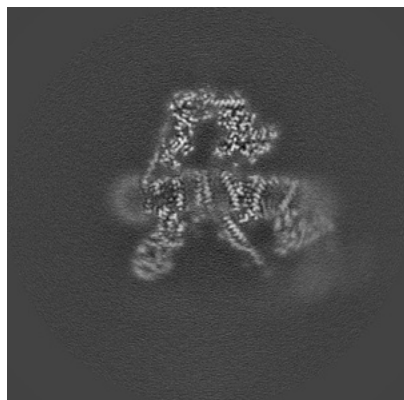


Y Index: 200

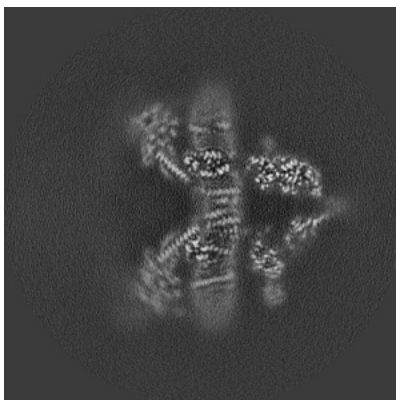


Z Index: 197

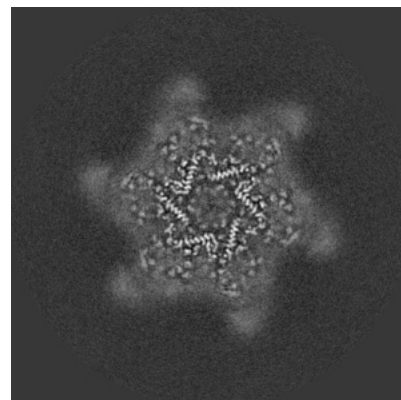
6.3.2 Raw map



X Index: 184



Y Index: 198

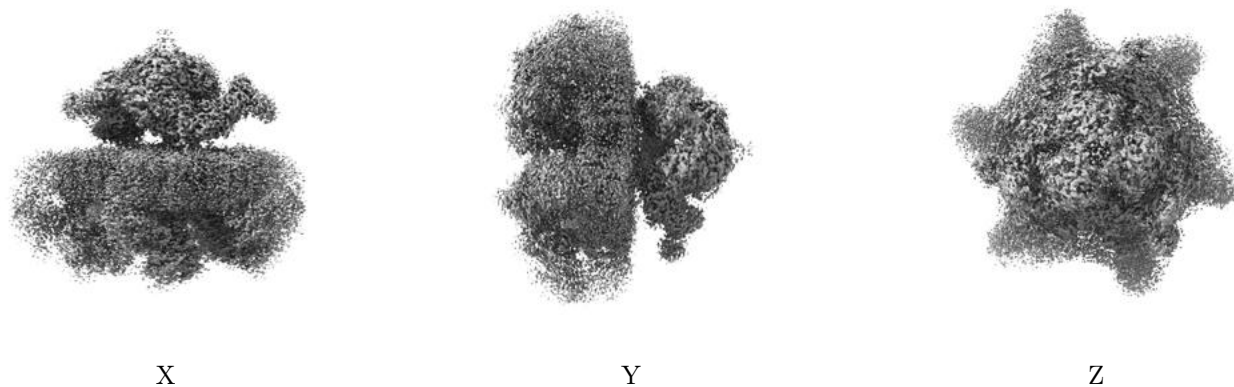


Z Index: 192

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

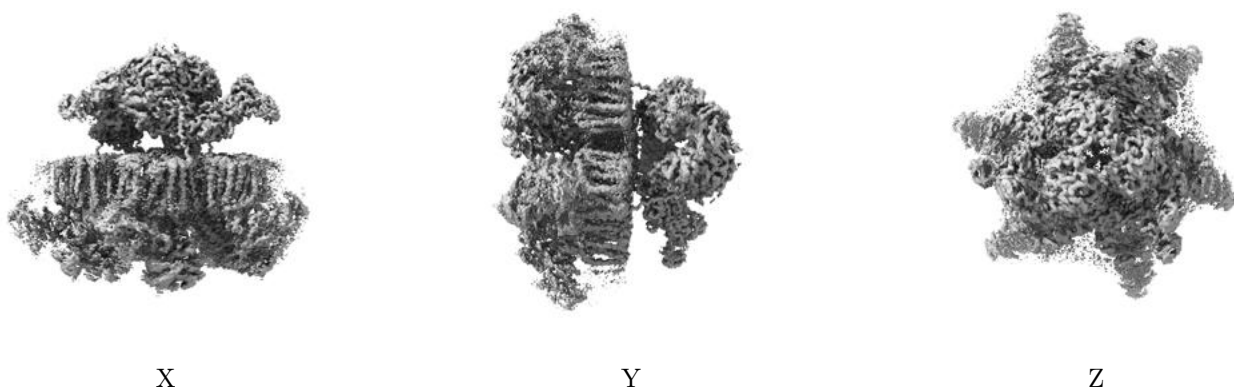
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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



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.

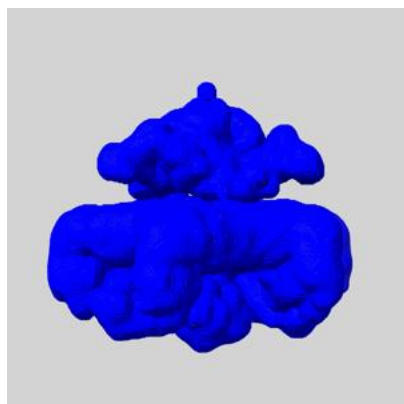
6.5 Mask visualisation [i](#)

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

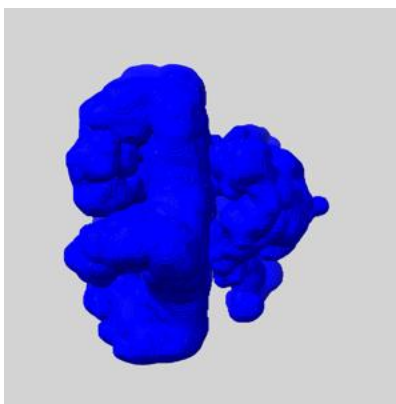
A mask typically either:

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

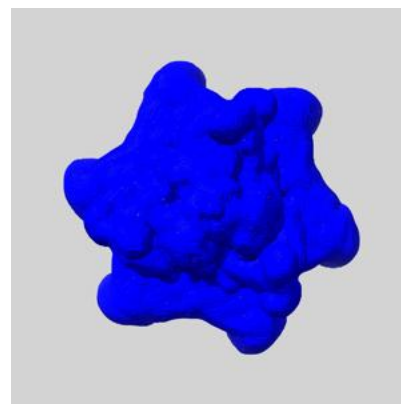
6.5.1 emd_12517_msk_1.map [i](#)



X



Y

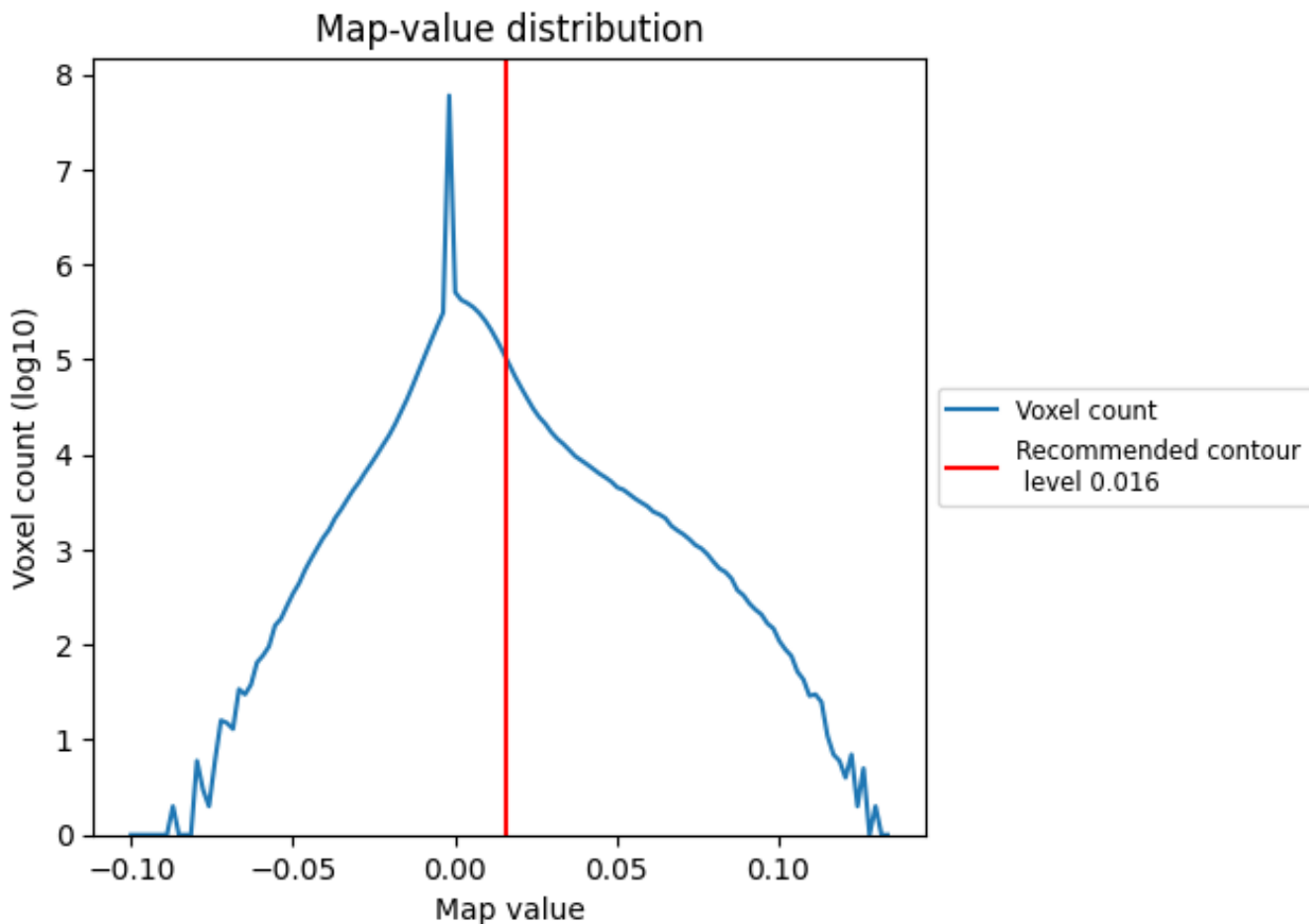


Z

7 Map analysis [i](#)

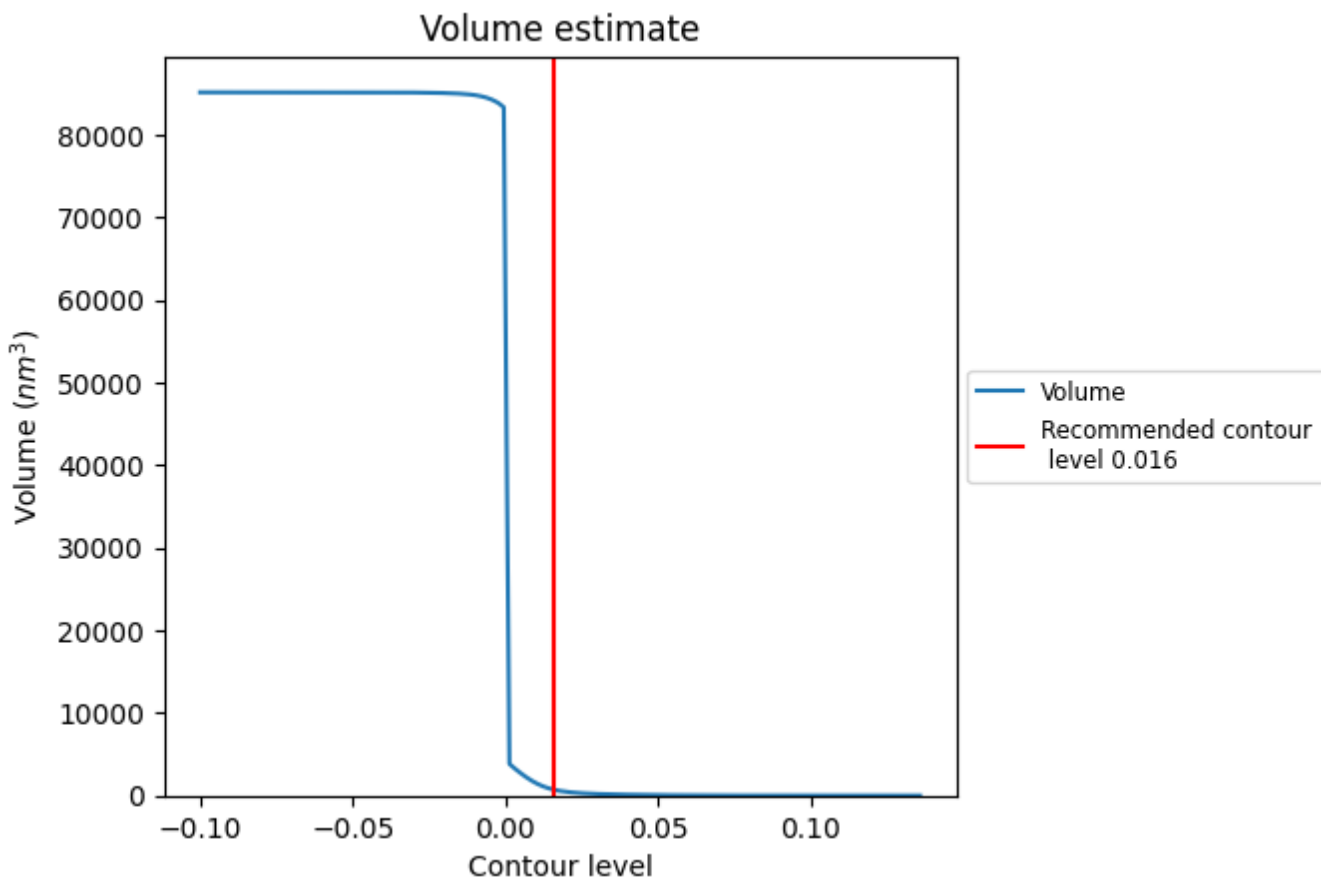
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

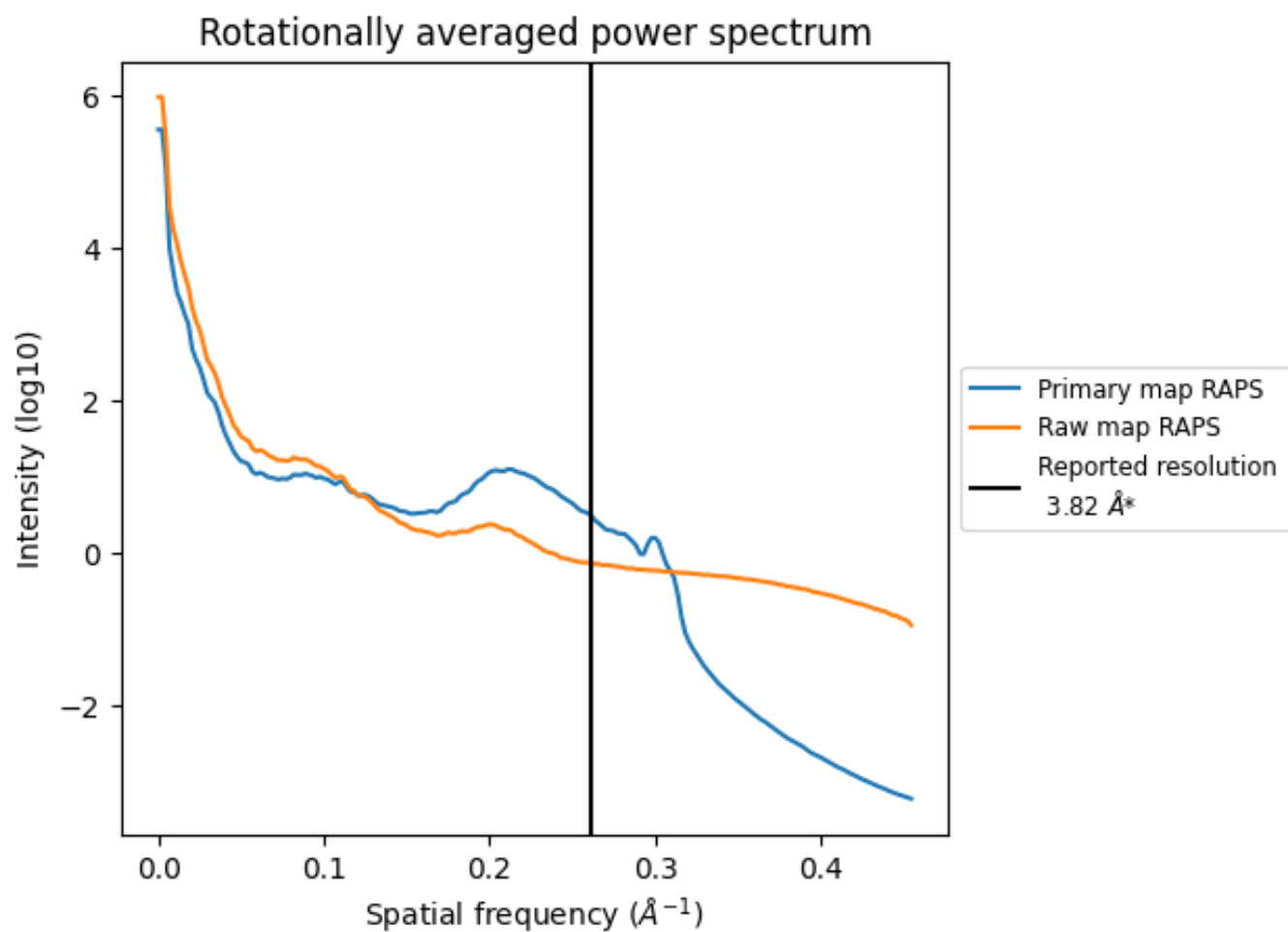
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 695 nm³; this corresponds to an approximate mass of 628 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

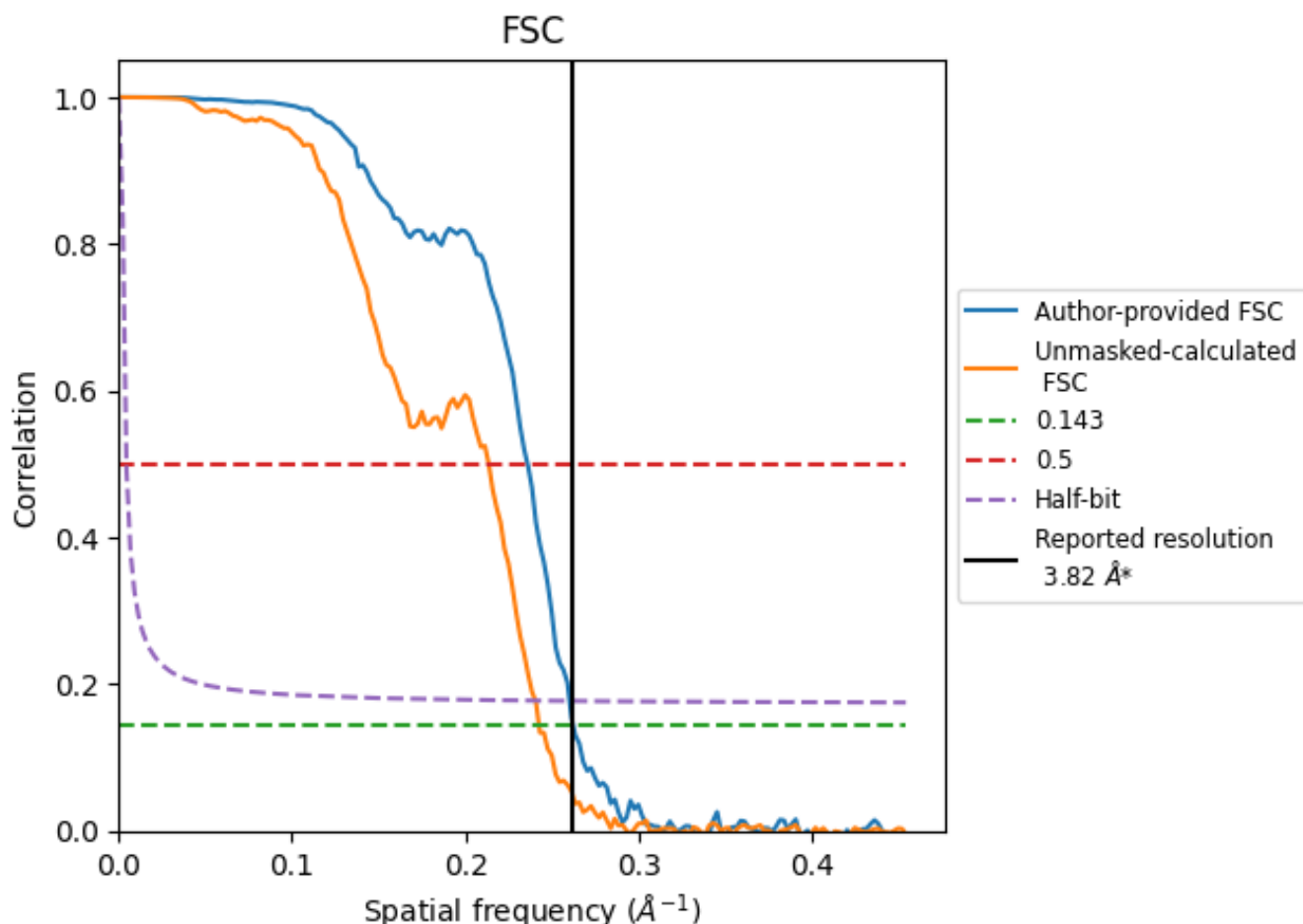


*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.262 \AA^{-1}

8.2 Resolution estimates [i](#)

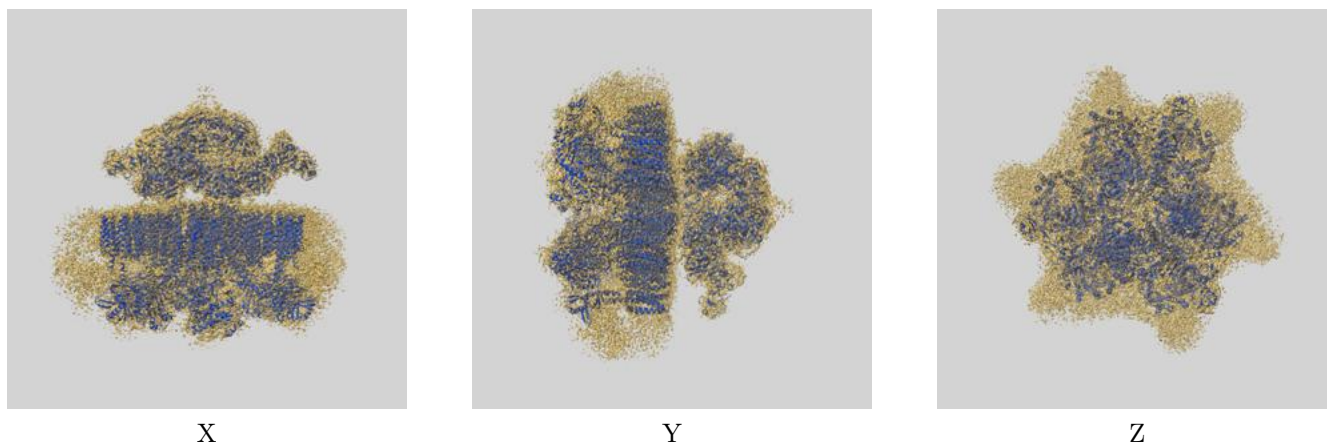
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.81	4.24	3.84
Unmasked-calculated*	4.12	4.68	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

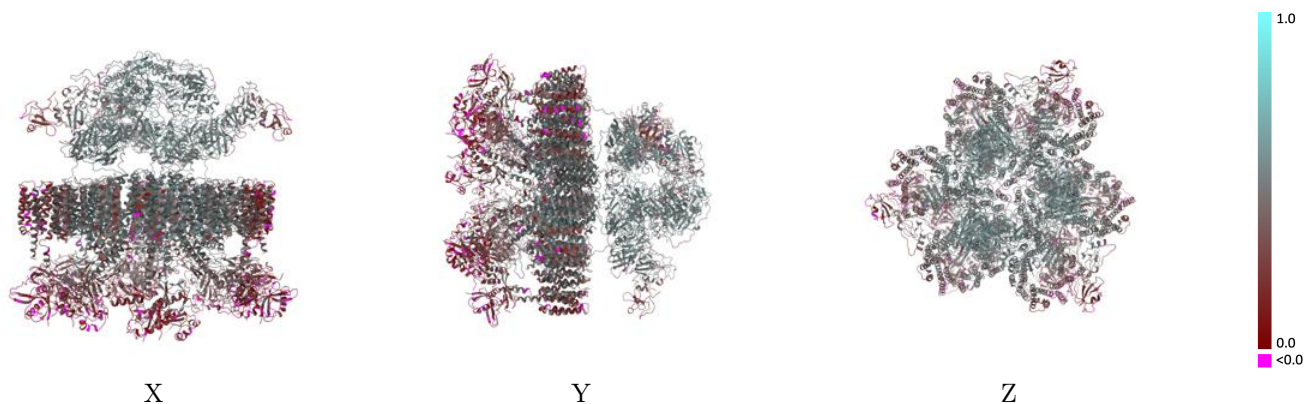
This section contains information regarding the fit between EMDB map EMD-12517 and PDB model 7NPR. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



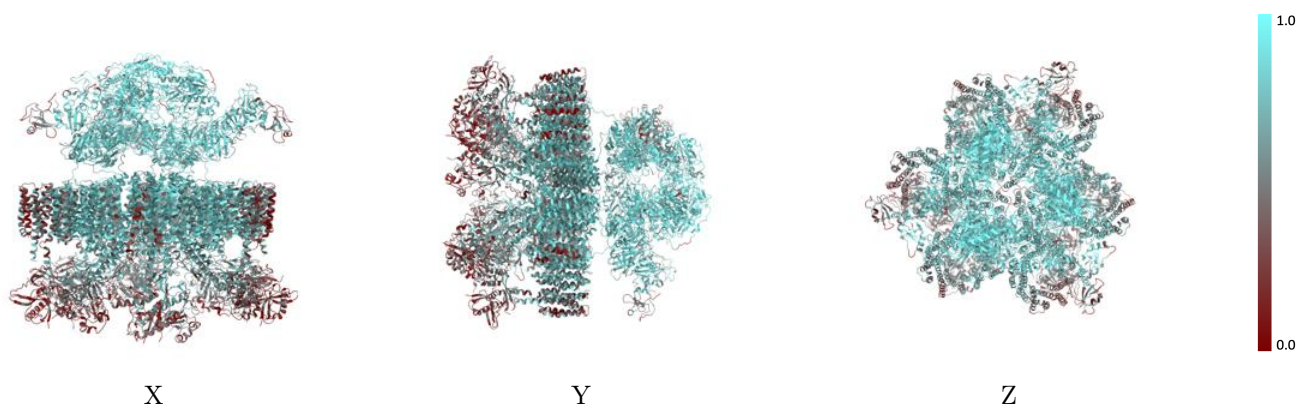
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



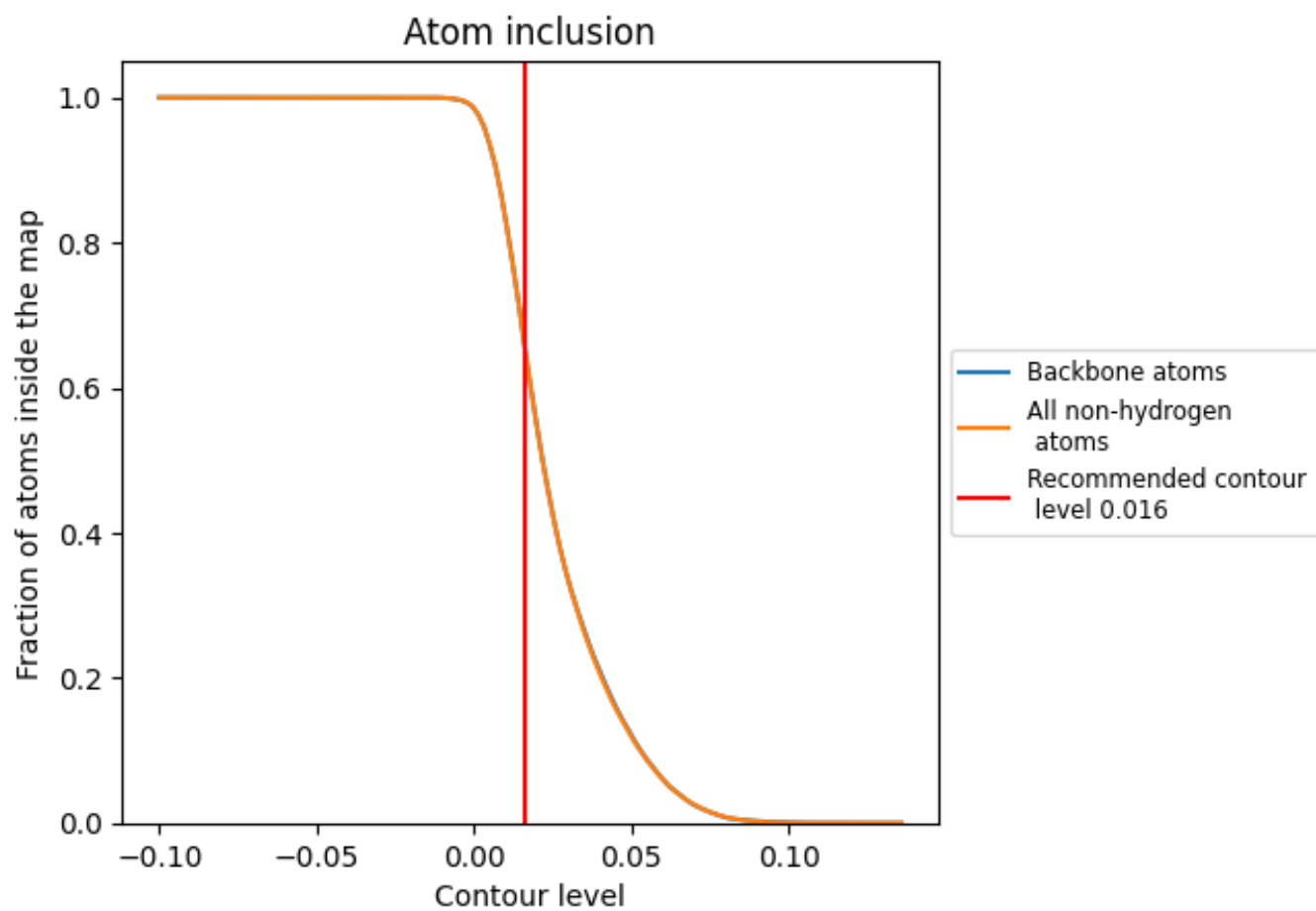
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.016).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.4070
B1	 0.7659	 0.4640
B2	 0.7662	 0.4640
B3	 0.7662	 0.4620
B4	 0.8256	 0.5060
B5	 0.8216	 0.5050
B6	 0.8210	 0.5040
C1	 0.5850	 0.3430
C2	 0.4837	 0.3080
C3	 0.5815	 0.3450
C4	 0.4767	 0.3050
C5	 0.5806	 0.3450
C6	 0.4815	 0.3040
D1	 0.6109	 0.3770
D2	 0.5122	 0.3190
D3	 0.6927	 0.4280
D4	 0.6032	 0.3780
D5	 0.6123	 0.3760
D6	 0.5139	 0.3230
D7	 0.6953	 0.4280
D8	 0.6071	 0.3800
D9	 0.6120	 0.3740
DA	 0.5142	 0.3170
DB	 0.6907	 0.4270
DC	 0.6051	 0.3790
P1	 0.8528	 0.5170
P2	 0.8531	 0.5150
P3	 0.8516	 0.5130

