



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 11:56 PM UTC

PDB ID : 9NGU / pdb_00009ngu
EMDB ID : EMD-49393
Title : In situ cryo-EM structure of outer membrane cap (OMC) of the Legionella Dot/Icm T4SS machine
Authors : Yue, J.; Jun, L.
Deposited on : 2025-02-22
Resolution : 2.96 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:

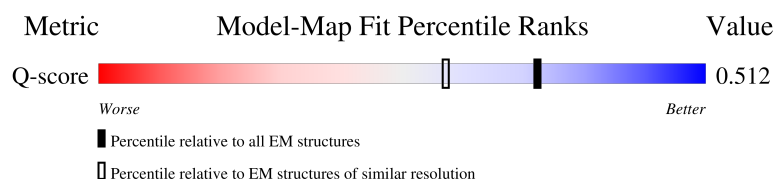
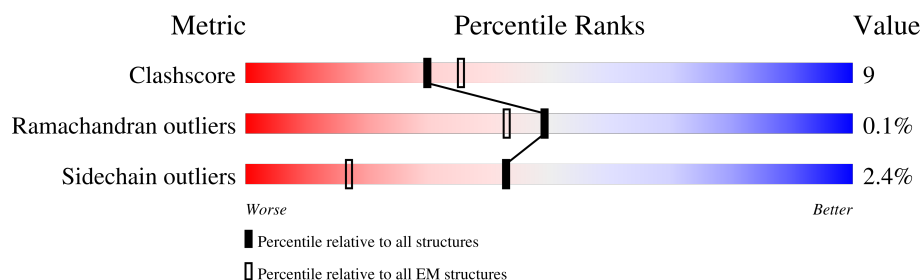
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.96 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.



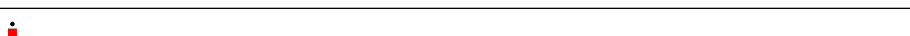
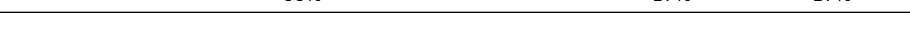
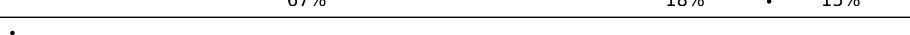
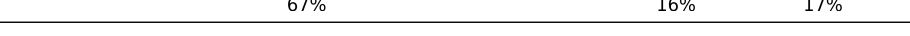
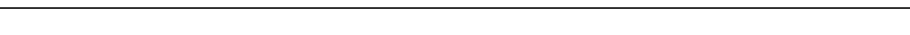
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13155 (2.46 - 3.46)

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	Aa	163	62% 23% 15%
1	Ae	163	64% 20% 17%
1	Ak	163	65% 20% 15%
1	Ao	163	67% 16% 17%

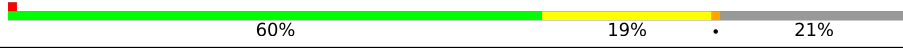
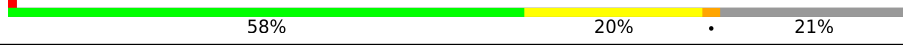
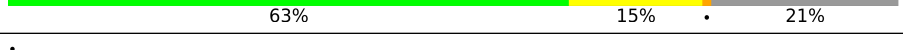
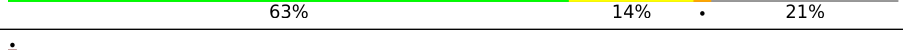
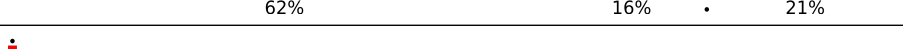
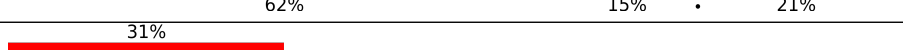
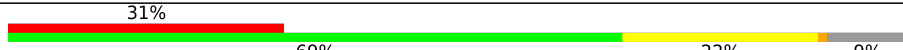
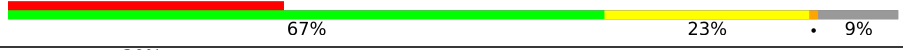
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Mol	Chain	Length	Quality of chain
1	Au	163	
1	Ay	163	
1	Be	163	
1	Bi	163	
1	Bo	163	
1	Bs	163	
1	By	163	
1	Cc	163	
1	Ci	163	
1	Cm	163	
1	Cs	163	
1	Cw	163	
1	Dc	163	
1	Dg	163	
1	Dm	163	
1	Dq	163	
1	Dw	163	
1	Ea	163	
1	Eg	163	
1	Ek	163	
1	Eq	163	
1	Eu	163	
2	Ab	189	
2	Al	189	
2	Av	189	

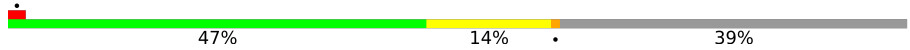
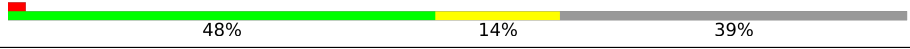
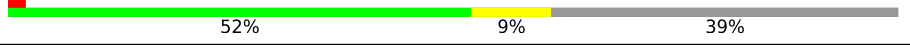
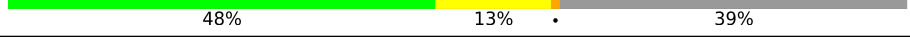
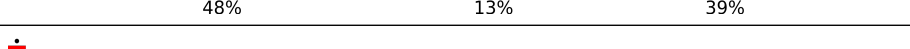
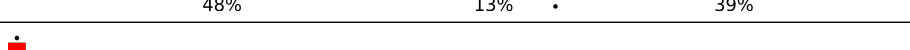
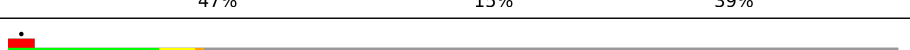
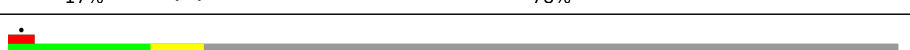
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Mol	Chain	Length	Quality of chain
2	Bf	189	
2	Bp	189	
2	Bz	189	
2	Cj	189	
2	Ct	189	
2	Dd	189	
2	Dn	189	
2	Dx	189	
2	Eh	189	
2	Er	189	
3	Ac	320	
3	Am	320	
3	Aw	320	
3	Bg	320	
3	Bq	320	
3	Ca	320	
3	Ck	320	
3	Cu	320	
3	De	320	
3	Do	320	
3	Dy	320	
3	Ei	320	
3	Es	320	
4	Ad	124	
4	An	124	

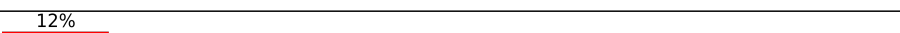
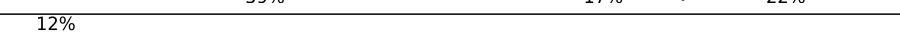
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Mol	Chain	Length	Quality of chain
4	Ax	124	
4	Bh	124	
4	Br	124	
4	Cb	124	
4	Cl	124	
4	Cv	124	
4	Df	124	
4	Dp	124	
4	Dz	124	
4	Ej	124	
4	Et	124	
5	Af	269	
5	Ap	269	
5	Az	269	
5	Bj	269	
5	Bt	269	
5	Cd	269	
5	Cn	269	
5	Cx	269	
5	Dh	269	
5	Dr	269	
5	Eb	269	
5	El	269	
5	Ev	269	
6	Ag	361	

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Mol	Chain	Length	Quality of chain
6	Aq	361	 19% 6% 75%
6	Ba	361	 20% 5% 75%
6	Bk	361	 20% 6% 75%
6	Bu	361	 19% 6% 75%
6	Ce	361	 19% 6% 75%
6	Co	361	 18% 7% 75%
6	Cy	361	 18% 7% 75%
6	Di	361	 20% 5% 75%
6	Ds	361	 19% 6% 75%
6	Ec	361	 19% 6% 75%
6	Em	361	 19% 7% 75%
6	Ew	361	 19% 6% 75%
7	Ah	249	 12% 57% 20% 22%
7	Ar	249	 12% 60% 17% 22%
7	Bb	249	 12% 59% 17% 22%
7	Bl	249	 12% 57% 19% 22%
7	Bv	249	 12% 59% 18% 22%
7	Cf	249	 13% 61% 16% 22%
7	Cp	249	 11% 59% 18% 22%
7	Cz	249	 12% 61% 16% 22%
7	Dj	249	 13% 60% 16% 22%
7	Dt	249	 12% 59% 18% 22%
7	Ed	249	 12% 59% 18% 22%
7	En	249	 12% 59% 18% 22%
7	Ex	249	 12% 61% 15% 22%

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Mol	Chain	Length	Quality of chain
8	Ai	303	
8	As	303	
8	Bc	303	
8	Bm	303	
8	Bw	303	
8	Cg	303	
8	Cq	303	
8	Da	303	
8	Dk	303	
8	Du	303	
8	Ee	303	
8	Eo	303	
8	Ey	303	
9	Aj	93	
9	At	93	
9	Bd	93	
9	Bn	93	
9	Bx	93	
9	Ch	93	
9	Cr	93	
9	Db	93	
9	Dl	93	
9	Dv	93	
9	Ef	93	
9	Ep	93	

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Mol	Chain	Length	Quality of chain
9	Ez	93	8% 48% 26% • 24%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 147498 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 DotD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ae	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Ak	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ao	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Au	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ay	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Be	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Bi	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Bo	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Bs	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	By	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cc	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Ci	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cm	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Cs	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Cw	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dc	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Dg	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dm	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Dq	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Dw	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ea	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Eg	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Ek	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		
1	Eq	139	Total	C	N	O	S	0	0
			1078	687	184	205	2		
1	Eu	136	Total	C	N	O	S	0	0
			1049	666	180	201	2		

- Molecule 2 is a protein called LphA (DotK).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Al	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Av	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bf	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bp	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Bz	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Cj	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Ct	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Dd	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Dn	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	Dx	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Eh	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		
2	Er	149	Total	C	N	O	S	0	0
			1161	737	207	213	4		

- Molecule 3 is a protein called Putative auto-transporter adhesin head GIN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ac	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Am	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Aw	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Bg	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Bq	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ca	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ck	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Cu	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	De	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Do	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Dy	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Ei	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		
3	Es	292	Total	C	N	O	S	0	0
			2321	1467	416	434	4		

- Molecule 4 is a protein called Neurogenic locus notch protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ad	76	Total	C	N	O	S	0	0
			565	347	96	109	13		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	An	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Ax	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Bh	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Br	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cb	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cl	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Cv	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Df	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Dp	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Dz	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Ej	76	Total 565	C 347	N 96	O 109	S 13	0	0
4	Et	76	Total 565	C 347	N 96	O 109	S 13	0	0

- Molecule 5 is a protein called IcmG (DotF).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Af	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Ap	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Az	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Bj	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Bt	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Cd	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Cn	59	Total 449	C 290	N 77	O 81	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Cx	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Dh	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Dr	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Eb	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	El	59	Total 449	C 290	N 77	O 81	S 1	0	0
5	Ev	59	Total 449	C 290	N 77	O 81	S 1	0	0

- Molecule 6 is a protein called IcmK (DotH).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ag	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Aq	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Ba	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Bk	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Bu	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Ce	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Co	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Cy	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Di	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Ds	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Ec	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Em	91	Total 691	C 440	N 121	O 126	S 4	0	0
6	Ew	91	Total 691	C 440	N 121	O 126	S 4	0	0

- Molecule 7 is a protein called Outer membrane protein, OmpA family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ah	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ar	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bb	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bl	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Bv	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cf	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cp	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Cz	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Dj	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Dt	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ed	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	En	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		
7	Ex	193	Total	C	N	O	S	0	0
			1500	947	273	275	5		

- Molecule 8 is a protein called DotC.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ai	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	As	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bc	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bm	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Bw	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		
8	Cg	249	Total	C	N	O	S	0	0
			1970	1249	345	369	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	Cq	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Da	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Dk	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Du	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Ee	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Eo	249	Total 1970	C 1249	N 345	O 369	S 7	0	0
8	Ey	249	Total 1970	C 1249	N 345	O 369	S 7	0	0

- Molecule 9 is a protein called Secreted protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Aj	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	At	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Bd	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Bn	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Bx	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Ch	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Cr	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Db	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Dl	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Dv	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Ef	71	Total 562	C 355	N 93	O 109	S 5	0	0
9	Ep	71	Total 562	C 355	N 93	O 109	S 5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ez	71	Total	C	N	O	S	0	0
			562	355	93	109	5		

There are 39 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Aj	43	ALA	GLY	conflict	UNP A0AAN5PM39
Aj	44	SER	ALA	conflict	UNP A0AAN5PM39
Aj	46	LEU	SER	conflict	UNP A0AAN5PM39
At	43	ALA	GLY	conflict	UNP A0AAN5PM39
At	44	SER	ALA	conflict	UNP A0AAN5PM39
At	46	LEU	SER	conflict	UNP A0AAN5PM39
Bd	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bd	44	SER	ALA	conflict	UNP A0AAN5PM39
Bd	46	LEU	SER	conflict	UNP A0AAN5PM39
Bn	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bn	44	SER	ALA	conflict	UNP A0AAN5PM39
Bn	46	LEU	SER	conflict	UNP A0AAN5PM39
Bx	43	ALA	GLY	conflict	UNP A0AAN5PM39
Bx	44	SER	ALA	conflict	UNP A0AAN5PM39
Bx	46	LEU	SER	conflict	UNP A0AAN5PM39
Ch	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ch	44	SER	ALA	conflict	UNP A0AAN5PM39
Ch	46	LEU	SER	conflict	UNP A0AAN5PM39
Cr	43	ALA	GLY	conflict	UNP A0AAN5PM39
Cr	44	SER	ALA	conflict	UNP A0AAN5PM39
Cr	46	LEU	SER	conflict	UNP A0AAN5PM39
Db	43	ALA	GLY	conflict	UNP A0AAN5PM39
Db	44	SER	ALA	conflict	UNP A0AAN5PM39
Db	46	LEU	SER	conflict	UNP A0AAN5PM39
Dl	43	ALA	GLY	conflict	UNP A0AAN5PM39
Dl	44	SER	ALA	conflict	UNP A0AAN5PM39
Dl	46	LEU	SER	conflict	UNP A0AAN5PM39
Dv	43	ALA	GLY	conflict	UNP A0AAN5PM39
Dv	44	SER	ALA	conflict	UNP A0AAN5PM39
Dv	46	LEU	SER	conflict	UNP A0AAN5PM39
Ef	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ef	44	SER	ALA	conflict	UNP A0AAN5PM39
Ef	46	LEU	SER	conflict	UNP A0AAN5PM39
Ep	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ep	44	SER	ALA	conflict	UNP A0AAN5PM39
Ep	46	LEU	SER	conflict	UNP A0AAN5PM39

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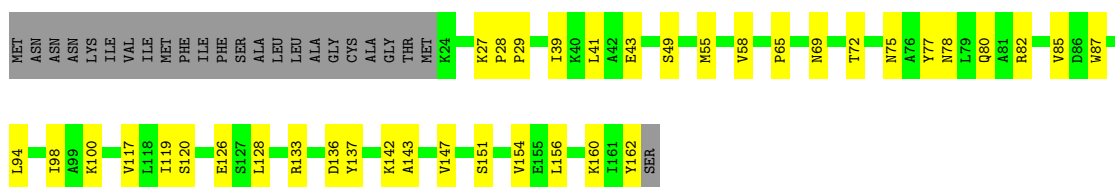
Chain	Residue	Modelled	Actual	Comment	Reference
Ez	43	ALA	GLY	conflict	UNP A0AAN5PM39
Ez	44	SER	ALA	conflict	UNP A0AAN5PM39
Ez	46	LEU	SER	conflict	UNP A0AAN5PM39

3 Residue-property plots

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.

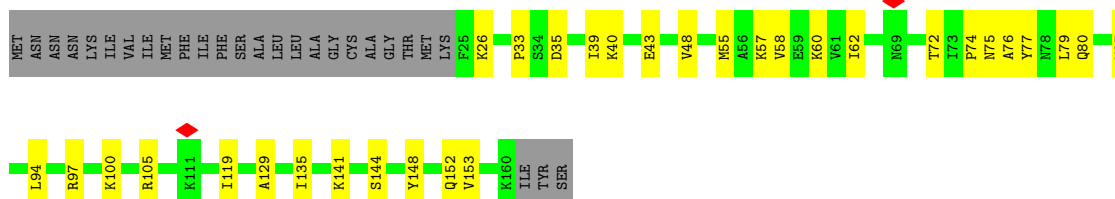
• Molecule 1: DotD

Chain Aa: 



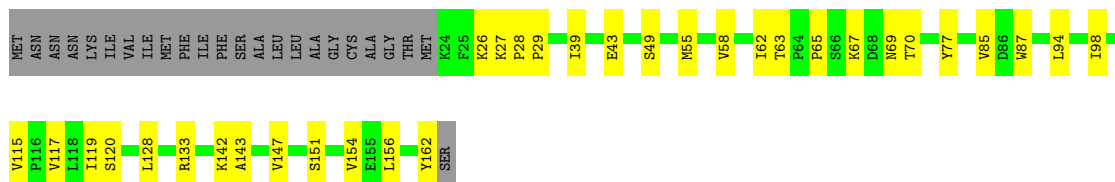
• Molecule 1: DotD

Chain Ae: 



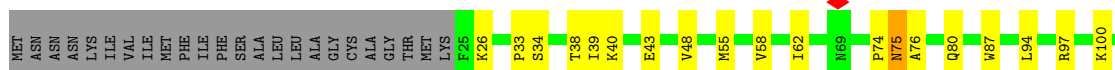
• Molecule 1: DotD

Chain Ak: 



• Molecule 1: DotD

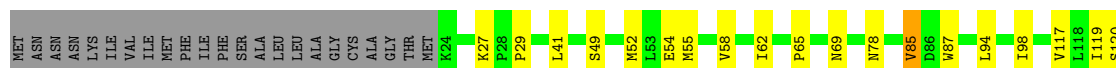
Chain Ao: 





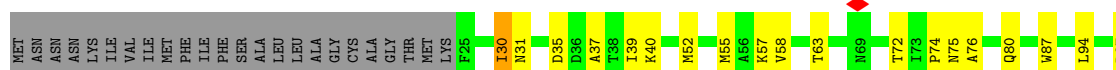
- Molecule 1: DotD

Chain Au: 69% 16% 15%



- Molecule 1: DotD

Chain Ay: 63% 20% 17%



- Molecule 1: DotD

Chain Be: 64% 20% 15%



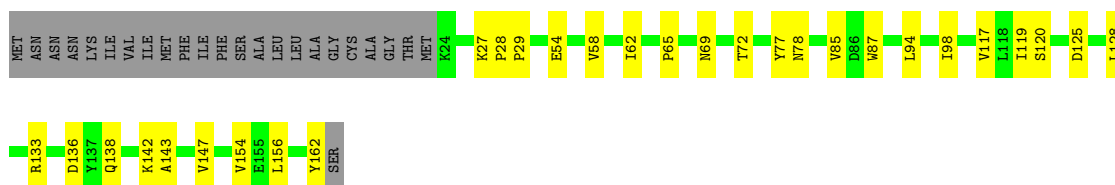
- Molecule 1: DotD

Chain Bi: 63% 19% 17%

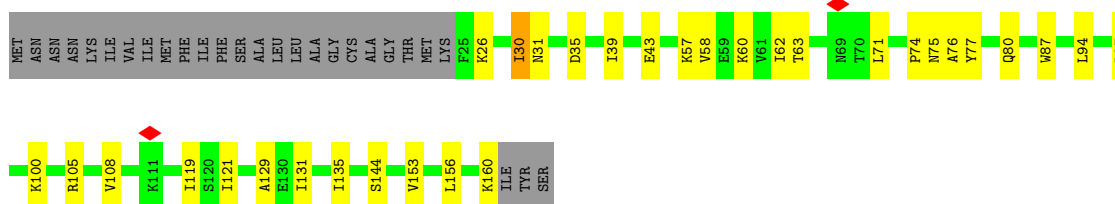


- Molecule 1: DotD

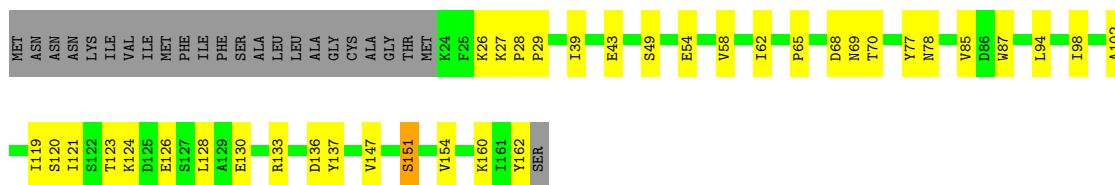
Chain Bo: 67% 18% 15%



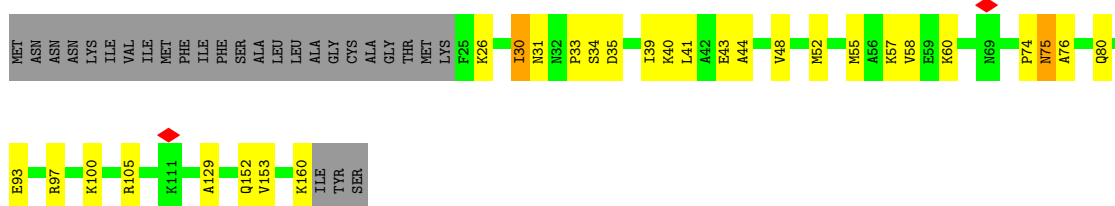
• Molecule 1: DotD



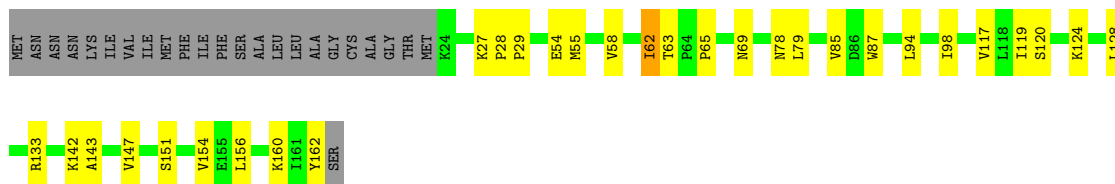
• Molecule 1: DotD



• Molecule 1: DotD

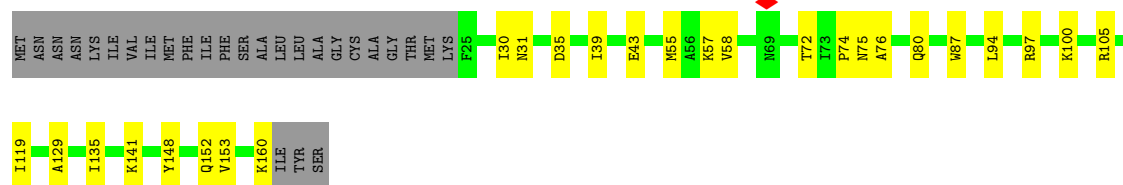


• Molecule 1: DotD



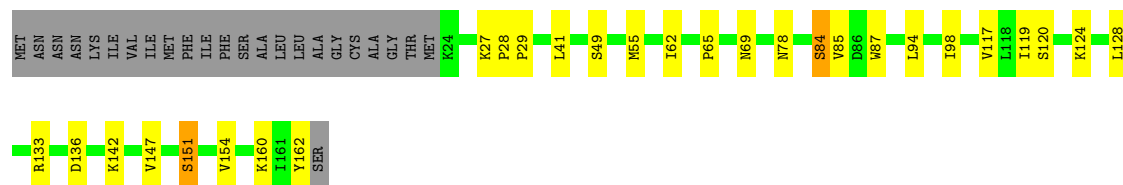
• Molecule 1: DotD

Chain Cm:  67% 16% 17%



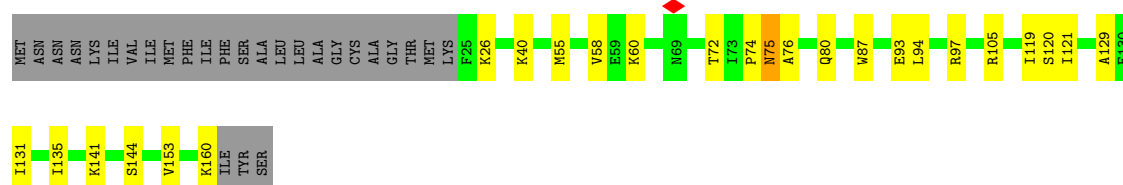
• Molecule 1: DotD

Chain Cs:  68% 16% 15%



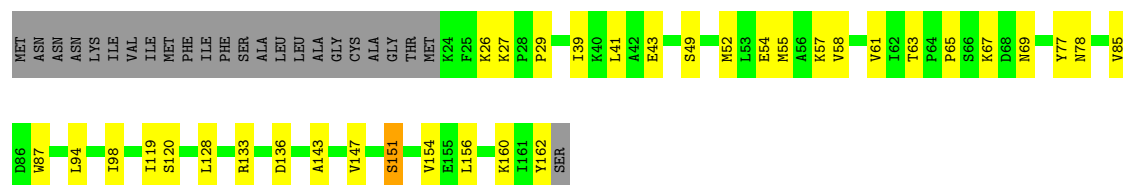
• Molecule 1: DotD

Chain Cw:  68% 15% 17%



• Molecule 1: DotD

Chain Dc:  64% 21% 15%



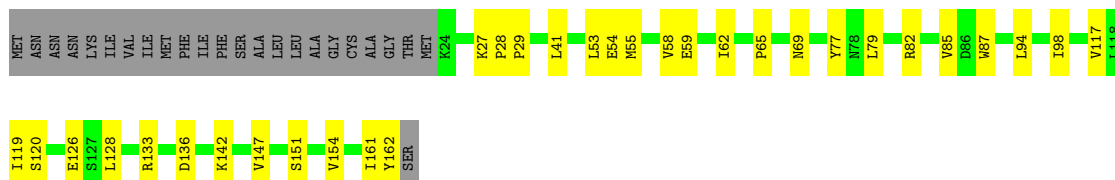
• Molecule 1: DotD

Chain Dg:  67% 16% 17%



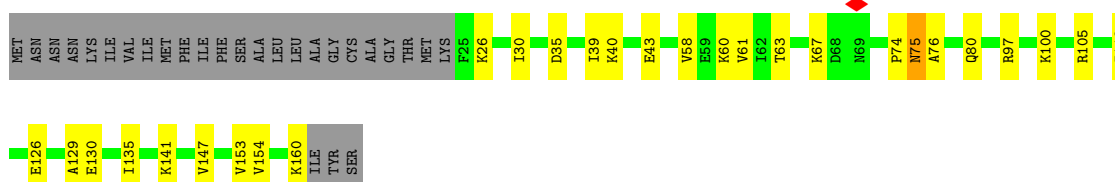
- Molecule 1: DotD

Chain Dm:  66% 20% 15%



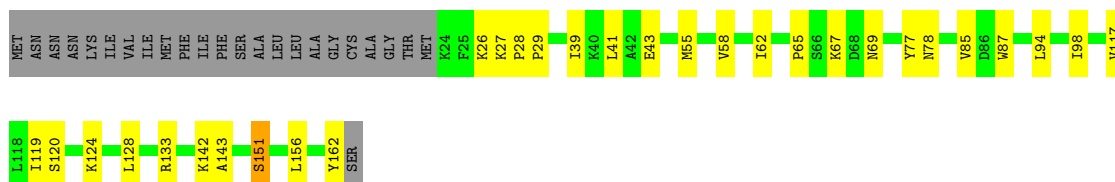
- Molecule 1: DotD

Chain Dq:  66% 17% 17%



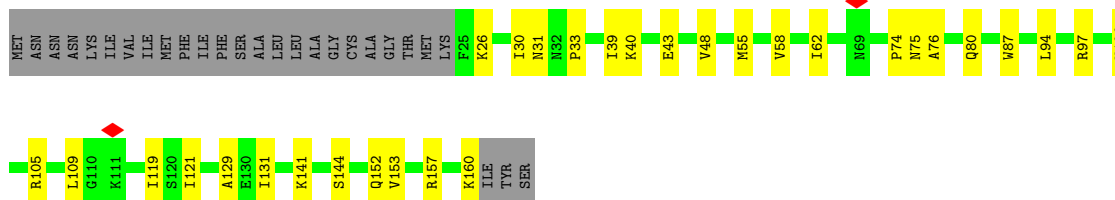
- Molecule 1: DotD

Chain Dw:  67% 18% 15%



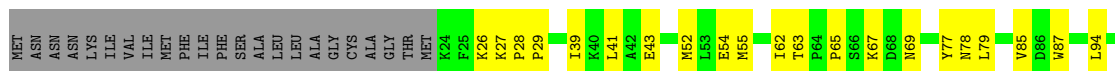
- Molecule 1: DotD

Chain Ea:  64% 19% 17%



- Molecule 1: DotD

Chain Eg:  63% 22% 15%





- Molecule 1: DotD



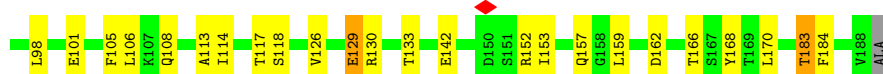
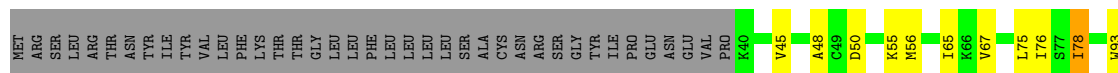
- Molecule 1: DotD



- Molecule 1: DotD

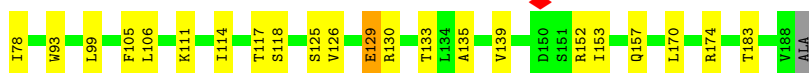
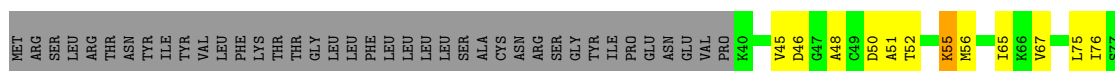


- Molecule 2: LphA (DotK)

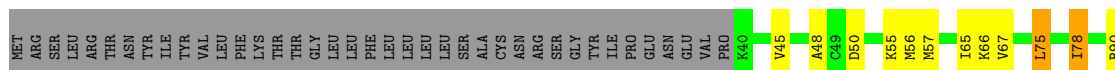


- Molecule 2: LphA (DotK)

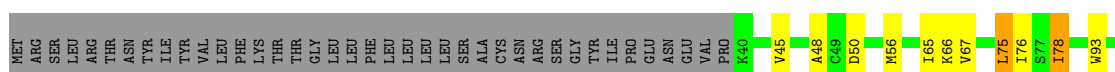




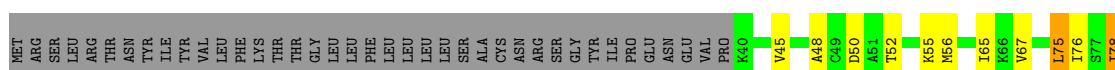
• Molecule 2: LphA (DotK)



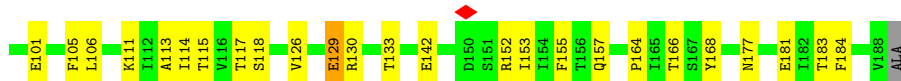
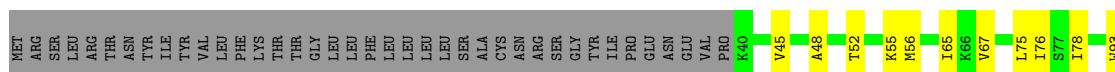
• Molecule 2: LphA (DotK)



• Molecule 2: LphA (DotK)



• Molecule 2: LphA (DotK)



● Molecule 2: LphA (DotK)

Chain Cj:  58% 20% 21%

MET	ARG	SER	LEU	ARG	THR	ASN	TYR	ILE	TYR	VAL	PHE	LYS	THR	GLY	LEU	LEU	PHE	LEU	LEU	LEU	SER	ALA	CYS	ASN	ARG	SER	GLY	TYR	ILE	PRO	GLU	ASN	GLU	VAL	PRO	K40	V45	V45	A48	C49	D50	A51	T52	I53	T54	K55	M56	M57	I65	K66	V67	L75	I76
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

S77	I78	R90	W93	L98	E101	L106	K111	I112	A113	I114	T117	S118	V126	E129	T133	L134	A135	V139	E142	G148	V149	D150	S151	R152	I153	Q157	T166	S167	Y168	T169	L170	T183	F184	V188	ALA
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● Molecule 2: LphA (DotK)

Chain Ct:  62% 15% 21%

MET	ARG	SER	LEU	ARG	THR	ASN	TYR	ILE	TYR	VAL	PHE	LYS	THR	GLY	LEU	LEU	PHE	LEU	LEU	LEU	SER	ALA	CYS	ASN	ARG	SER	GLY	TYR	ILE	PRO	GLU	ASN	GLU	VAL	PRO	K40	V45	V45	A48	C49	D50	A51	T52	K55	M56	I65	K66	V67	L75	I76	S77	I78
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

W93	L99	L106	K111	I112	A113	I114	S118	K122	V126	E129	T133	D150	S151	I153	T166	S167	Y168	T169	L170	R174	T183	F184	V188	ALA
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● Molecule 2: LphA (DotK)

Chain Dd:  60% 18% 21%

MET	ARG	SER	LEU	ARG	THR	ASN	TYR	ILE	TYR	VAL	PHE	LYS	THR	GLY	LEU	LEU	PHE	LEU	LEU	LEU	SER	ALA	CYS	ASN	ARG	SER	GLY	TYR	ILE	PRO	GLU	ASN	GLU	VAL	PRO	K40	V45	V45	A48	C49	D50	A51	T52	M56	I65	K66	V67	L75	I76	S77	I78
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

W93	L98	F105	L106	R110	K111	T112	A113	I114	T117	S118	K127	R130	T133	L134	A135	V139	E142	D150	S151	I153	Q157	I165	R174	T183	F184	V188	ALA
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● Molecule 2: LphA (DotK)

Chain Dn:  63% 15% 21%

MET	ARG	SER	LEU	ARG	THR	ASN	TYR	ILE	TYR	VAL	PHE	LYS	THR	GLY	LEU	LEU	PHE	LEU	LEU	LEU	SER	ALA	CYS	ASN	ARG	SER	GLY	TYR	ILE	PRO	GLU	ASN	GLU	VAL	PRO	K40	V45	D46	G47	A48	C49	D50	A51	K55	I65	K66	V67	L75	I76	S77	I78
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W93	E101	L106	K111	T112	A113	I114	T117	R130	S146	Q147	G148	V149	D150	S151	I153	Q157	P164	I165	T166	S167	Y168	N177	T183	F184	V188	ALA
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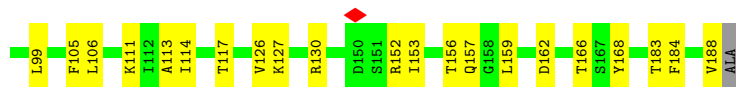
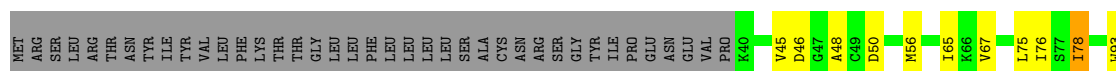
● Molecule 2: LphA (DotK)

Chain Dx:  63% 14% 21%

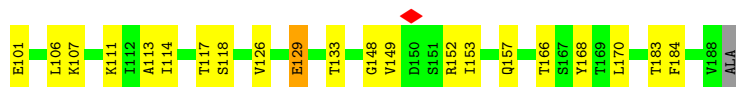
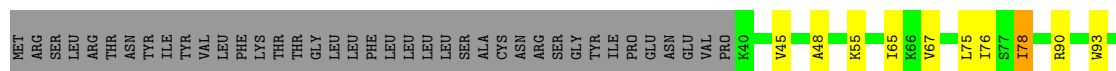
MET	ARG	SER	LEU	ARG	THR	ASN	TYR	ILE	TYR	VAL	PHE	LYS	THR	GLY	LEU	LEU	PHE	LEU	LEU	LEU	SER	ALA	CYS	ASN	ARG	SER	GLY	TYR	ILE	PRO	GLU	ASN	GLU	VAL	PRO	K40	V45	V45	A48	K55	M56	I65	K66	V67	L75	I76	S77	I78	W93	L99
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



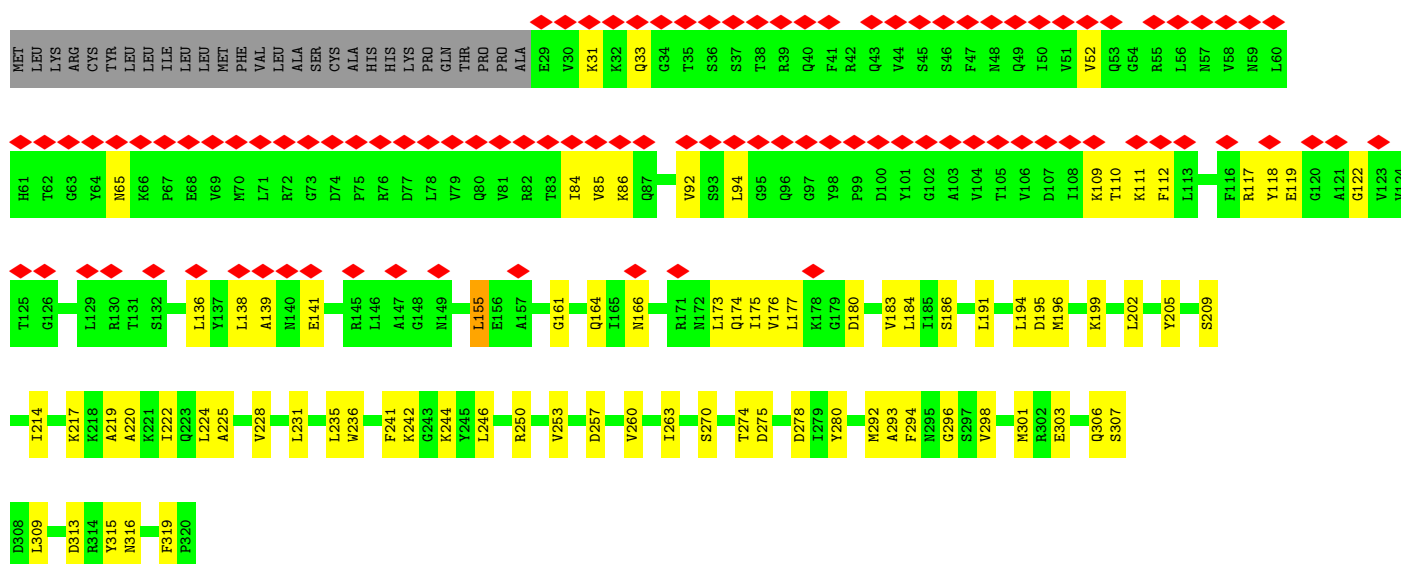
• Molecule 2: LphA (DotK)



• Molecule 2: LphA (DotK)

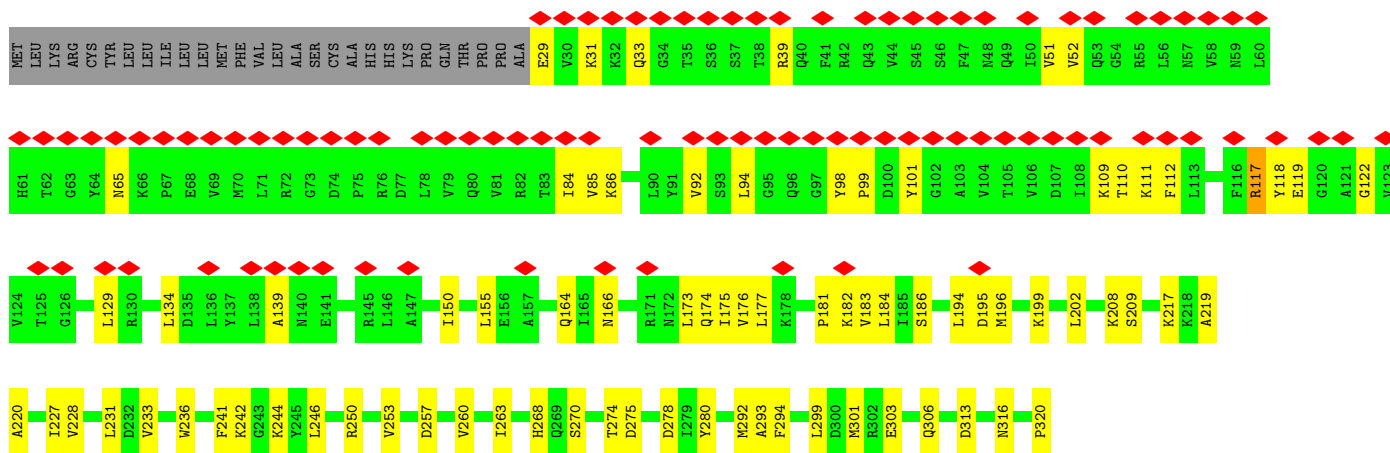


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

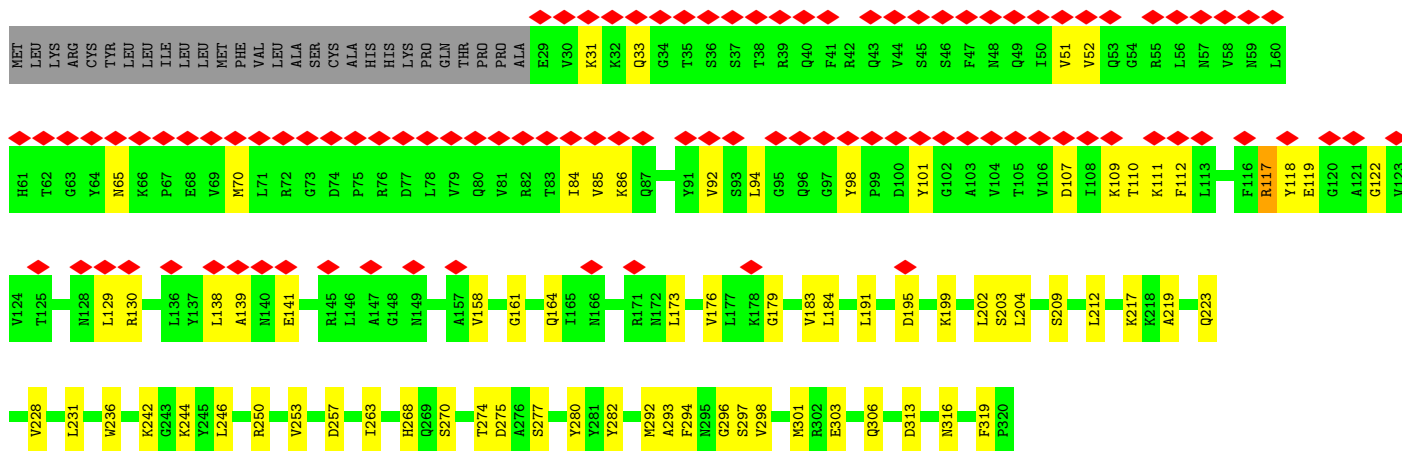


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

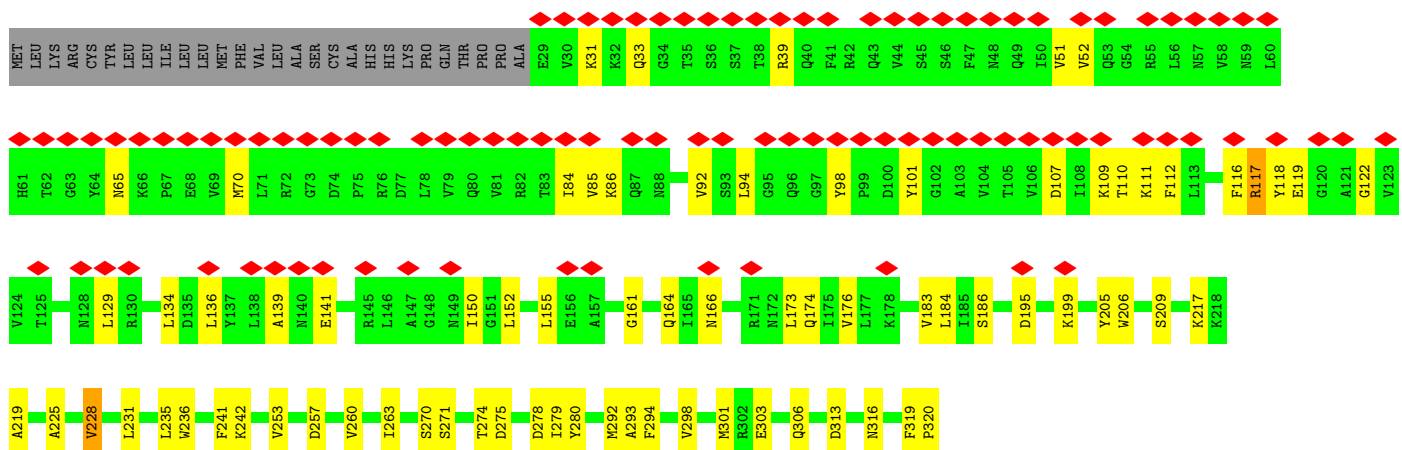




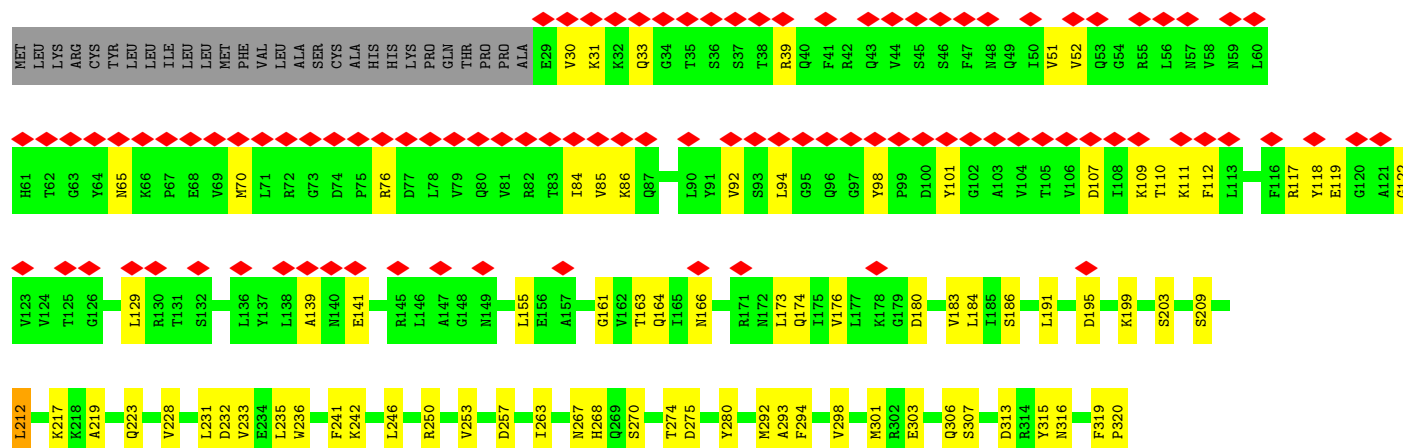
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein



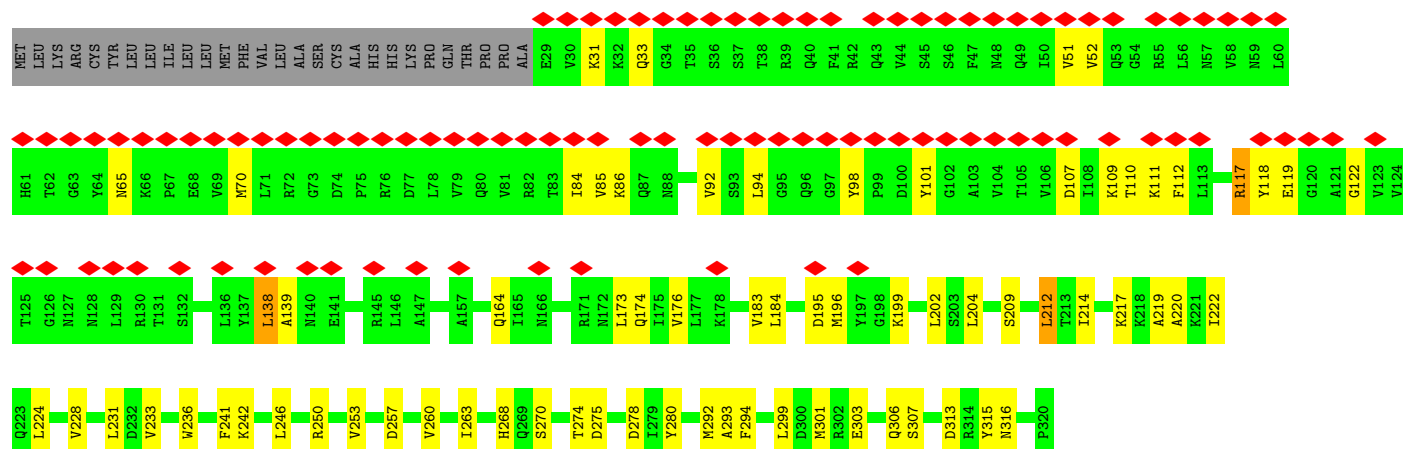
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein



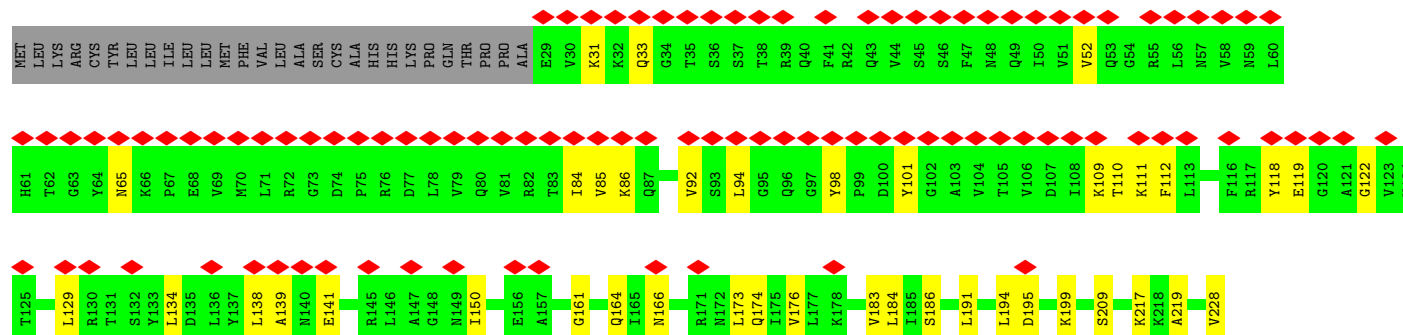
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein



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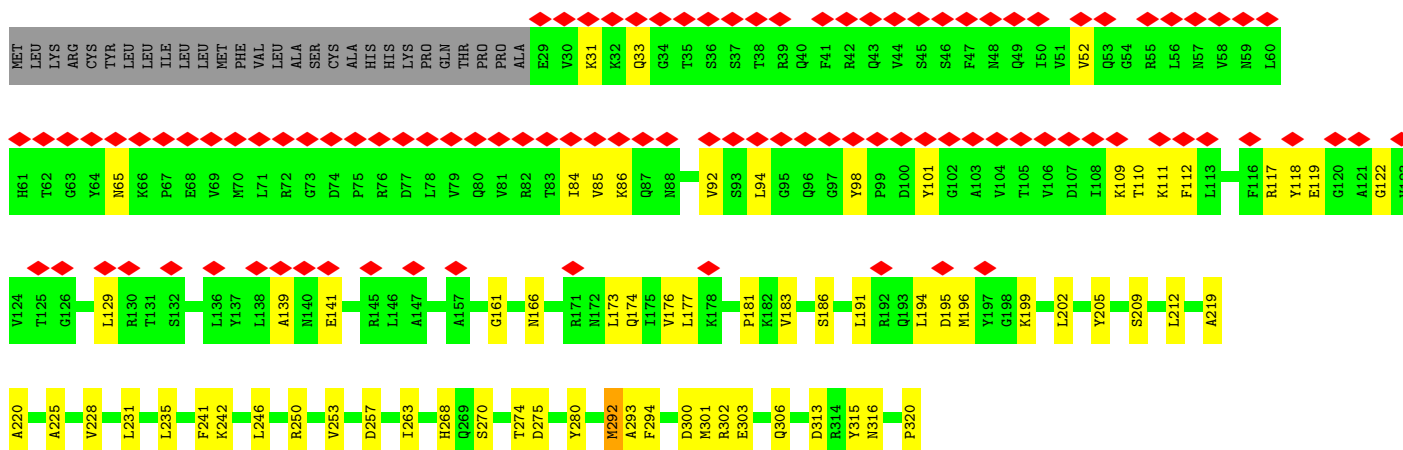


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

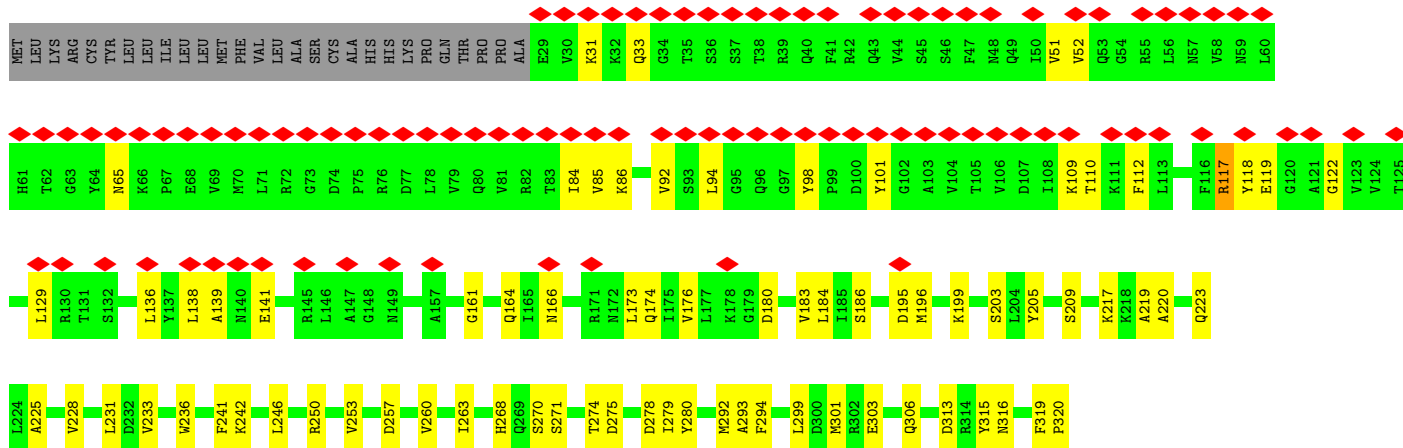




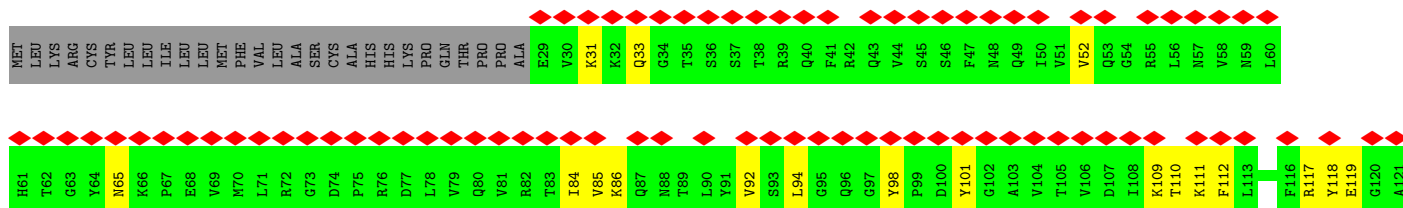
• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

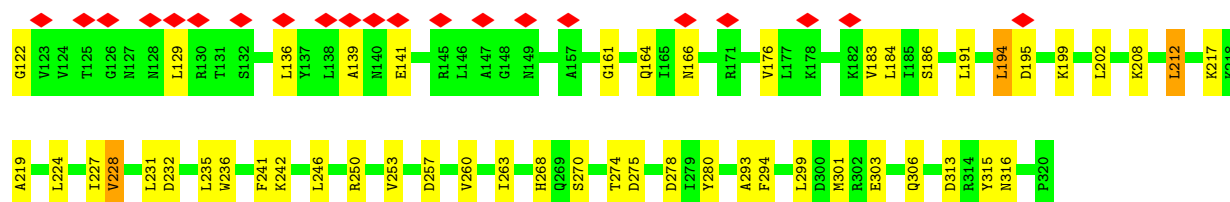


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

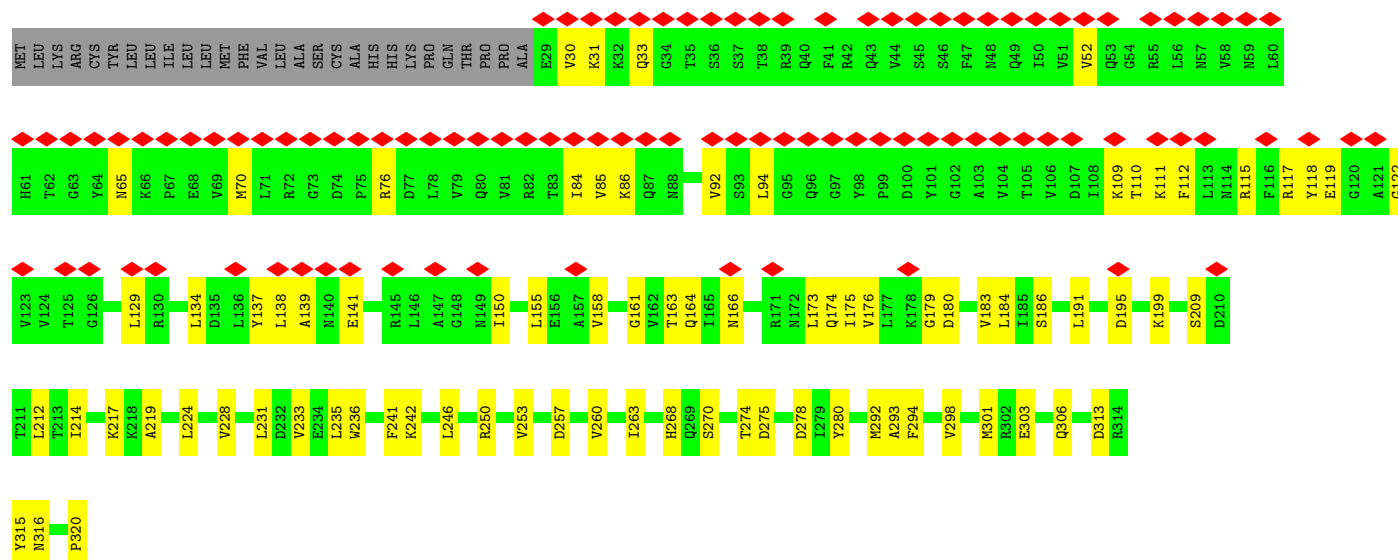


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

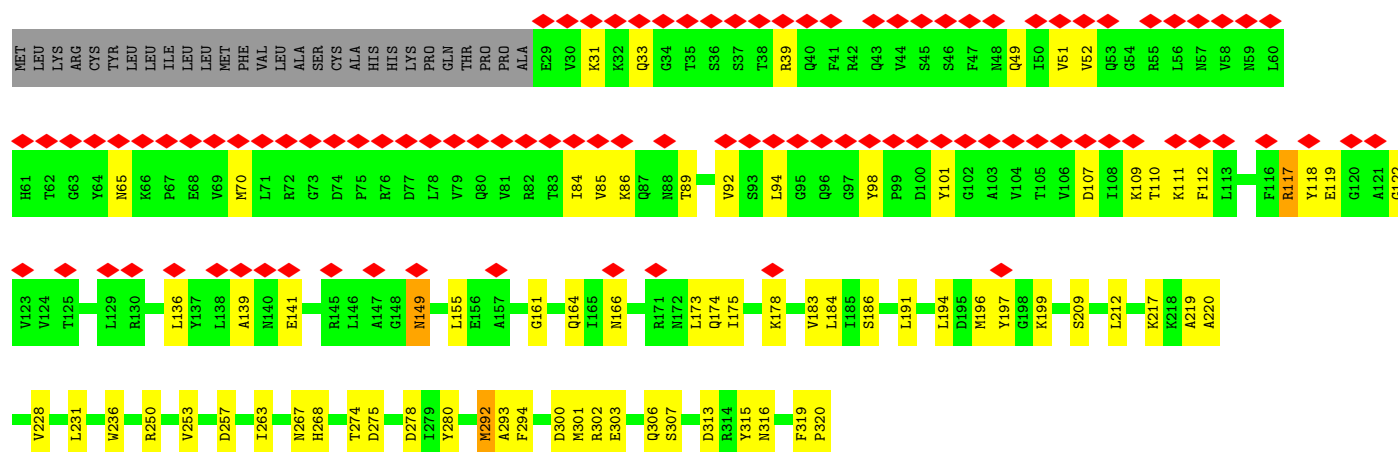




• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

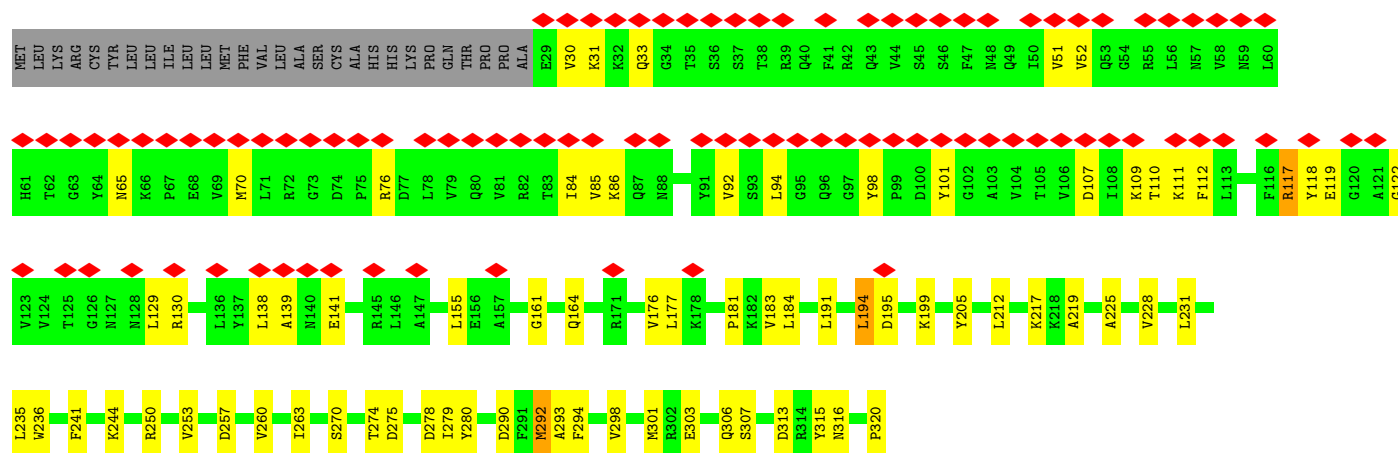


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

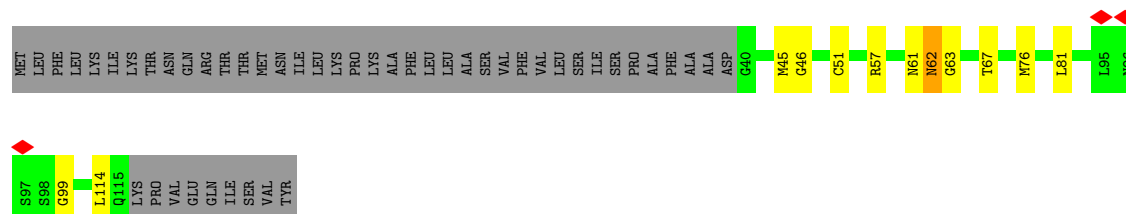


• Molecule 3: Putative auto-transporter adhesin head GIN domain-containing protein

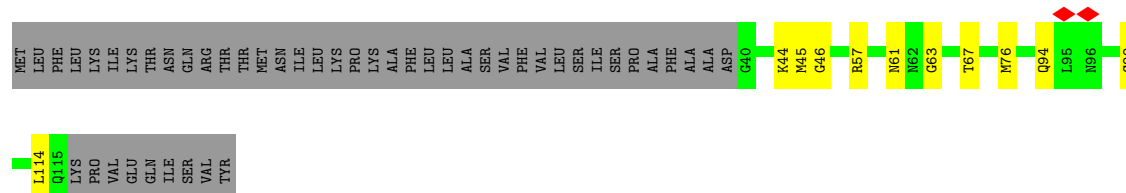




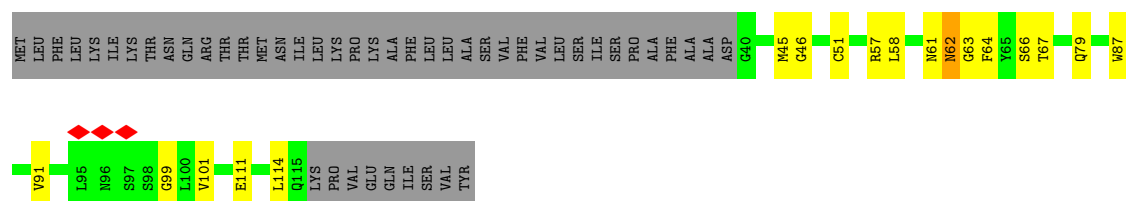
- Molecule 4: Neurogenic locus notch protein homolog



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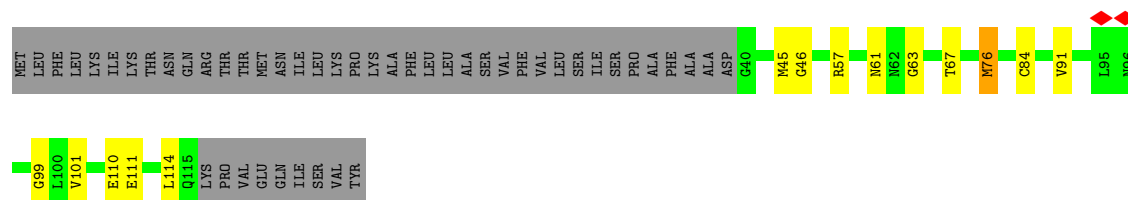


- Molecule 4: Neurogenic locus notch protein homolog

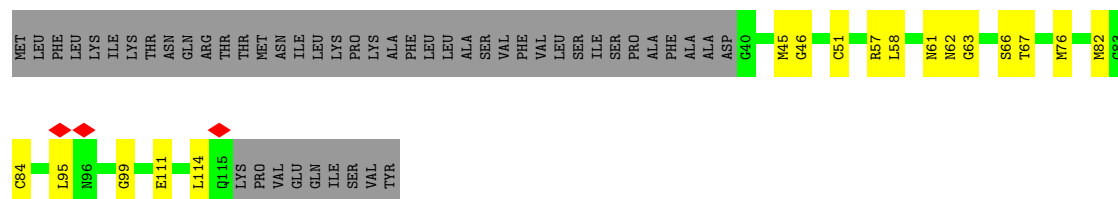


- Molecule 4: Neurogenic locus notch protein homolog

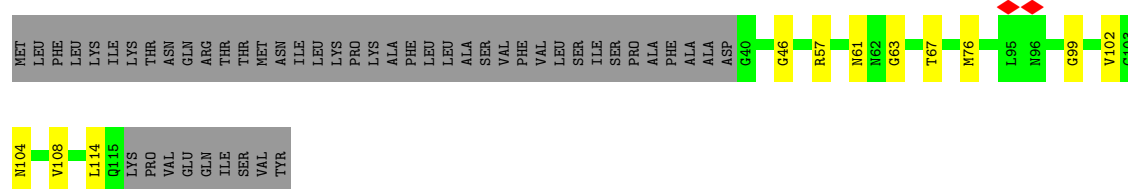




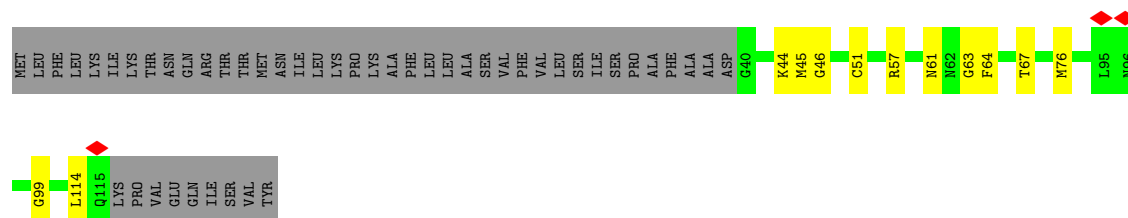
- Molecule 4: Neurogenic locus notch protein homolog



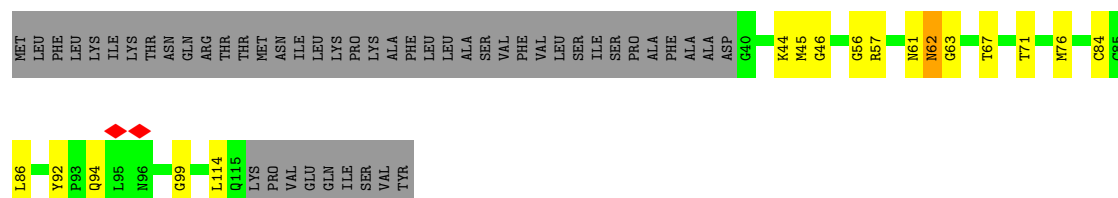
- Molecule 4: Neurogenic locus notch protein homolog



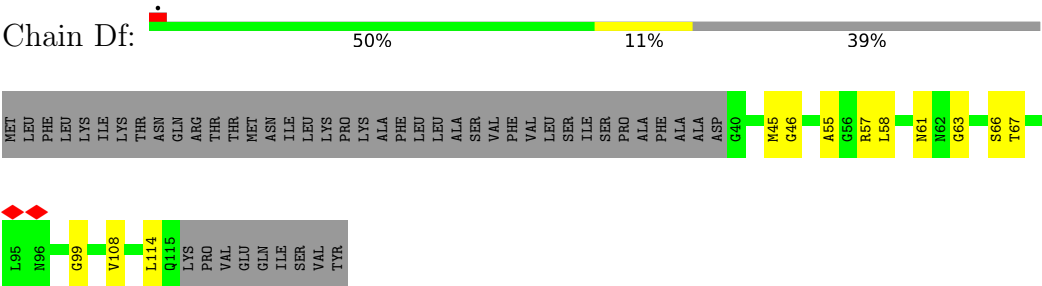
- Molecule 4: Neurogenic locus notch protein homolog



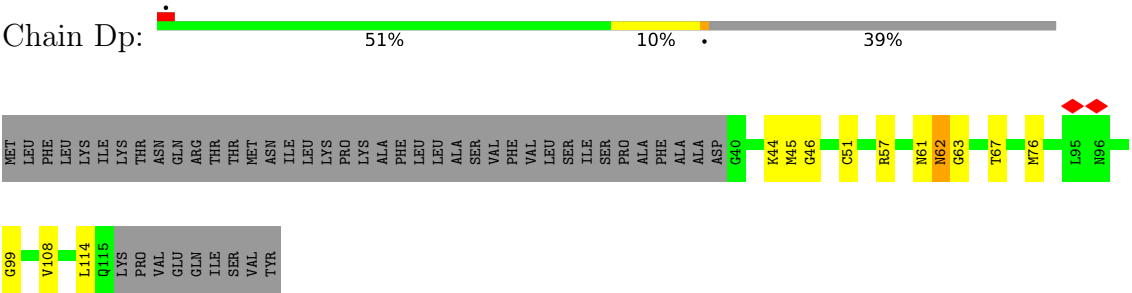
- Molecule 4: Neurogenic locus notch protein homolog



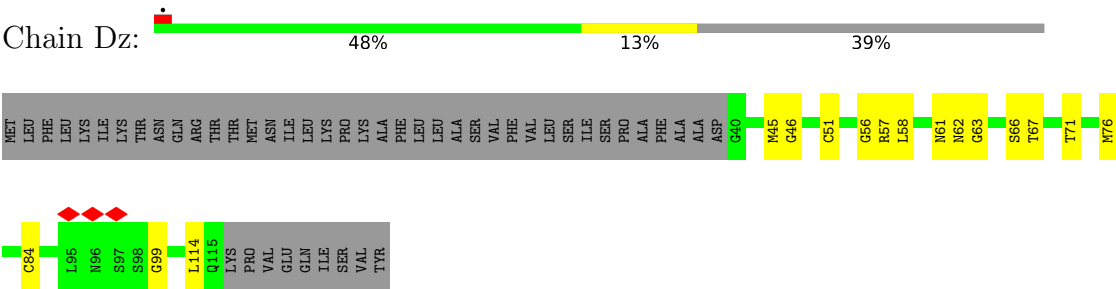
• Molecule 4: Neurogenic locus notch protein homolog



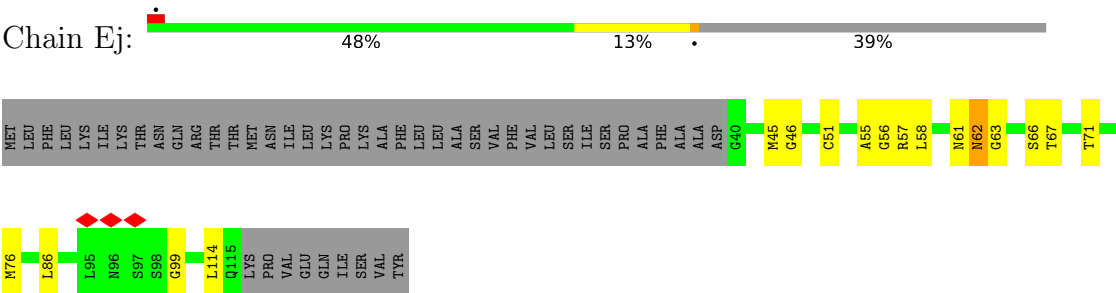
• Molecule 4: Neurogenic locus notch protein homolog



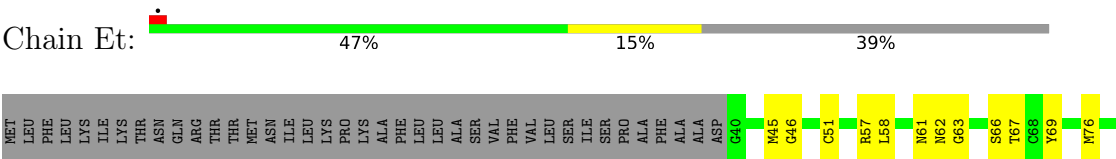
• Molecule 4: Neurogenic locus notch protein homolog

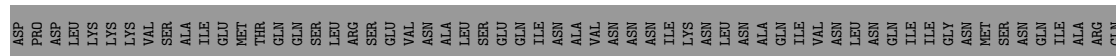


• Molecule 4: Neurogenic locus notch protein homolog



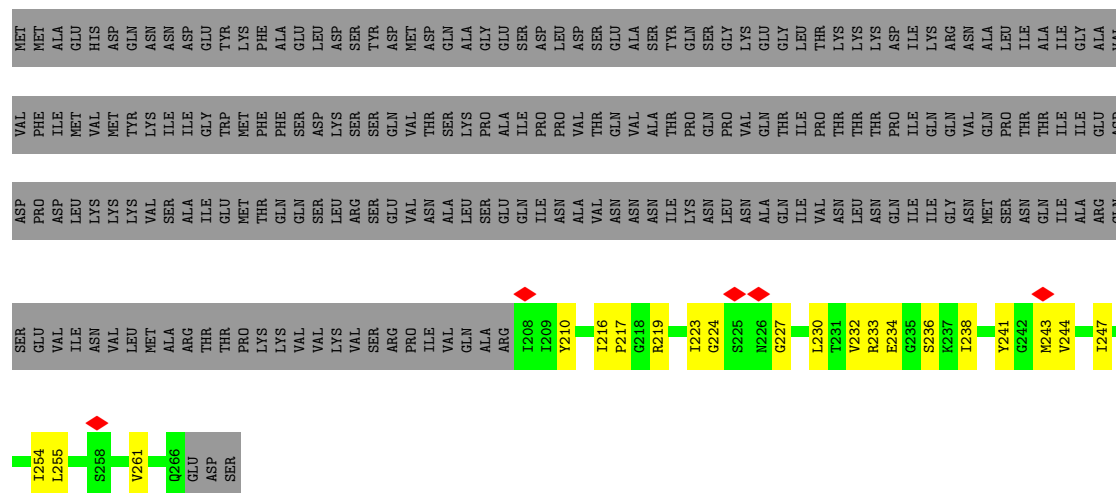
• Molecule 4: Neurogenic locus notch protein homolog





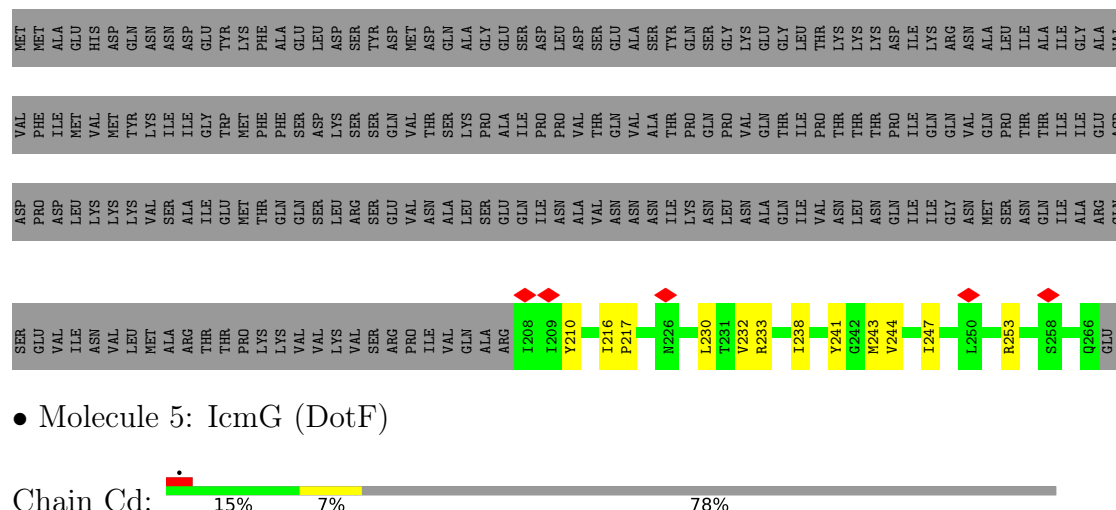
- Molecule 5: IcmG (DotF)

Chain Bi: 14% 8% 78%

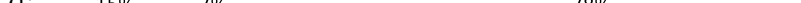


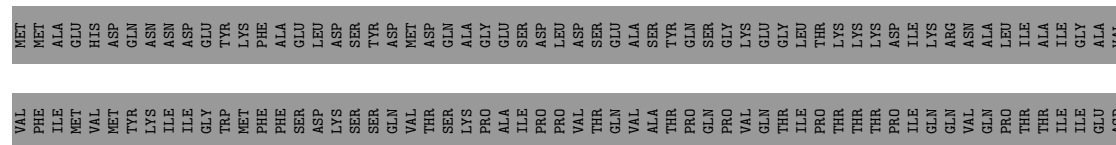
- Molecule 5: IcmG (DotF)

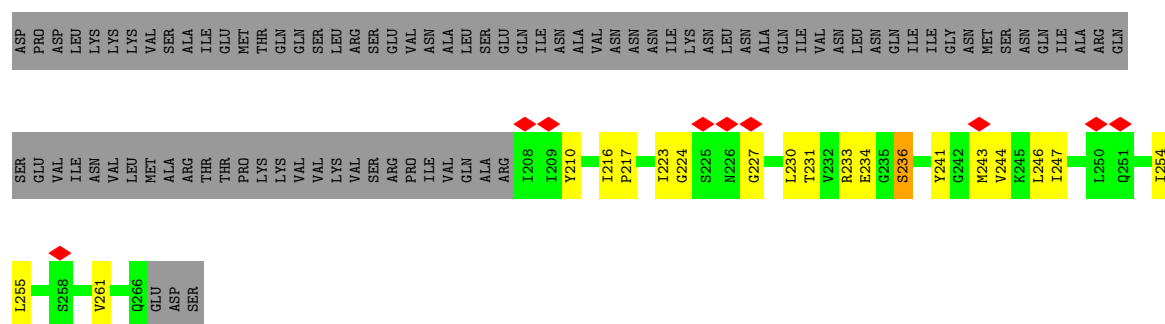
Chain Bt: 17% 78%



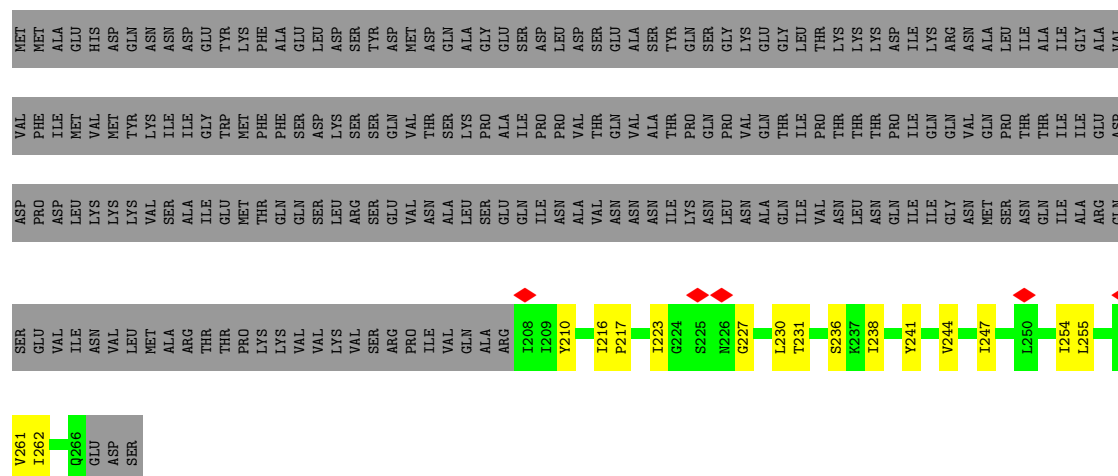
- Molecule 5: IcmG (DotF)

Chain Cd: 

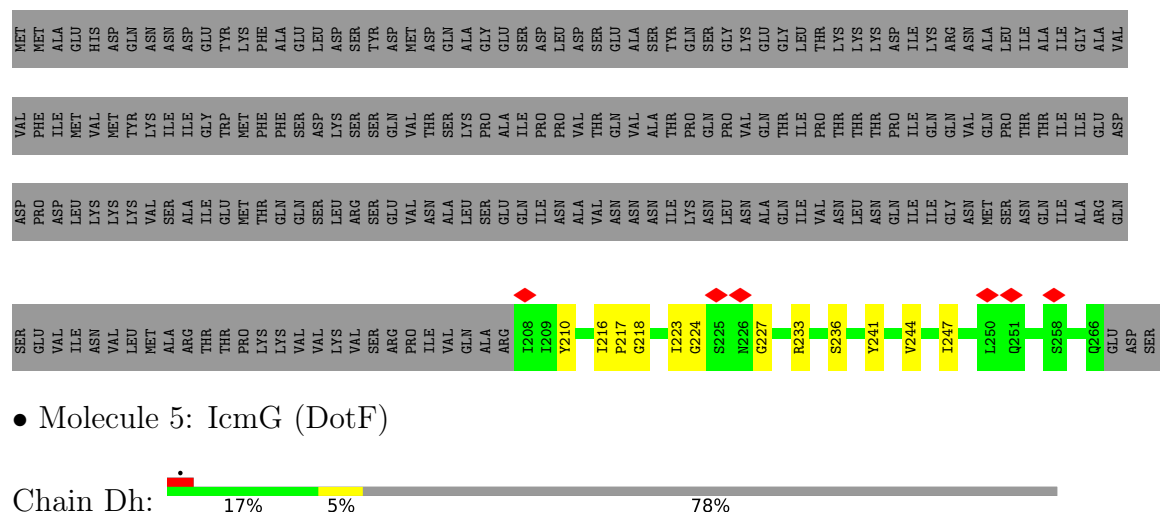




- Molecule 5: IcmG (DotF)



- Molecule 5: IcmG (DotF)



- Molecule 5: IcmG (DotF)









• Molecule 6: IcmK (DotH)



MET	MET	LYS	LYS	TYR	ASP	GLN	LEU	CYS	TYR	TYR	CYS	LEU	VAL	ILE	GLY	LEU	THR	PHE	SER	MET	CYS	ALA	ASP	THR	ILE	ALA	GLN	LEU	GLN	LEU	GLN	LEU	ASP	ARG	MET	LEU	GLN	GLN	PRO	PHE	LYS	PRO	ASP	PRO	ASP	ALA	GLN	SER	GLY	ALA			
GLY	ASP	GLY	GLY	ASP	ASN	ALA	ALA	SER	ASP	THR	THR	GLN	GLN	PRO	ASN	GLY	SER	GLY	ALA	GLN	ALA	ASN	ALA	ASN	ALA	PRO	ALA	ALA	ASN	GLN	THR	THR	ALA	THR	ALA	THR	ALA	GLY	GLY	GLN	GLN	GLY	ILE	ILE	SER	GLN	LEU	ASP	ASP	GLY	THR	VAL	TYR
PRO	LEU	ASN	PRO	GLY	GLN	VAL	VAL	LYS	PRO	LYS	GLN	ILE	TYR	GLY	THR	SER	ALA	PRO	TYR	ALA	LYS	ALA	ALA	ALA	PRO	GLY	THR	ASN	PRO	LYS	THR	THR	PRO	THR	THR	THR	ALA	ALA	THR	ILE	ASN	LEU	LEU	TYR	ASN	PRO	GLY	THR	VAL	THR			
PHE	LEU	ASP	SER	THR	GLY	ALA	ALA	PRO	TRP	PRO	ILE	ALA	ALA	TYR	ASP	GLY	GLY	ASP	PRO	SER	SER	PHE	ASN	ILE	TRP	GLN	TRP	ASP	LYS	THR	THR	SER	GLY	ASN	THR	THR	LEU	MET	ILE	THR	GLN	GLY	ALA	ALA	THR	LYS	THR	ASN	LEU	THR			
LEU	ILE	PRO	GLY	GLN	LYS	VAL	VAL	ASP	TYR	ARG	VAL	ASP	LEU	ARG	VAL	GLN	GLY	TYR	GLY	PRO	ASN	ALA	LYS	SER	MET	PRO	THR	GLY	GLU	GLU	G271	S275	V283	L284	E285	P289	P290	V297	S298	G299	A302	L306	Y312	I319	L320	S321	M328	T329	S330	M339			



• Molecule 6: IcmK (DotH)



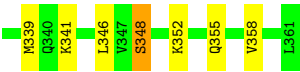
LEU	ILE	PRO	GLY	GLN	LYS	VAL	ASP	TYR	ASP	ARG	VAL	ASP	LEU	ARG	VAL	GLN	GLY	TYR	GLY	PRO	ASN	ASN	PRO	THR	THR	GLY	GLU	GLU	G271	S275	V283	L284	E285	P289	P290	V297	S298	A302	Y312	L317	T318	I319	L320	S321	M328	T329	S330	L346	V347		
PHE	LEU	ASP	SER	THR	GLY	ALA	ALA	PRO	TRP	PRO	ILE	ALA	ALA	TYR	ASP	GLY	GLY	ASP	PRO	SER	SER	PHE	ASN	ILE	TRP	GLN	TRP	ASP	LYS	THR	THR	SER	GLY	ASN	THR	THR	LEU	MET	ILE	THR	GLN	GLY	ALA	ALA	THR	LYS	THR	ASN	LEU	THR	
PRO	LEU	ASN	PRO	GLY	GLN	VAL	VAL	LYS	PRO	LYS	GLN	ILE	TYR	GLY	THR	SER	ALA	PRO	TYR	ALA	ALA	ALA	ASN	ALA	ALA	ALA	PRO	GLY	THR	ASN	PRO	LYS	ALA	THR	THR	THR	ALA	THR	ILE	SER	GLN	GLY	GLY	GLN	VAL	VAL	ILE	SER	GLN	GLY	THR
GLY	ASP	GLY	ASP	ASN	ASP	ALA	ALA	ALA	LEU	ASP	THR	THR	GLN	GLN	PRO	ASN	GLN	GLY	GLY	ALA	ALA	ASN	ALA	ALA	ALA	ALA	THR	THR	ALA	GLY	GLY	ASP	ALA	ASP	ALA	ASP	ALA	ALA	GLN	GLN	GLN	GLN	GLN	LEU	LEU	LEU	LEU	LEU	GLY	TYR	



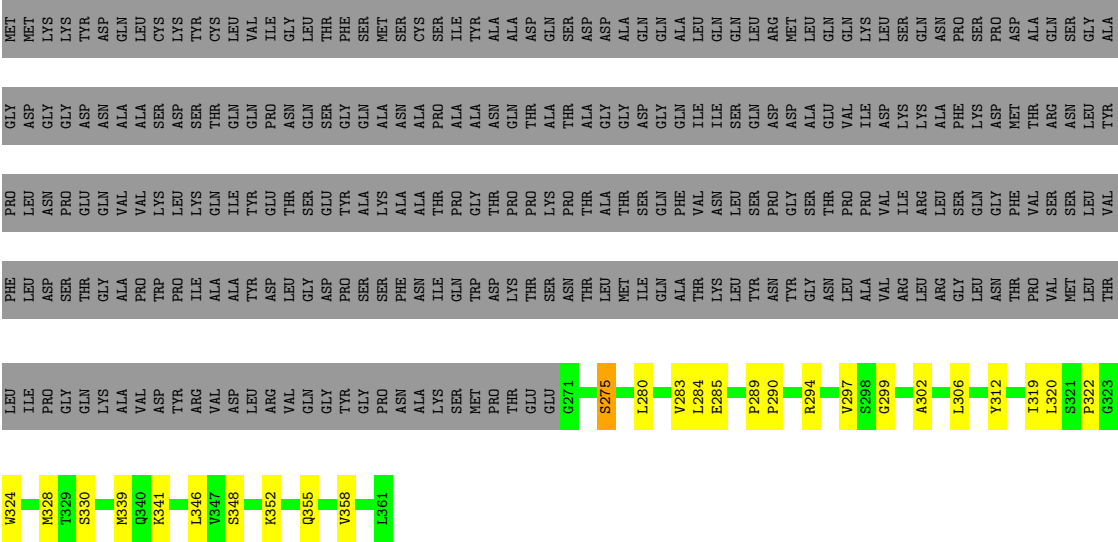
• Molecule 6: IcmK (DotH)



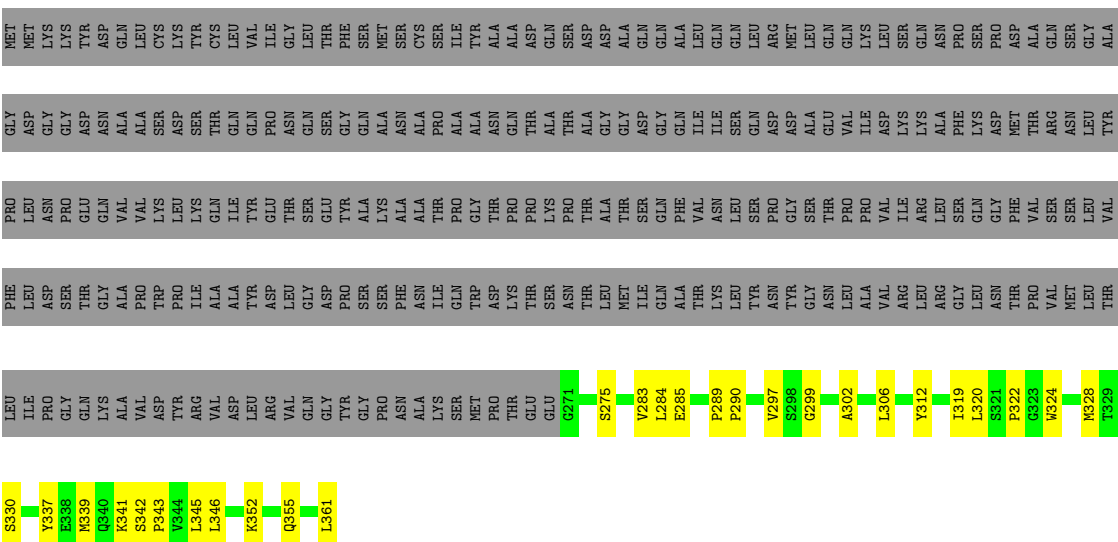
MET	MET	LYS	LYS	TYR	ASP	GLN	LEU	CYS	TYR	TYR	CYS	LEU	VAL	ILE	GLY	LEU	THR	PHE	SER	MET	CYS	ALA	ASP	THR	ILE	ALA	GLN	LEU	GLN	LEU	GLN	LEU	ARG	MET	LEU	GLN	GLN	PRO	PHE	LYS	PRO	ASP	PRO	ASP	ALA	GLN	SER	GLY	ALA
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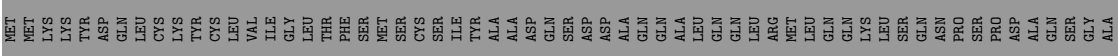
• Molecule 6: IcmK (DotH)



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• Molecule 6: IcmK (DotH)



Q355	L361	LEU	ILE	LEU	PHE	PRO	GLY
		ILE	LEU	LEU	LEU	LEU	GLY
L361		GLN	GLY	ASP	THR	GLU	ASP
		GLN	THR	THR	THR	GLN	GLN
		LYS	ALA	GLY	GLY	VAL	ALA
		ALA	ALA	PRO	ALA	VAL	ALA
		VAL	ASP	TRP	TRP	LYS	SER
		ASP	TYR	PRO	PRO	LEU	ASP
		ARG	ARG	ILE	ILE	LYS	SER
		VAL	VAL	ALA	ALA	THR	THR
		ASP	ASP	ALA	ALA	GLN	GLN
		VAL	VAL	TYR	TYR	ILE	GLN
		LEU	LEU	ASP	ASP	GLU	GLN
		VAL	VAL	GLY	GLY	THR	ASN
		GLN	GLN	PRO	PRO	THR	GLN
		GLY	GLY	ASP	ASP	GLY	SER
		TYR	TYR	THR	THR	TYR	GLY
		GLY	GLY	SER	SER	ALA	GLN
		PRO	PRO	SER	SER	LYS	ALA
		ASN	ASN	PHE	PHE	ALA	ASN
		ALA	ALA	ASN	ASN	ALA	ALA
		LYS	LYS	ILE	ILE	THR	PRO
		SER	SER	GLN	GLN	ALA	ALA
		MET	MET	TRP	TRP	GLY	PRO
		PRO	PRO	ASP	ASP	THR	ASN
		THR	THR	LYS	LYS	PRO	GLN
		GLU	GLU	THR	THR	PRO	THR
		GLY	GLY	SER	SER	LYS	ALA
		S271	S271	ASN	ASN	PRO	THR
		S275	S275	THR	THR	THR	ALA
		V263	V263	ILE	ILE	SER	ASP
		L284	L284	GLN	GLN	GLN	GLY
		E285	E285	ALA	ALA	PHE	GLN
		G259	G259	THR	THR	VAL	ILE
				LYS	LYS	ASN	SER
				LEU	LEU	LEU	THR
		Y312	Y312	TYR	TYR	SER	GLN
		L320	L320	ASN	ASN	PRO	ASP
		S321	S321	TYR	TYR	GLY	ASP
		M328	M328	GLY	GLY	SER	ALA
		T329	T329	ASN	ASN	THR	GLU
		S330	S330	LEU	LEU	PRO	VAL
				ALA	ALA	PRO	ILE
		Y337	Y337	ARG	ARG	VAL	ASP
		K341	K341	LEU	LEU	ILE	LYS
		L346	L346	ARG	ARG	ARG	LYS
		V347	V347	GLY	GLY	LEU	ALA
		S348	S348	LEU	LEU	SER	PHE
				THR	THR	GLN	LYS
		K352	K352	ASN	ASN	GLY	ASP
		V353	V353	THR	THR	PHE	MET
		M354	M354	PRO	PRO	VAL	THR
				VAL	VAL	SER	ASN
				LEU	LEU	SER	THR
				THR	THR	ILE	THR
				THR	THR	VAL	THR

- Molecule 6: IcmK (DotH)

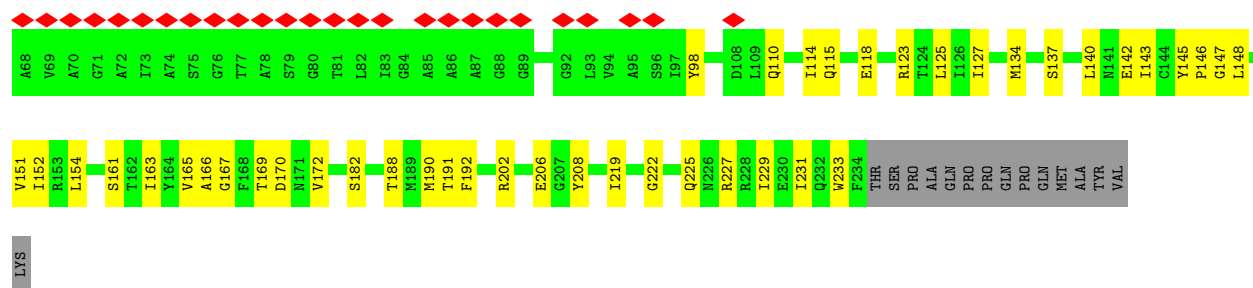
Chain Ds:

L346	L350	L354	L358	L361	L365	L369	L373	L377	L381	L385	L389	L393	L397	L401	L405	L409	L413	L417	L421	L425	L429	L433	L437	L441	L445	L449	L453	L457	L461	L465	L469	L473	L477	L481	L485	L489	L493	L497	L501	L505	L509	L513	L517	L521	L525	L529	L533	L537	L541	L545	L549	L553	L557	L561	L565	L569	L573	L577	L581	L585	L589	L593	L597	L601	L605	L609	L613	L617	L621	L625	L629	L633	L637	L641	L645	L649	L653	L657	L661	L665	L669	L673	L677	L681	L685	L689	L693	L697	L701	L705	L709	L713	L717	L721	L725	L729	L733	L737	L741	L745	L749	L753	L757	L761	L765	L769	L773	L777	L781	L785	L789	L793	L797	L801	L805	L809	L813	L817	L821	L825	L829	L833	L837	L841	L845	L849	L853	L857	L861	L865	L869	L873	L877	L881	L885	L889	L893	L897	L901	L905	L909	L913	L917	L921	L925	L929	L933	L937	L941	L945	L949	L953	L957	L961	L965	L969	L973	L977	L981	L985	L989	L993	L997	L1001	L1005	L1009	L1013	L1017	L1021	L1025	L1029	L1033	L1037	L1041	L1045	L1049	L1053	L1057	L1061	L1065	L1069	L1073	L1077	L1081	L1085	L1089	L1093	L1097	L1101	L1105	L1109	L1113	L1117	L1121	L1125	L1129	L1133	L1137	L1141	L1145	L1149	L1153	L1157	L1161	L1165	L1169	L1173	L1177	L1181	L1185	L1189	L1193	L1197	L1201	L1205	L1209	L1213	L1217	L1221	L1225	L1229	L1233	L1237	L1241	L1245	L1249	L1253	L1257	L1261	L1265	L1269	L1273	L1277	L1281	L1285	L1289	L1293	L1297	L1301	L1305	L1309	L1313	L1317	L1321	L1325	L1329	L1333	L1337	L1341	L1345	L1349	L1353	L1357	L1361	L1365	L1369	L1373	L1377	L1381	L1385	L1389	L1393	L1397	L1401	L1405	L1409	L1413	L1417	L1421	L1425	L1429	L1433	L1437	L1441	L1445	L1449	L1453	L1457	L1461	L1465	L1469	L1473	L1477	L1481	L1485	L1489	L1493	L1497	L1501	L1505	L1509	L1513	L1517	L1521	L1525	L1529	L1533	L1537	L1541	L1545	L1549	L1553	L1557	L1561	L1565	L1569	L1573	L1577	L1581	L1585	L1589	L1593	L1597	L1601	L1605	L1609	L1613	L1617	L1621	L1625	L1629	L1633	L1637	L1641	L1645	L1649	L1653	L1657	L1661	L1665	L1669	L1673	L1677	L1681	L1685	L1689	L1693	L1697	L1701	L1705	L1709	L1713	L1717	L1721	L1725	L1729	L1733	L1737	L1741	L1745	L1749	L1753	L1757	L1761	L1765	L1769	L1773	L1777	L1781	L1785	L1789	L1793	L1797	L1801	L1805	L1809	L1813	L1817	L1821	L1825	L1829	L1833	L1837	L1841	L1845	L1849	L1853	L1857	L1861	L1865	L1869	L1873	L1877	L1881	L1885	L1889	L1893	L1897	L1901	L1905	L1909	L1913	L1917	L1921	L1925	L1929	L1933	L1937	L1941	L1945	L1949	L1953	L1957	L1961	L1965	L1969	L1973	L1977	L1981	L1985	L1989	L1993	L1997	L2001	L2005	L2009	L2013	L2017	L2021	L2025	L2029	L2033	L2037	L2041	L2045	L2049	L2053	L2057	L2061	L2065	L2069	L2073	L2077	L2081	L2085	L2089	L2093	L2097	L2101	L2105	L2109	L2113	L2117	L2121	L2125	L2129	L2133	L2137	L2141	L2145	L2149	L2153	L2157	L2161	L2165	L2169	L2173	L2177	L2181	L2185	L2189	L2193	L2197	L2201	L2205	L2209	L2213	L2217	L2221	L2225	L2229	L2233	L2237	L2241	L2245	L2249	L2253	L2257	L2261	L2265	L2269	L2273	L2277	L2281	L2285	L2289	L2293	L2297	L2301	L2305	L2309	L2313	L2317	L2321	L2325	L2329	L2333	L2337	L2341	L2345	L2349	L2353	L2357	L2361	L2365	L2369	L2373	L2377	L2381	L2385	L2389	L2393	L2397	L2401	L2405	L2409	L2413	L2417	L2421	L2425	L2429	L2433	L2437	L2441	L2445	L2449	L2453	L2457	L2461	L2465	L2469	L2473	L2477	L2481	L2485	L2489	L2493	L2497	L2501	L2505	L2509	L2513	L2517	L2521	L2525	L2529	L2533	L2537	L2541	L2545	L2549	L2553	L2557	L2561	L2565	L2569	L2573	L2577	L2581	L2585	L2589	L2593	L2597	L2601	L2605	L2609	L2613	L2617	L2621	L2625	L2629	L2633	L2637	L2641	L2645	L2649	L2653	L2657	L2661	L2665	L2669	L2673	L2677	L2681	L2685	L2689	L2693	L2697	L2701	L2705	L2709	L2713	L2717	L2721	L2725	L2729	L2733	L2737	L2741	L2745	L2749	L2753	L2757	L2761	L2765	L2769	L2773	L2777	L2781	L2785	L2789	L2793	L2797	L2801	L2805	L2809	L2813	L2817	L2821	L2825	L2829	L2833	L2837	L2841	L2845	L2849	L2853	L2857	L2861	L2865	L2869	L2873	L2877	L2881	L2885	L2889	L2893	L2897	L2901	L2905	L2909	L2913	L2917	L2921	L2925	L2929	L2933	L2937	L2941	L2945	L2949	L2953	L2957	L2961	L2965	L2969	L2973	L2977	L2981	L2985	L2989	L2993	L2997	L3001	L3005	L3009	L3013	L3017	L3021	L3025	L3029	L3033	L3037	L3041	L3045	L3049	L3053	L3057	L3061	L3065	L3069	L3073	L3077	L3081	L3085	L3089	L3093	L3097	L3101	L3105	L3109	L3113	L3117	L3121	L3125	L3129	L3133	L3137	L3141	L3145	L3149	L3153	L3157	L3161	L3165	L3169	L3173	L3177	L3181	L3185	L3189	L3193	L3197	L3201	L3205	L3209	L3213	L3217	L3221	L3225	L3229	L3233	L3237	L3241	L3245	L3249	L3253	L3257	L3261	L3265	L3269	L3273	L3277	L3281	L3285	L3289	L3293	L3297	L3301	L3305	L3309	L3313	L3317	L3321	L3325	L3329	L3333	L3337	L3341	L3345	L3349	L3353	L3357	L3361	L3365	L3369	L3373	L3377	L3381	L3385	L3389	L3393	L3397	L3401	L3405	L3409	L3413	L3417	L3421	L3425	L3429	L3433	L3437	L3441	L3445	L3449	L3453	L3457	L3461	L3465	L3469	L3473	L3477	L3481	L3485	L3489	L3493	L3497	L3501	L3505	L3509	L3513	L3517	L3521	L3525	L3529	L3533	L3537	L3541	L3545	L3549	L3553	L3557	L3561	L3565	L3569	L3573	L3577	L3581	L3585	L3589	L3593	L3597	L3601	L3605	L3609	L3613	L3617	L3621	L3625	L3629	L3633	L3637	L3641	L3645	L3649	L3653	L3657	L3661	L3665	L3669	L3673	L3677	L3681	L3685	L3689	L3693	L3697	L3701	L3705	L3709	L3713	L3717	L3721	L3725	L3729	L3733	L3737	L3741	L3745	L3749	L3753	L3757	L3761	L3765	L3769	L3773	L3777	L3781	L378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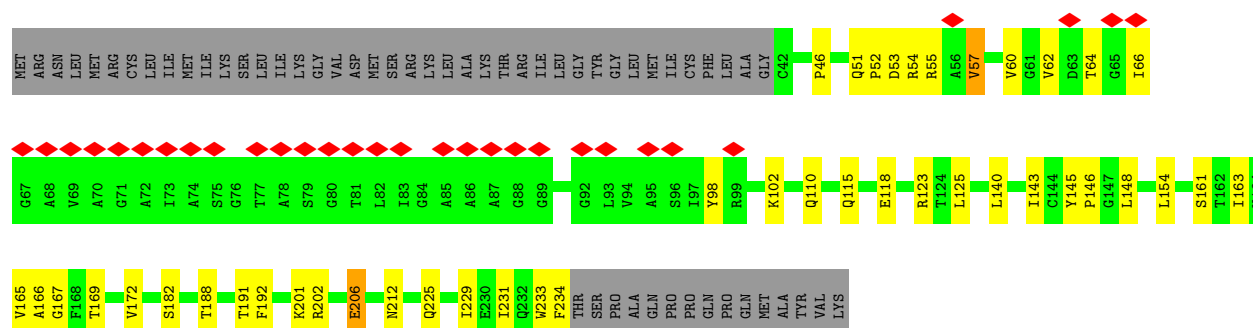
- Molecule 6: IcmK (DotH)

Chain Ec:

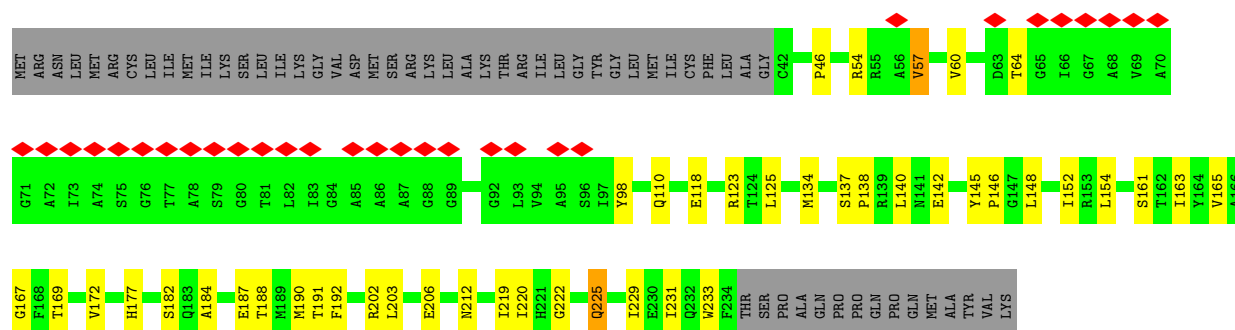
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PRO	ASP	ASP	ASN	GLY	LYS
GLY	PRO	SER	PRO	GLY	GLY
GLN	GLN	THR	GLU	ASP	TYR
LYS	LYS	GLY	GLN	ASN	ASP
ALA	ALA	ALA	VAL	ALA	GLN
VAL	VAL	PRO	VAL	ALA	LEU
ASP	ASP	THR	LEU	SER	CYS
TYR	TYR	PRO	LEU	ASP	LYS
ARG	ARG	ILE	LYS	THR	TYR
VAL	VAL	ALA	GLN	SER	CYS
ASP	ASP	ALA	ILE	GLN	LEU
LEU	LEU	TYR	TYR	GLN	VAL
ARG	ARG	ASP	GLU	PRO	ILE
GLN	GLN	LEU	THR	ASN	GLY
VAL	VAL	GLY	SER	GLN	LEU
GLY	GLY	ASP	GLU	SER	THR
TYR	PRO	PRO	TYR	GLY	PHE
GLY	GLY	SER	ALA	GLN	SER
PRO	PRO	SER	LYS	ALA	MET
ASN	ASN	PHE	ALA	ASN	SER
ALA	ALA	ASN	ALA	CYS	CYS
LYS	LYS	ILE	THR	ALA	SER
SER	SER	GLN	PRO	PRO	ILE
MET	MET	THR	GLY	ALA	TYR
THR	THR	TRP	THR	ASN	ALA
GLU	GLU	LYS	PRO	GLN	ALA
GLY	GLY	SER	PRO	THR	ASP
GLN	GLN	ASN	LYS	ALA	GLN
6271	6271	6271	PRO	THR	SER
S275	S275	6275	THR	ALA	ASP
V283	V283	6283	THR	ASP	ASP
L284	L284	6284	ALA	GLY	ASP
E285	E285	6285	ILE	GLY	ALA
V297	V297	6297	THR	ASP	GLN
S298	S298	6298	LYS	GLN	GLN
G299	G299	6299	LEU	ILE	LEU
A302	A302	6302	SER	GLN	LEU
W305	W305	6305	PRO	ASP	ARG
Y312	Y312	6312	GLY	ASP	MET
L317	L317	6317	THR	ASP	LEU
L320	L320	6320	GLN	ASP	GLN
W324	W324	6324	THR	ASP	LYS
M328	M328	6328	GLY	ASP	SER
T329	T329	6329	ASN	LEU	GLN
S330	S330	6330	THR	GLN	ASN
M339	M339	6339	VAL	THR	PRO
			THR	THR	ASP
			LEU	ARG	ALA
			GLY	ASN	GLN
			LEU	GLY	GLY
			VAL	TYR	ALA



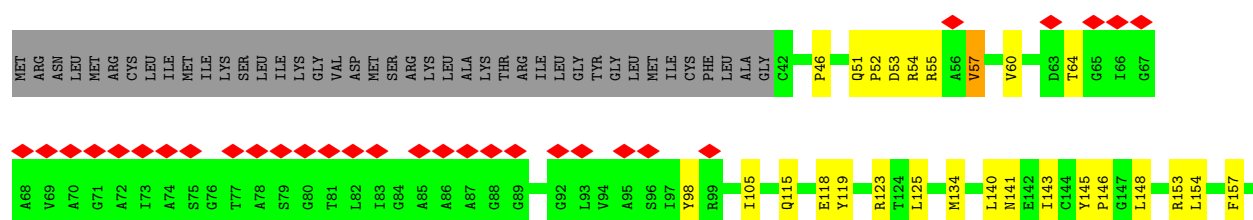
- Molecule 7: Outer membrane protein, OmpA family protein



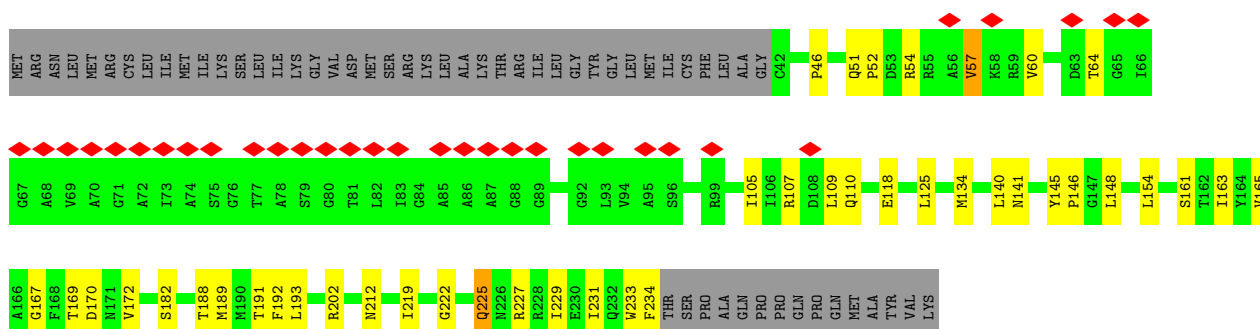
- Molecule 7: Outer membrane protein, OmpA family protein



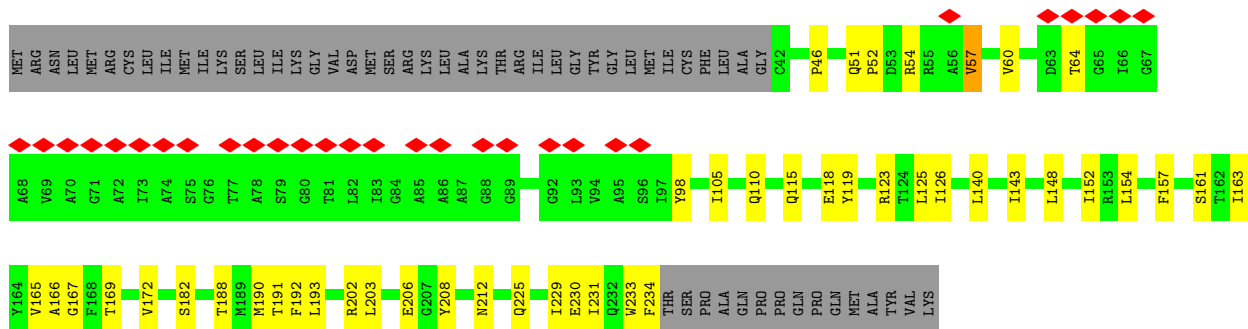
- Molecule 7: Outer membrane protein, OmpA family protein



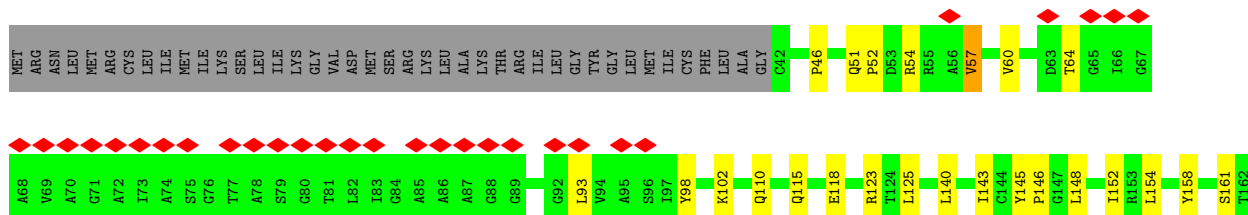
- Molecule 7: Outer membrane protein, OmpA family protein



- Molecule 7: Outer membrane protein, OmpA family protein

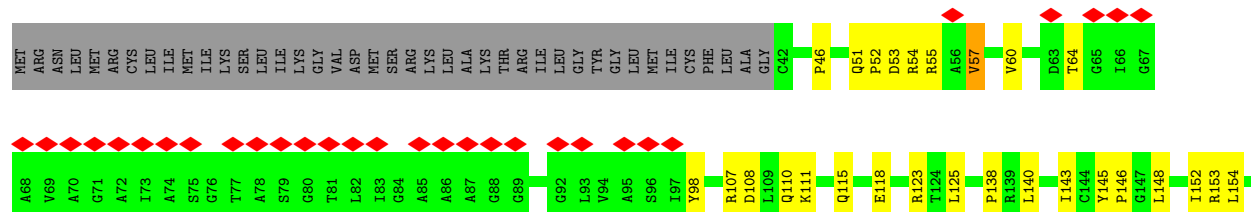


- Molecule 7: Outer membrane protein, OmpA family protein

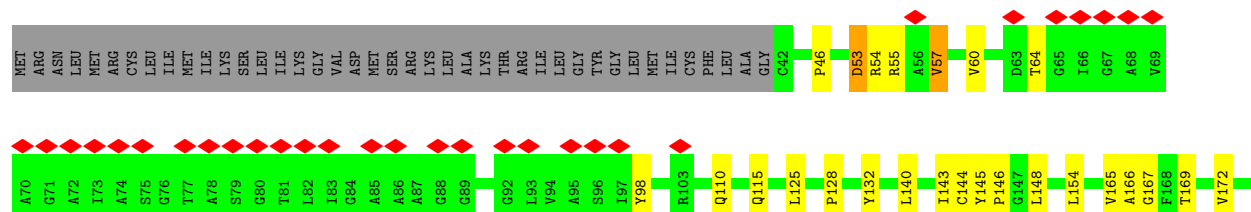




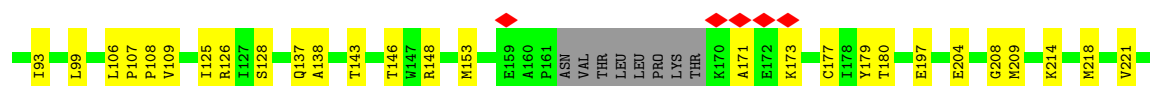
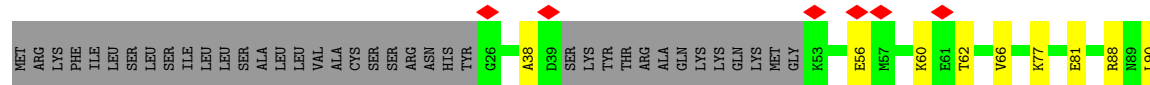
• Molecule 7: Outer membrane protein, OmpA family protein



• Molecule 7: Outer membrane protein, OmpA family protein

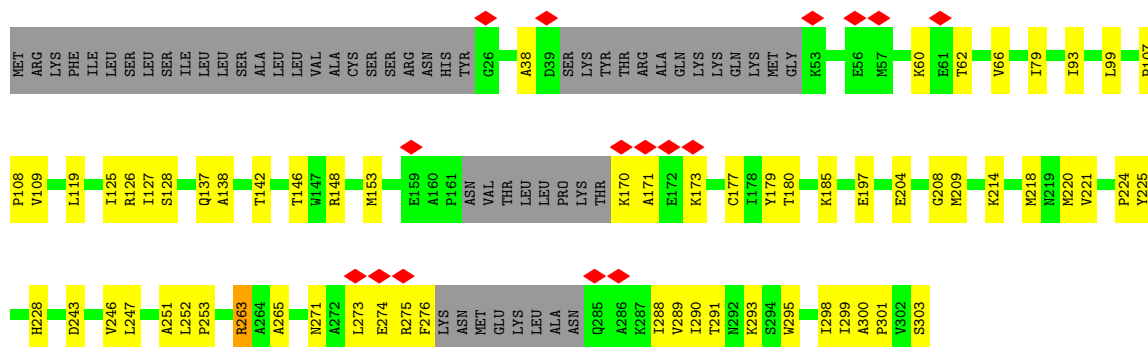


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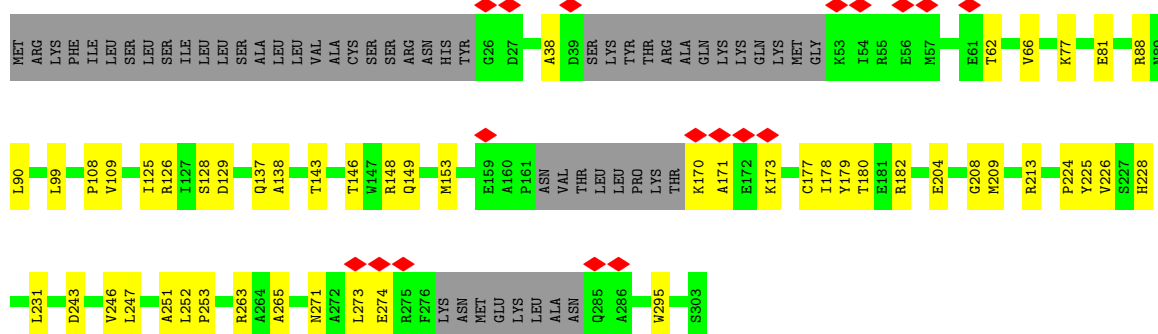


• Molecule 8: DotC

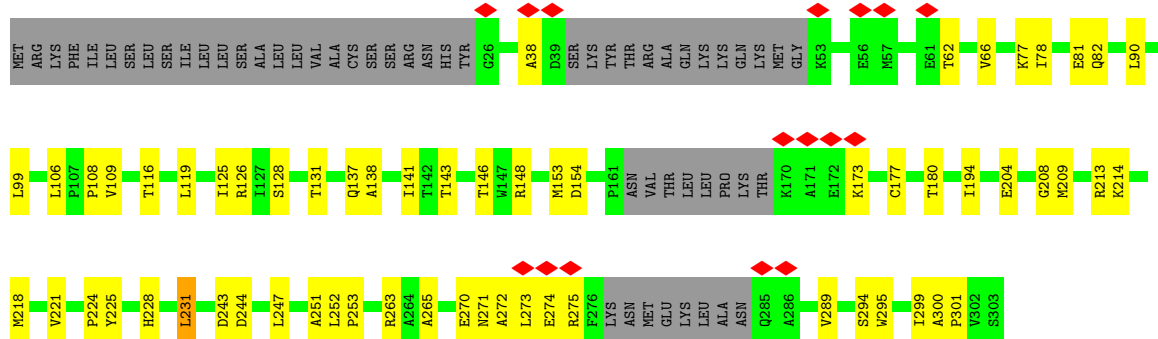




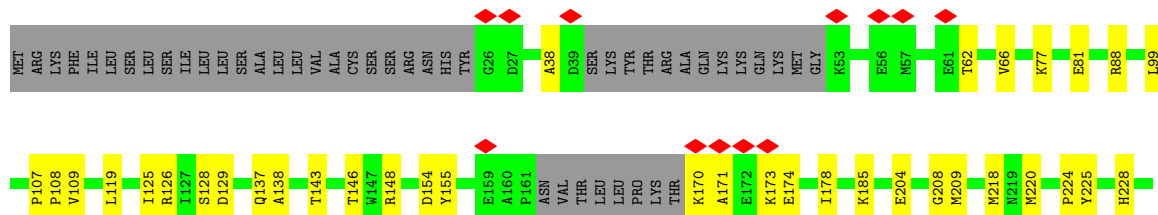
• Molecule 8: DotC



• Molecule 8: DotC

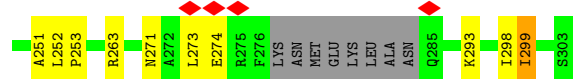


• Molecule 8: DotC

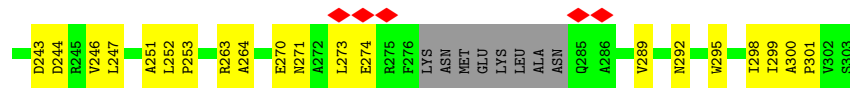
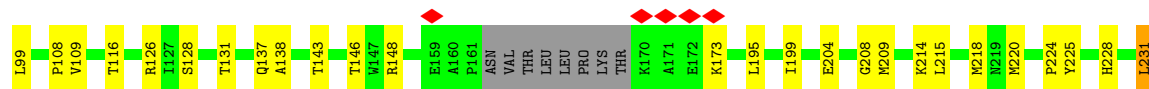
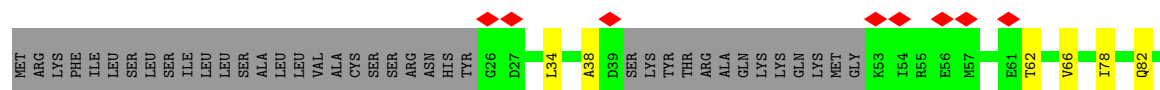




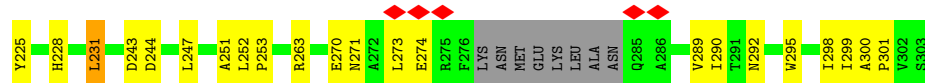
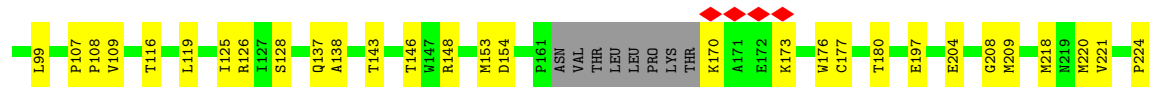
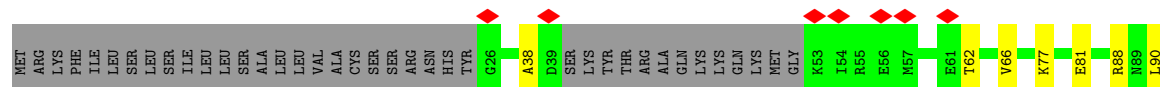
- Molecule 8: DotC



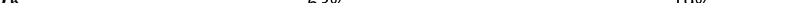
- Molecule 8: DotC

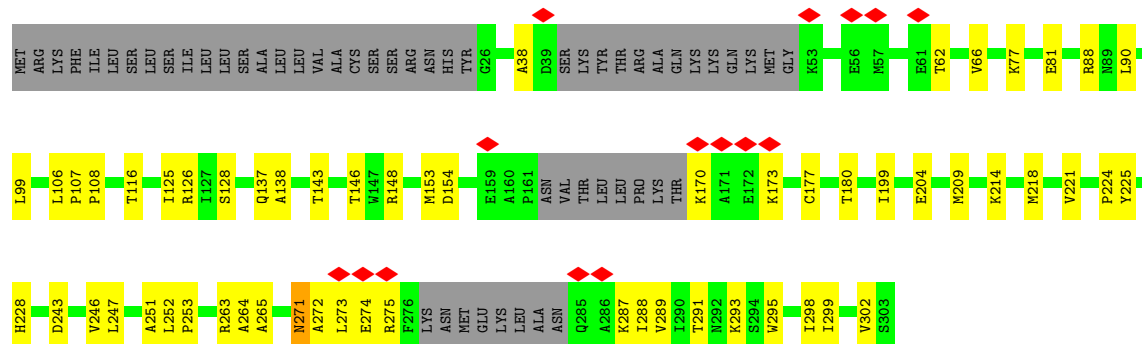


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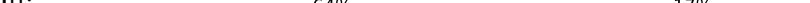


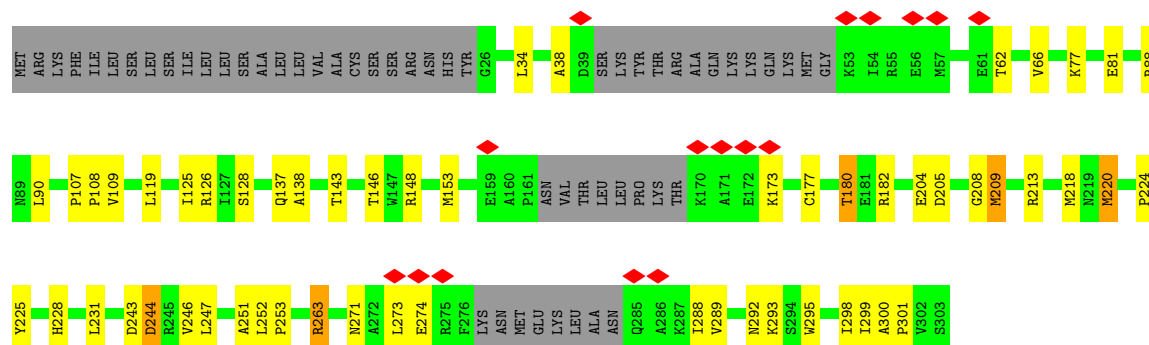
- Molecule 8: DotC

Chain Dk: 

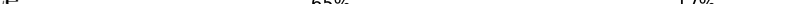


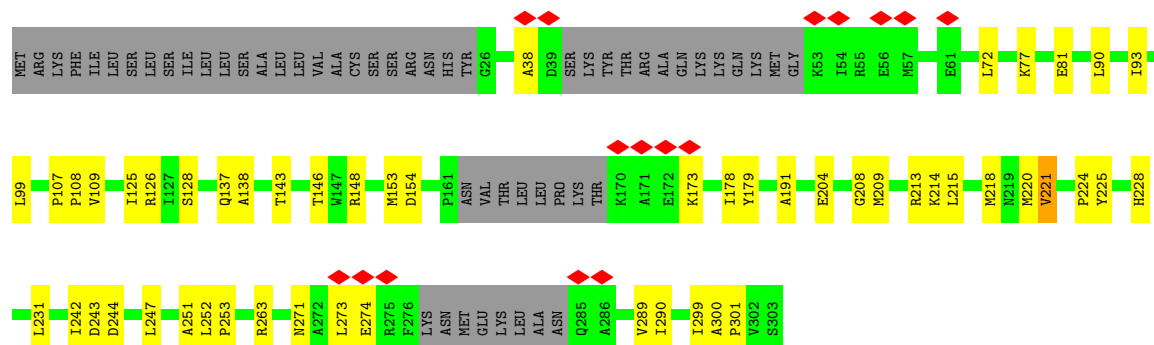
- Molecule 8: DotC

Chain Du: 

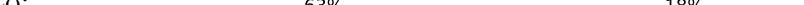


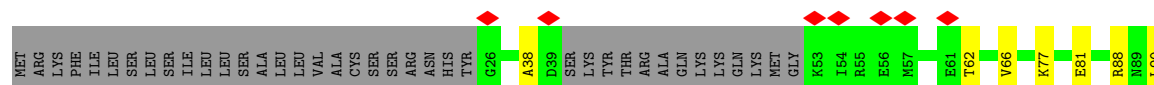
- Molecule 8: DotC

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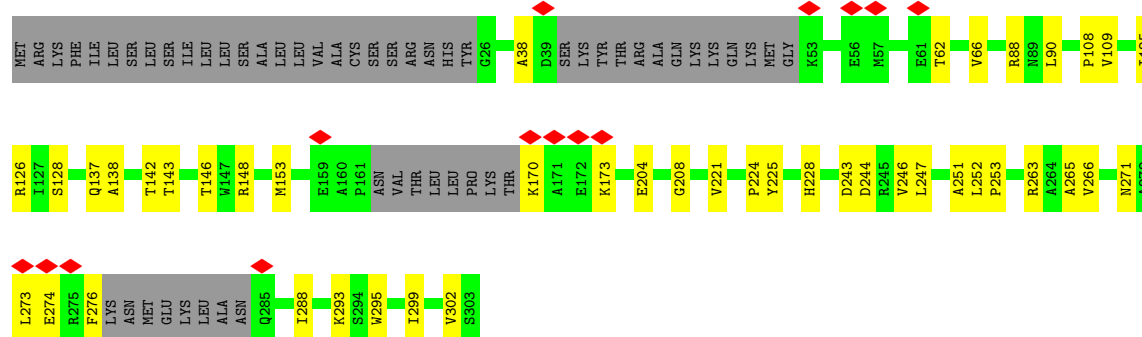


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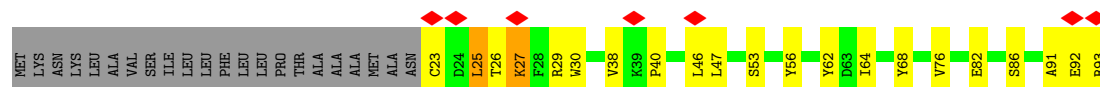
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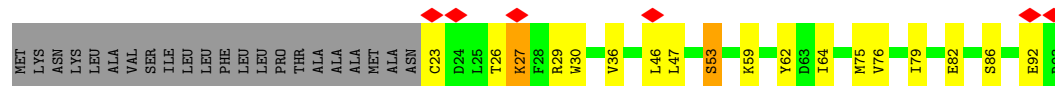
- Molecule 8: DotC



- Molecule 9: Secreted protein



- Molecule 9: Secreted protein

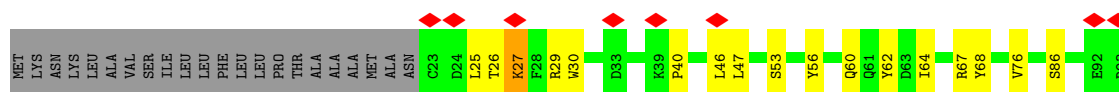


- Molecule 9: Secreted protein



- Molecule 9: Secreted protein





- Molecule 9: Secreted protein



- Molecule 9: Secreted protein



- Molecule 9: Secreted protein



- Molecule 9: Secreted protein

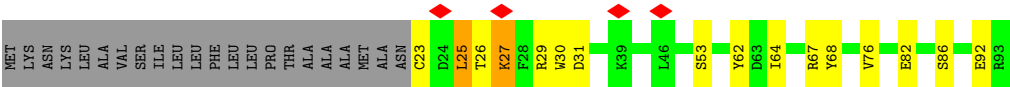


- Molecule 9: Secreted protein

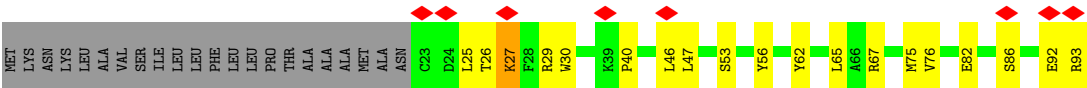


- Molecule 9: Secreted protein

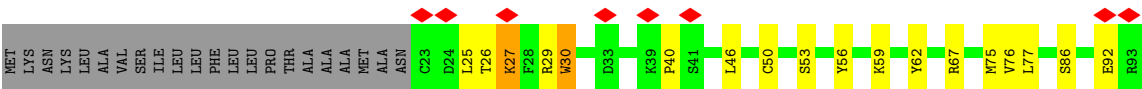




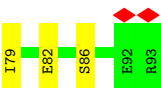
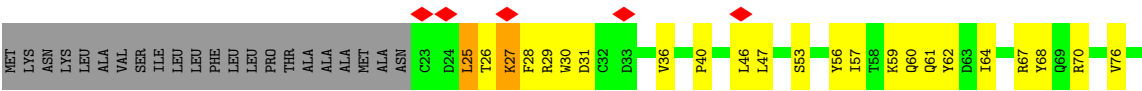
• Molecule 9: Secreted protein



• Molecule 9: Secreted protein



• Molecule 9: Secreted protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76409	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	73	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.656	Depositor
Minimum map value	-0.995	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	598.08, 598.08, 598.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.335, 1.335, 1.335	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	Aa	0.22	0/1099	0.36	0/1492
1	Ae	0.20	0/1069	0.37	0/1452
1	Ak	0.21	0/1099	0.37	0/1492
1	Ao	0.19	0/1069	0.33	0/1452
1	Au	0.21	0/1099	0.35	0/1492
1	Ay	0.19	0/1069	0.32	0/1452
1	Be	0.25	0/1099	0.38	0/1492
1	Bi	0.20	0/1069	0.38	0/1452
1	Bo	0.21	0/1099	0.36	0/1492
1	Bs	0.19	0/1069	0.32	0/1452
1	By	0.22	0/1099	0.36	0/1492
1	Cc	0.19	0/1069	0.35	0/1452
1	Ci	0.21	0/1099	0.37	0/1492
1	Cm	0.21	0/1069	0.39	0/1452
1	Cs	0.21	0/1099	0.36	0/1492
1	Cw	0.18	0/1069	0.31	0/1452
1	Dc	0.22	0/1099	0.35	0/1492
1	Dg	0.19	0/1069	0.34	0/1452
1	Dm	0.21	0/1099	0.35	0/1492
1	Dq	0.19	0/1069	0.33	0/1452
1	Dw	0.21	0/1099	0.34	0/1492
1	Ea	0.19	0/1069	0.33	0/1452
1	Eg	0.21	0/1099	0.37	0/1492
1	Ek	0.19	0/1069	0.32	0/1452
1	Eq	0.21	0/1099	0.35	0/1492
1	Eu	0.19	0/1069	0.33	0/1452
2	Ab	0.21	0/1180	0.32	0/1594
2	Al	0.21	0/1180	0.35	0/1594
2	Av	0.22	0/1180	0.35	0/1594
2	Bf	0.21	0/1180	0.34	0/1594
2	Bp	0.20	0/1180	0.31	0/1594
2	Bz	0.21	0/1180	0.34	0/1594
2	Cj	0.22	0/1180	0.37	0/1594
2	Ct	0.21	0/1180	0.32	0/1594

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Dd	0.21	0/1180	0.32	0/1594
2	Dn	0.21	0/1180	0.34	0/1594
2	Dx	0.21	0/1180	0.35	0/1594
2	Eh	0.21	0/1180	0.35	0/1594
2	Er	0.22	0/1180	0.36	0/1594
3	Ac	0.15	0/2360	0.35	0/3183
3	Am	0.15	0/2360	0.35	0/3183
3	Aw	0.14	0/2360	0.35	0/3183
3	Bg	0.15	0/2360	0.35	0/3183
3	Bq	0.15	0/2360	0.35	0/3183
3	Ca	0.14	0/2360	0.35	0/3183
3	Ck	0.14	0/2360	0.34	0/3183
3	Cu	0.15	0/2360	0.34	0/3183
3	De	0.14	0/2360	0.35	0/3183
3	Do	0.14	0/2360	0.36	0/3183
3	Dy	0.16	0/2360	0.35	0/3183
3	Ei	0.16	0/2360	0.38	0/3183
3	Es	0.15	0/2360	0.35	0/3183
4	Ad	0.21	0/576	0.33	0/777
4	An	0.22	0/576	0.35	0/777
4	Ax	0.22	0/576	0.34	0/777
4	Bh	0.22	0/576	0.40	0/777
4	Br	0.23	0/576	0.38	0/777
4	Cb	0.22	0/576	0.34	0/777
4	Cl	0.22	0/576	0.34	0/777
4	Cv	0.23	0/576	0.40	0/777
4	Df	0.22	0/576	0.35	0/777
4	Dp	0.22	0/576	0.33	0/777
4	Dz	0.22	0/576	0.35	0/777
4	Ej	0.22	0/576	0.37	0/777
4	Et	0.22	0/576	0.38	0/777
5	Af	0.16	0/456	0.33	0/615
5	Ap	0.15	0/456	0.31	0/615
5	Az	0.12	0/456	0.32	0/615
5	Bj	0.13	0/456	0.34	0/615
5	Bt	0.14	0/456	0.34	0/615
5	Cd	0.17	0/456	0.37	0/615
5	Cn	0.17	0/456	0.33	0/615
5	Cx	0.17	0/456	0.31	0/615
5	Dh	0.17	0/456	0.36	0/615
5	Dr	0.16	0/456	0.36	0/615
5	Eb	0.16	0/456	0.34	0/615
5	El	0.15	0/456	0.36	0/615

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	Ev	0.15	0/456	0.33	0/615
6	Ag	0.24	0/708	0.37	0/963
6	Aq	0.25	0/708	0.39	0/963
6	Ba	0.25	0/708	0.37	0/963
6	Bk	0.24	0/708	0.37	0/963
6	Bu	0.24	0/708	0.34	0/963
6	Ce	0.24	0/708	0.38	0/963
6	Co	0.24	0/708	0.37	0/963
6	Cy	0.25	0/708	0.38	0/963
6	Di	0.24	0/708	0.37	0/963
6	Ds	0.24	0/708	0.35	0/963
6	Ec	0.24	0/708	0.36	0/963
6	Em	0.24	0/708	0.36	0/963
6	Ew	0.25	0/708	0.36	0/963
7	Ah	0.19	0/1530	0.35	0/2068
7	Ar	0.19	0/1530	0.35	0/2068
7	Bb	0.19	0/1530	0.33	0/2068
7	Bl	0.19	0/1530	0.34	0/2068
7	Bv	0.20	0/1530	0.34	0/2068
7	Cf	0.19	0/1530	0.33	0/2068
7	Cp	0.19	0/1530	0.36	0/2068
7	Cz	0.19	0/1530	0.36	0/2068
7	Dj	0.19	0/1530	0.34	0/2068
7	Dt	0.19	0/1530	0.36	0/2068
7	Ed	0.19	0/1530	0.37	0/2068
7	En	0.19	0/1530	0.35	0/2068
7	Ex	0.19	0/1530	0.36	0/2068
8	Ai	0.20	0/2006	0.33	0/2718
8	As	0.21	0/2006	0.33	0/2718
8	Bc	0.20	0/2006	0.32	0/2718
8	Bm	0.21	0/2006	0.31	0/2718
8	Bw	0.21	0/2006	0.34	0/2718
8	Cg	0.20	0/2006	0.30	0/2718
8	Cq	0.20	0/2006	0.31	0/2718
8	Da	0.20	0/2006	0.31	0/2718
8	Dk	0.20	0/2006	0.33	0/2718
8	Du	0.20	0/2006	0.33	0/2718
8	Ee	0.20	0/2006	0.31	0/2718
8	Eo	0.21	0/2006	0.31	0/2718
8	Ey	0.21	0/2006	0.33	0/2718
9	Aj	0.17	0/574	0.38	0/778
9	At	0.17	0/574	0.38	0/778
9	Bd	0.16	0/574	0.39	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	Bn	0.18	0/574	0.42	0/778
9	Bx	0.18	0/574	0.41	0/778
9	Ch	0.18	0/574	0.43	0/778
9	Cr	0.18	0/574	0.39	0/778
9	Db	0.17	0/574	0.41	0/778
9	Dl	0.18	0/574	0.41	0/778
9	Dv	0.16	0/574	0.38	0/778
9	Ef	0.19	0/574	0.43	0/778
9	Ep	0.18	0/574	0.44	0/778
9	Ez	0.20	0/574	0.46	0/778
All	All	0.19	0/150254	0.35	0/203320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	Aa	1078	0	1112	30	0
1	Ae	1049	0	1079	25	0
1	Ak	1078	0	1112	26	0
1	Ao	1049	0	1079	23	0
1	Au	1078	0	1112	23	0
1	Ay	1049	0	1079	31	0
1	Be	1078	0	1112	31	0
1	Bi	1049	0	1079	26	0
1	Bo	1078	0	1112	23	0
1	Bs	1049	0	1079	25	0
1	By	1078	0	1112	31	0
1	Cc	1049	0	1079	23	0
1	Ci	1078	0	1112	23	0
1	Cm	1049	0	1079	21	0
1	Cs	1078	0	1112	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Cw	1049	0	1079	19	0
1	Dc	1078	0	1112	28	0
1	Dg	1049	0	1079	18	0
1	Dm	1078	0	1112	25	0
1	Dq	1049	0	1079	24	0
1	Dw	1078	0	1112	26	0
1	Ea	1049	0	1079	24	0
1	Eg	1078	0	1112	29	0
1	Ek	1049	0	1079	30	0
1	Eq	1078	0	1112	26	0
1	Eu	1049	0	1079	20	0
2	Ab	1161	0	1205	26	0
2	Al	1161	0	1205	26	0
2	Av	1161	0	1205	26	0
2	Bf	1161	0	1205	29	0
2	Bp	1161	0	1205	23	0
2	Bz	1161	0	1205	25	0
2	Cj	1161	0	1205	33	0
2	Ct	1161	0	1205	24	0
2	Dd	1161	0	1205	30	0
2	Dn	1161	0	1205	24	0
2	Dx	1161	0	1205	23	0
2	Eh	1161	0	1205	26	0
2	Er	1161	0	1205	22	0
3	Ac	2321	0	2343	48	0
3	Am	2321	0	2343	47	0
3	Aw	2321	0	2343	47	0
3	Bg	2321	0	2343	45	0
3	Bq	2321	0	2343	46	0
3	Ca	2321	0	2343	42	0
3	Ck	2321	0	2343	45	0
3	Cu	2321	0	2343	42	0
3	De	2321	0	2343	41	0
3	Do	2321	0	2343	38	0
3	Dy	2321	0	2343	53	0
3	Ei	2321	0	2343	45	0
3	Es	2321	0	2343	42	0
4	Ad	565	0	513	9	0
4	An	565	0	513	9	0
4	Ax	565	0	513	14	0
4	Bh	565	0	513	13	0
4	Br	565	0	513	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Cb	565	0	513	7	0
4	Cl	565	0	513	11	0
4	Cv	565	0	513	15	0
4	Df	565	0	513	10	0
4	Dp	565	0	513	12	0
4	Dz	565	0	513	11	0
4	Ej	565	0	513	13	0
4	Et	565	0	513	12	0
5	Af	449	0	474	11	0
5	Ap	449	0	474	11	0
5	Az	449	0	474	11	0
5	Bj	449	0	474	13	0
5	Bt	449	0	474	7	0
5	Cd	449	0	474	15	0
5	Cn	449	0	474	12	0
5	Cx	449	0	474	8	0
5	Dh	449	0	474	10	0
5	Dr	449	0	474	10	0
5	Eb	449	0	474	9	0
5	El	449	0	474	13	0
5	Ev	449	0	474	12	0
6	Ag	691	0	703	13	0
6	Aq	691	0	703	16	0
6	Ba	691	0	703	15	0
6	Bk	691	0	703	14	0
6	Bu	691	0	703	14	0
6	Ce	691	0	703	16	0
6	Co	691	0	703	17	0
6	Cy	691	0	703	19	0
6	Di	691	0	703	14	0
6	Ds	691	0	703	15	0
6	Ec	691	0	703	16	0
6	Em	691	0	703	16	0
6	Ew	691	0	703	17	0
7	Ah	1500	0	1499	32	0
7	Ar	1500	0	1499	29	0
7	Bb	1500	0	1499	28	0
7	Bl	1500	0	1499	34	0
7	Bv	1500	0	1499	32	0
7	Cf	1500	0	1499	26	0
7	Cp	1500	0	1499	34	0
7	Cz	1500	0	1499	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Dj	1500	0	1499	28	0
7	Dt	1500	0	1499	34	0
7	Ed	1500	0	1499	32	0
7	En	1500	0	1499	29	0
7	Ex	1500	0	1499	30	0
8	Ai	1970	0	1980	43	0
8	As	1970	0	1980	53	0
8	Bc	1970	0	1980	43	0
8	Bm	1970	0	1980	51	0
8	Bw	1970	0	1980	44	0
8	Cg	1970	0	1980	38	0
8	Cq	1970	0	1980	37	0
8	Da	1970	0	1980	51	0
8	Dk	1970	0	1980	44	0
8	Du	1970	0	1980	43	0
8	Ee	1970	0	1980	43	0
8	Eo	1970	0	1980	42	0
8	Ey	1970	0	1980	35	0
9	Aj	562	0	545	16	0
9	At	562	0	545	17	0
9	Bd	562	0	545	12	0
9	Bn	562	0	545	16	0
9	Bx	562	0	545	22	0
9	Ch	562	0	545	17	0
9	Cr	562	0	545	15	0
9	Db	562	0	545	22	0
9	Dl	562	0	545	19	0
9	Dv	562	0	545	16	0
9	Ef	562	0	545	17	0
9	Ep	562	0	545	15	0
9	Ez	562	0	545	21	0
All	All	147498	0	148889	2688	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 9.

The worst 5 of 2688 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)
8:As:107:PRO:HG2	8:As:209:MET:HG2	1.52	0.89
8:Ai:107:PRO:HG2	8:Ai:209:MET:HG2	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Bi:75:ASN:HD22	1:Bi:75:ASN:C	1.78	0.89
4:Cv:45:MET:HB3	4:Cv:62:ASN:HD21	1.38	0.88
3:Et:149:ASN:O	3:Et:149:ASN:ND2	2.06	0.88

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	Aa	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ae	134/163 (82%)	131 (98%)	3 (2%)	0	100	100
1	Ak	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Ao	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Au	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ay	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Be	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Bi	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Bo	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Bs	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	By	137/163 (84%)	131 (96%)	6 (4%)	0	100	100
1	Cc	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Ci	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Cm	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Cs	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Cw	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Dc	137/163 (84%)	130 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Dg	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Dm	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Dq	134/163 (82%)	130 (97%)	4 (3%)	0	100	100
1	Dw	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ea	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
1	Eg	137/163 (84%)	129 (94%)	8 (6%)	0	100	100
1	Ek	134/163 (82%)	131 (98%)	3 (2%)	0	100	100
1	Eq	137/163 (84%)	130 (95%)	7 (5%)	0	100	100
1	Eu	134/163 (82%)	129 (96%)	5 (4%)	0	100	100
2	Ab	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Al	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Av	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
2	Bf	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Bp	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Bz	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Cj	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Ct	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Dd	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Dn	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
2	Dx	147/189 (78%)	144 (98%)	3 (2%)	0	100	100
2	Eh	147/189 (78%)	143 (97%)	4 (3%)	0	100	100
2	Er	147/189 (78%)	145 (99%)	2 (1%)	0	100	100
3	Ac	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Am	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Aw	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Bg	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Bq	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Ca	290/320 (91%)	272 (94%)	18 (6%)	0	100	100
3	Ck	290/320 (91%)	271 (93%)	19 (7%)	0	100	100
3	Cu	290/320 (91%)	271 (93%)	19 (7%)	0	100	100
3	De	290/320 (91%)	270 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Do	290/320 (91%)	267 (92%)	23 (8%)	0	100	100
3	Dy	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
3	Ei	290/320 (91%)	270 (93%)	20 (7%)	0	100	100
3	Es	290/320 (91%)	269 (93%)	21 (7%)	0	100	100
4	Ad	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	An	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Ax	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Bh	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Br	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Cb	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Cl	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
4	Cv	74/124 (60%)	69 (93%)	5 (7%)	0	100	100
4	Df	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
4	Dp	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
4	Dz	74/124 (60%)	70 (95%)	4 (5%)	0	100	100
4	Ej	74/124 (60%)	68 (92%)	6 (8%)	0	100	100
4	Et	74/124 (60%)	67 (90%)	7 (10%)	0	100	100
5	Af	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Ap	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Az	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Bj	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Bt	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Cd	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Cn	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Cx	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Dh	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
5	Dr	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	Eb	57/269 (21%)	55 (96%)	2 (4%)	0	100	100
5	El	57/269 (21%)	54 (95%)	3 (5%)	0	100	100
5	Ev	57/269 (21%)	53 (93%)	4 (7%)	0	100	100
6	Ag	89/361 (25%)	83 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Aq	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ba	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Bk	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Bu	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ce	89/361 (25%)	85 (96%)	4 (4%)	0	100	100
6	Co	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Cy	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Di	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ds	89/361 (25%)	83 (93%)	6 (7%)	0	100	100
6	Ec	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Em	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
6	Ew	89/361 (25%)	84 (94%)	5 (6%)	0	100	100
7	Ah	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Ar	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Bb	191/249 (77%)	185 (97%)	6 (3%)	0	100	100
7	Bl	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Bv	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Cf	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Cp	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Cz	191/249 (77%)	183 (96%)	8 (4%)	0	100	100
7	Dj	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Dt	191/249 (77%)	185 (97%)	6 (3%)	0	100	100
7	Ed	191/249 (77%)	186 (97%)	5 (3%)	0	100	100
7	En	191/249 (77%)	184 (96%)	7 (4%)	0	100	100
7	Ex	191/249 (77%)	183 (96%)	8 (4%)	0	100	100
8	Ai	241/303 (80%)	224 (93%)	17 (7%)	0	100	100
8	As	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Bc	241/303 (80%)	228 (95%)	13 (5%)	0	100	100
8	Bm	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Bw	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Cg	241/303 (80%)	226 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Cq	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Da	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
8	Dk	241/303 (80%)	228 (95%)	13 (5%)	0	100	100
8	Du	241/303 (80%)	226 (94%)	15 (6%)	0	100	100
8	Ee	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
8	Eo	241/303 (80%)	227 (94%)	14 (6%)	0	100	100
8	Ey	241/303 (80%)	225 (93%)	16 (7%)	0	100	100
9	Aj	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	At	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	24
9	Bd	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	Bn	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	24
9	Bx	69/93 (74%)	60 (87%)	8 (12%)	1 (1%)	9	24
9	Ch	69/93 (74%)	59 (86%)	9 (13%)	1 (1%)	9	24
9	Cr	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	Db	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	Dl	69/93 (74%)	60 (87%)	8 (12%)	1 (1%)	9	24
9	Dv	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	Ef	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	24
9	Ep	69/93 (74%)	62 (90%)	6 (9%)	1 (1%)	9	24
9	Ez	69/93 (74%)	61 (88%)	7 (10%)	1 (1%)	9	24
All	All	18577/29042 (64%)	17556 (94%)	1008 (5%)	13 (0%)	49	72

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Aj	27	LYS
9	At	27	LYS
9	Bd	27	LYS
9	Bn	27	LYS
9	Bx	27	LYS

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	Aa	120/139 (86%)	118 (98%)	2 (2%)	53	73
1	Ae	117/139 (84%)	115 (98%)	2 (2%)	53	73
1	Ak	120/139 (86%)	118 (98%)	2 (2%)	53	73
1	Ao	117/139 (84%)	114 (97%)	3 (3%)	40	65
1	Au	120/139 (86%)	118 (98%)	2 (2%)	53	73
1	Ay	117/139 (84%)	113 (97%)	4 (3%)	32	58
1	Be	120/139 (86%)	117 (98%)	3 (2%)	42	66
1	Bi	117/139 (84%)	112 (96%)	5 (4%)	26	52
1	Bo	120/139 (86%)	120 (100%)	0	100	100
1	Bs	117/139 (84%)	112 (96%)	5 (4%)	26	52
1	By	120/139 (86%)	118 (98%)	2 (2%)	53	73
1	Cc	117/139 (84%)	111 (95%)	6 (5%)	21	47
1	Ci	120/139 (86%)	118 (98%)	2 (2%)	53	73
1	Cm	117/139 (84%)	116 (99%)	1 (1%)	70	83
1	Cs	120/139 (86%)	117 (98%)	3 (2%)	42	66
1	Cw	117/139 (84%)	113 (97%)	4 (3%)	32	58
1	Dc	120/139 (86%)	117 (98%)	3 (2%)	42	66
1	Dg	117/139 (84%)	115 (98%)	2 (2%)	53	73
1	Dm	120/139 (86%)	120 (100%)	0	100	100
1	Dq	117/139 (84%)	113 (97%)	4 (3%)	32	58
1	Dw	120/139 (86%)	119 (99%)	1 (1%)	73	85
1	Ea	117/139 (84%)	115 (98%)	2 (2%)	53	73
1	Eg	120/139 (86%)	119 (99%)	1 (1%)	73	85
1	Ek	117/139 (84%)	114 (97%)	3 (3%)	40	65
1	Eq	120/139 (86%)	116 (97%)	4 (3%)	33	58
1	Eu	117/139 (84%)	113 (97%)	4 (3%)	32	58
2	Ab	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Al	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Av	127/163 (78%)	123 (97%)	4 (3%)	35	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Bf	127/163 (78%)	122 (96%)	5 (4%)	28	54
2	Bp	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Bz	127/163 (78%)	124 (98%)	3 (2%)	43	67
2	Cj	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Ct	127/163 (78%)	124 (98%)	3 (2%)	43	67
2	Dd	127/163 (78%)	126 (99%)	1 (1%)	73	85
2	Dn	127/163 (78%)	124 (98%)	3 (2%)	43	67
2	Dx	127/163 (78%)	123 (97%)	4 (3%)	35	59
2	Eh	127/163 (78%)	125 (98%)	2 (2%)	55	75
2	Er	127/163 (78%)	122 (96%)	5 (4%)	28	54
3	Ac	251/276 (91%)	243 (97%)	8 (3%)	34	59
3	Am	251/276 (91%)	245 (98%)	6 (2%)	43	67
3	Aw	251/276 (91%)	245 (98%)	6 (2%)	43	67
3	Bg	251/276 (91%)	244 (97%)	7 (3%)	38	62
3	Bq	251/276 (91%)	244 (97%)	7 (3%)	38	62
3	Ca	251/276 (91%)	242 (96%)	9 (4%)	31	56
3	Ck	251/276 (91%)	246 (98%)	5 (2%)	48	71
3	Cu	251/276 (91%)	246 (98%)	5 (2%)	48	71
3	De	251/276 (91%)	243 (97%)	8 (3%)	34	59
3	Do	251/276 (91%)	242 (96%)	9 (4%)	31	56
3	Dy	251/276 (91%)	245 (98%)	6 (2%)	43	67
3	Ei	251/276 (91%)	242 (96%)	9 (4%)	31	56
3	Es	251/276 (91%)	241 (96%)	10 (4%)	28	53
4	Ad	64/107 (60%)	61 (95%)	3 (5%)	23	49
4	An	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Ax	64/107 (60%)	62 (97%)	2 (3%)	35	59
4	Bh	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Br	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Cb	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Cl	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Cv	64/107 (60%)	63 (98%)	1 (2%)	55	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Df	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Dp	64/107 (60%)	61 (95%)	3 (5%)	23	49
4	Dz	64/107 (60%)	63 (98%)	1 (2%)	55	75
4	Ej	64/107 (60%)	62 (97%)	2 (3%)	35	59
4	Et	64/107 (60%)	63 (98%)	1 (2%)	55	75
5	Af	49/237 (21%)	47 (96%)	2 (4%)	27	53
5	Ap	49/237 (21%)	47 (96%)	2 (4%)	27	53
5	Az	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	Bj	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	Bt	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	Cd	49/237 (21%)	47 (96%)	2 (4%)	27	53
5	Cn	49/237 (21%)	49 (100%)	0	100	100
5	Cx	49/237 (21%)	49 (100%)	0	100	100
5	Dh	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	Dr	49/237 (21%)	45 (92%)	4 (8%)	10	27
5	Eb	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	El	49/237 (21%)	48 (98%)	1 (2%)	48	71
5	Ev	49/237 (21%)	49 (100%)	0	100	100
6	Ag	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Aq	76/300 (25%)	76 (100%)	0	100	100
6	Ba	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Bk	76/300 (25%)	76 (100%)	0	100	100
6	Bu	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Ce	76/300 (25%)	74 (97%)	2 (3%)	40	65
6	Co	76/300 (25%)	74 (97%)	2 (3%)	40	65
6	Cy	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Di	76/300 (25%)	76 (100%)	0	100	100
6	Ds	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Ec	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Em	76/300 (25%)	75 (99%)	1 (1%)	61	78
6	Ew	76/300 (25%)	74 (97%)	2 (3%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	Ah	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Ar	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Bb	155/203 (76%)	149 (96%)	6 (4%)	28	54
7	Bl	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Bv	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Cf	155/203 (76%)	149 (96%)	6 (4%)	28	54
7	Cp	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Cz	155/203 (76%)	153 (99%)	2 (1%)	61	78
7	Dj	155/203 (76%)	152 (98%)	3 (2%)	50	71
7	Dt	155/203 (76%)	153 (99%)	2 (1%)	61	78
7	Ed	155/203 (76%)	150 (97%)	5 (3%)	34	59
7	En	155/203 (76%)	151 (97%)	4 (3%)	40	65
7	Ex	155/203 (76%)	151 (97%)	4 (3%)	40	65
8	Ai	208/257 (81%)	205 (99%)	3 (1%)	59	77
8	As	208/257 (81%)	204 (98%)	4 (2%)	50	71
8	Bc	208/257 (81%)	205 (99%)	3 (1%)	59	77
8	Bm	208/257 (81%)	204 (98%)	4 (2%)	50	71
8	Bw	208/257 (81%)	201 (97%)	7 (3%)	32	58
8	Cg	208/257 (81%)	206 (99%)	2 (1%)	68	82
8	Cq	208/257 (81%)	203 (98%)	5 (2%)	43	67
8	Da	208/257 (81%)	204 (98%)	4 (2%)	50	71
8	Dk	208/257 (81%)	203 (98%)	5 (2%)	43	67
8	Du	208/257 (81%)	199 (96%)	9 (4%)	26	52
8	Ee	208/257 (81%)	205 (99%)	3 (1%)	59	77
8	Eo	208/257 (81%)	202 (97%)	6 (3%)	37	61
8	Ey	208/257 (81%)	204 (98%)	4 (2%)	50	71
9	Aj	63/80 (79%)	60 (95%)	3 (5%)	23	48
9	At	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Bd	63/80 (79%)	60 (95%)	3 (5%)	23	48
9	Bn	63/80 (79%)	62 (98%)	1 (2%)	55	75
9	Bx	63/80 (79%)	61 (97%)	2 (3%)	34	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	Ch	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Cr	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Db	63/80 (79%)	62 (98%)	1 (2%)	55	75
9	Dl	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Dv	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Ef	63/80 (79%)	61 (97%)	2 (3%)	34	59
9	Ep	63/80 (79%)	62 (98%)	1 (2%)	55	75
9	Ez	63/80 (79%)	60 (95%)	3 (5%)	23	48
All	All	15990/24713 (65%)	15599 (98%)	391 (2%)	43	67

5 of 391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Da	228	HIS
7	Dt	110	GLN
2	Dd	78	ILE
9	Dl	31	ASP
2	Dx	75	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 198 such sidechains are listed below:

Mol	Chain	Res	Type
3	Cu	166	ASN
1	Dm	75	ASN
5	Cx	251	GLN
3	De	164	GLN
6	Ds	316	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

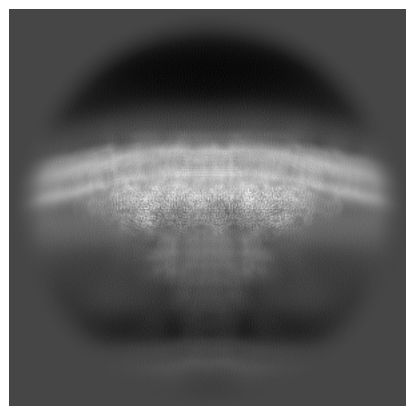
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49393. These allow visual inspection of the internal detail of the map and identification of artifacts.

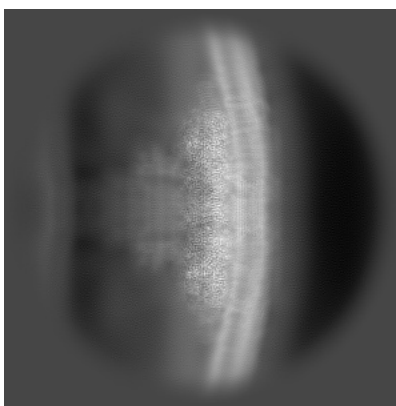
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

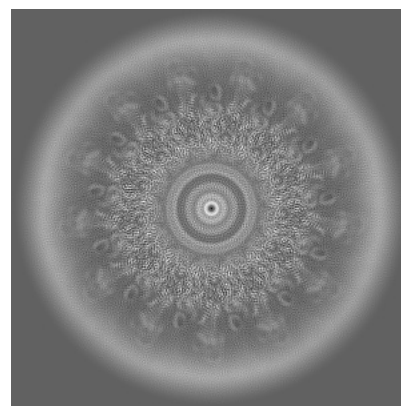
6.1.1 Primary map



X

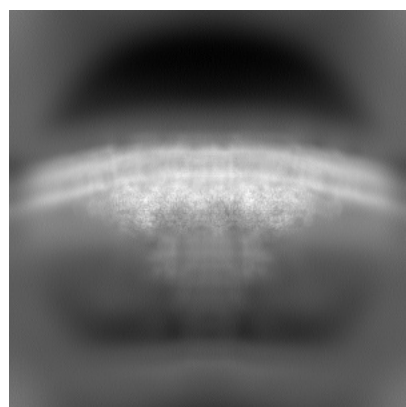


Y

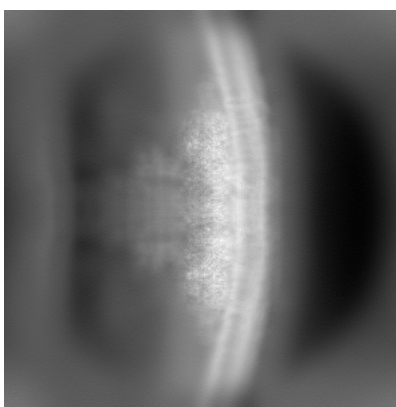


Z

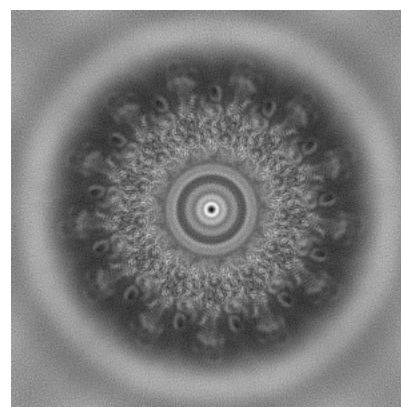
6.1.2 Raw map



X



Y

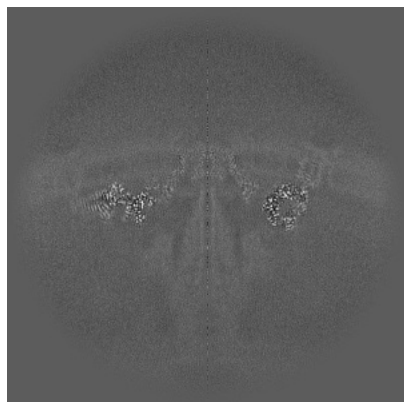


Z

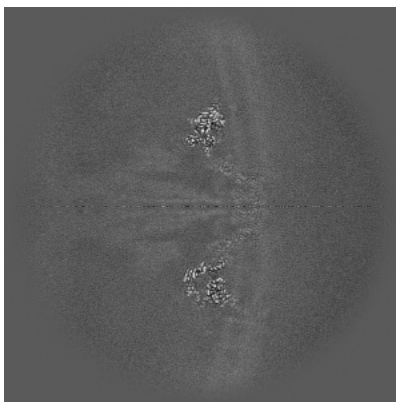
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

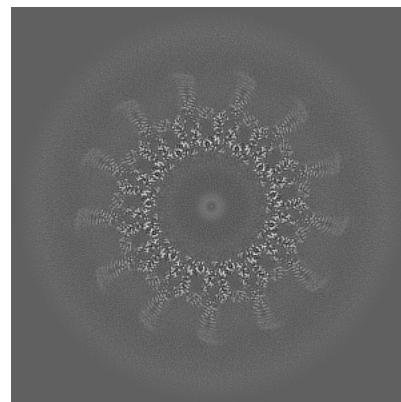
6.2.1 Primary map



X Index: 224

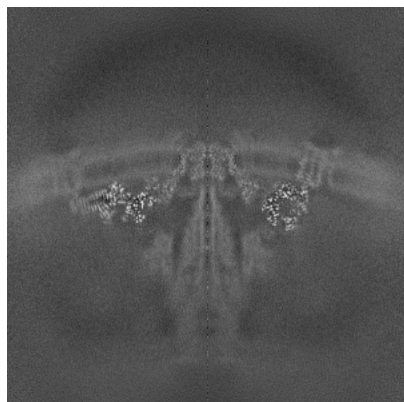


Y Index: 224

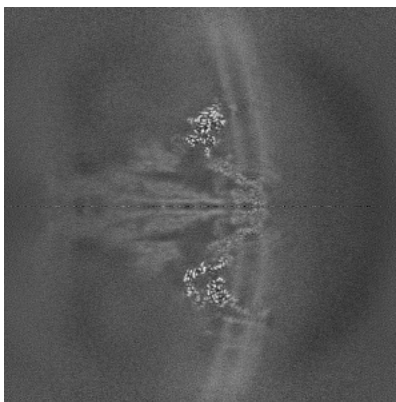


Z Index: 224

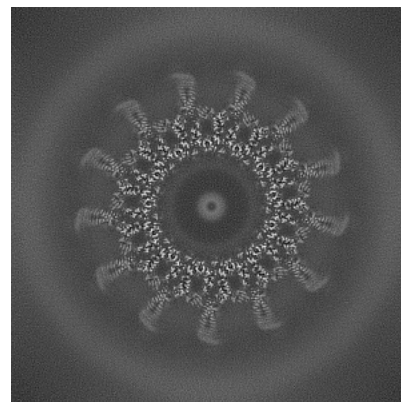
6.2.2 Raw map



X Index: 224



Y Index: 224

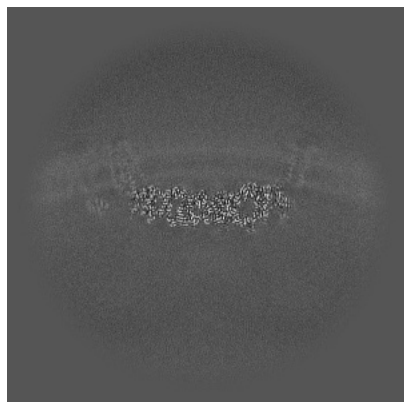


Z Index: 224

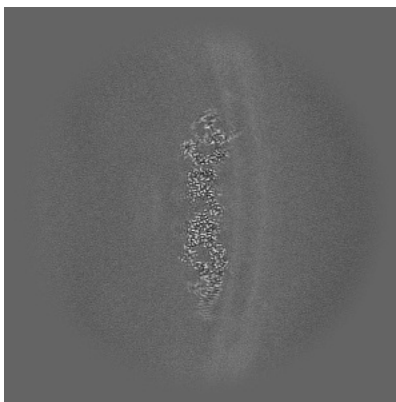
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

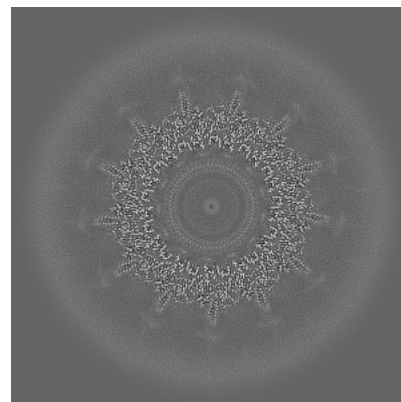
6.3.1 Primary map



X Index: 152

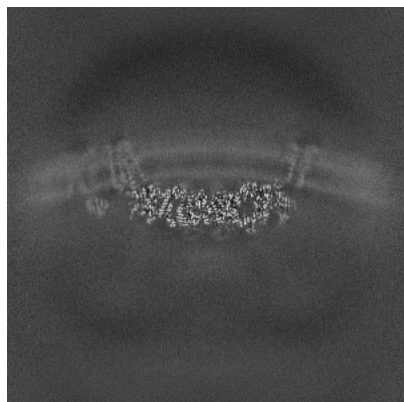


Y Index: 155

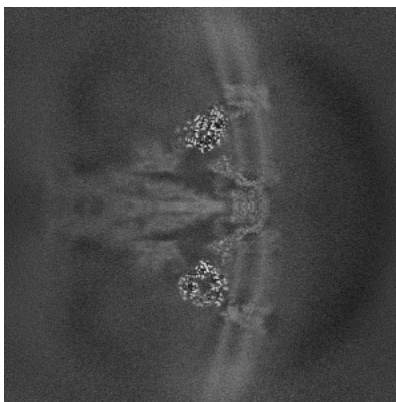


Z Index: 235

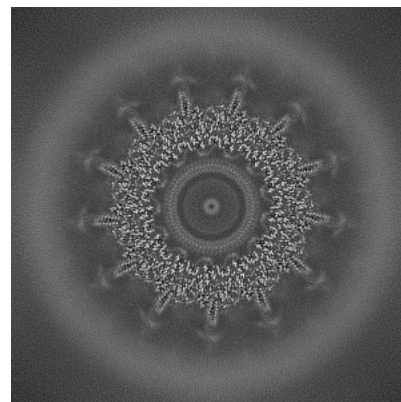
6.3.2 Raw map



X Index: 152



Y Index: 230

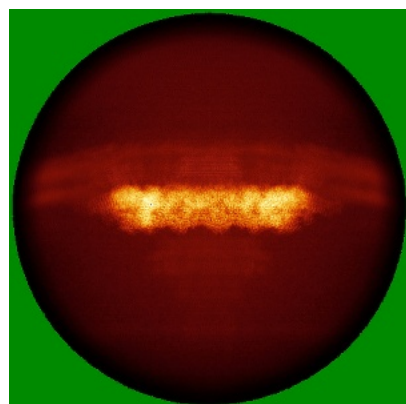


Z Index: 235

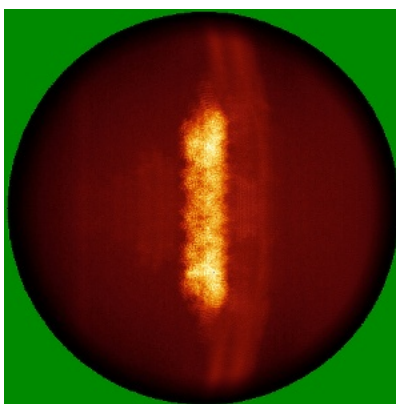
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

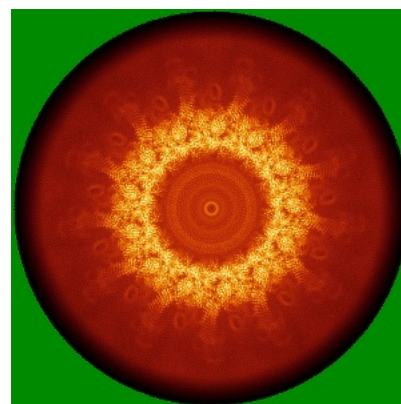
6.4.1 Primary map



X

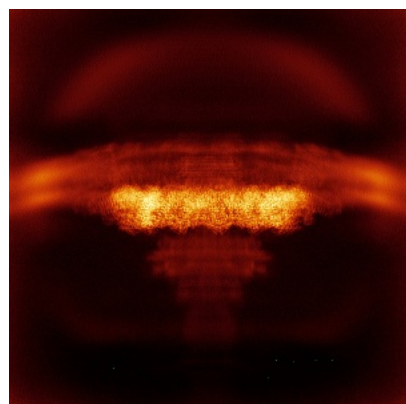


Y

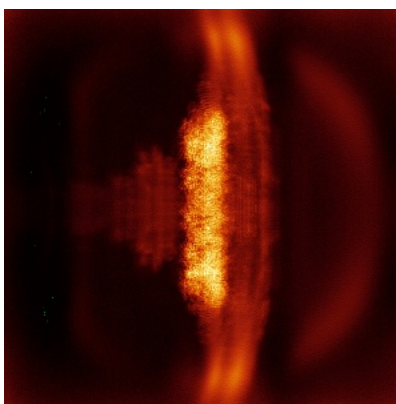


Z

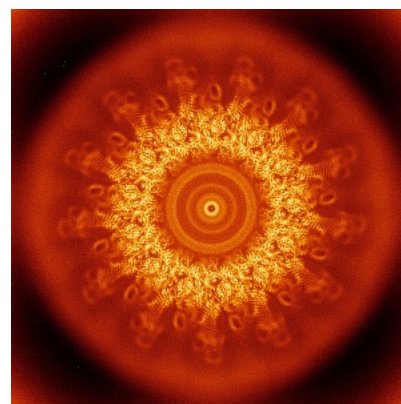
6.4.2 Raw map



X



Y

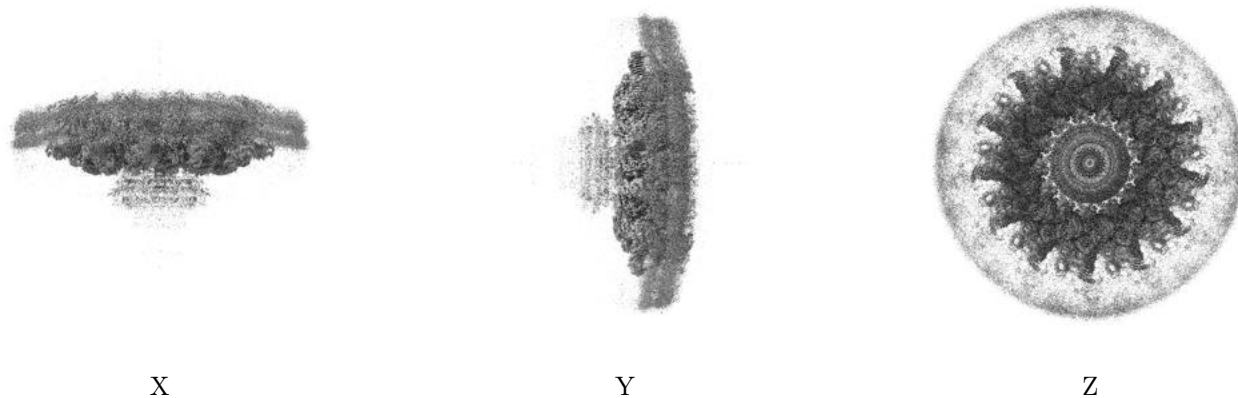


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

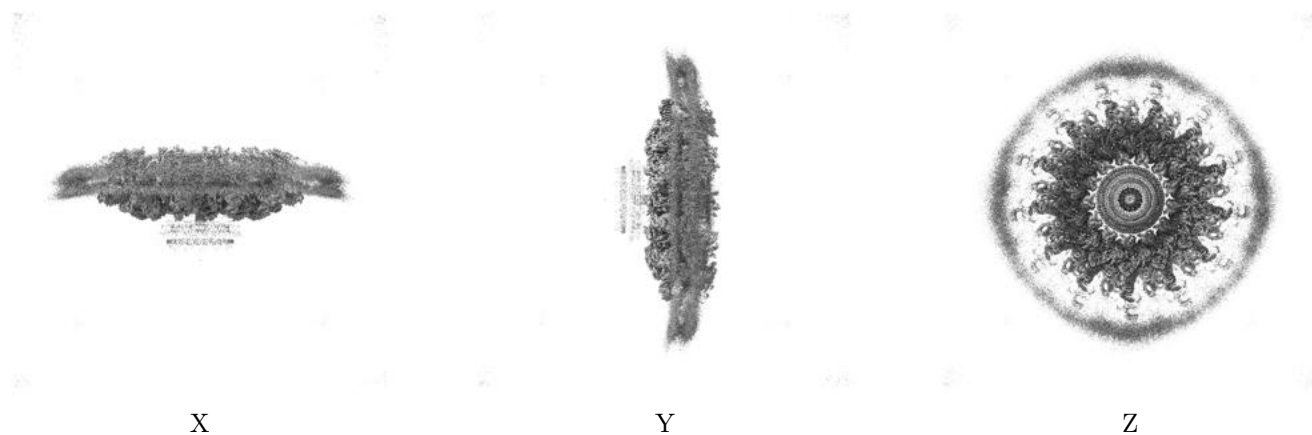
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

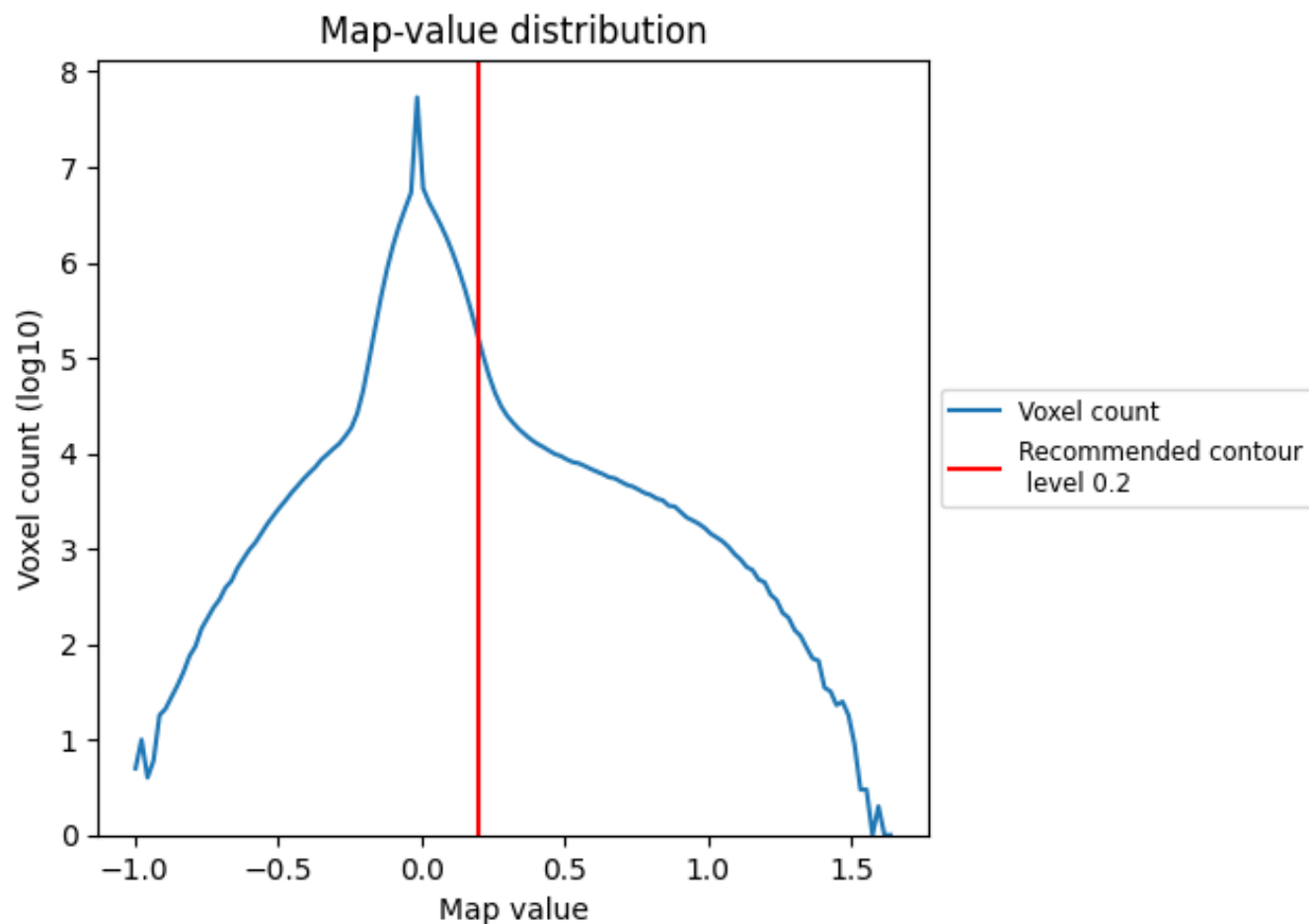
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

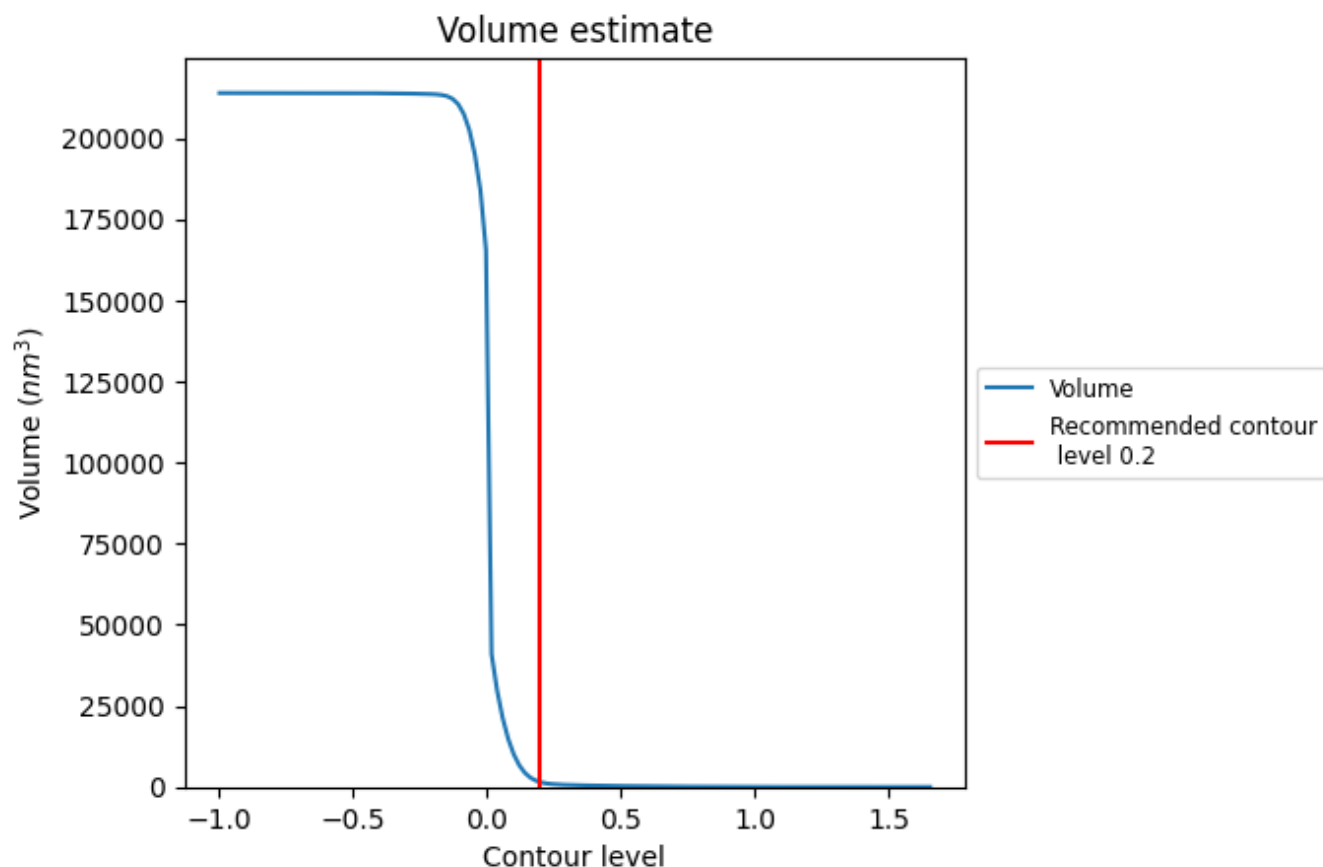
This section contains the results of statistical analysis of the map.

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.

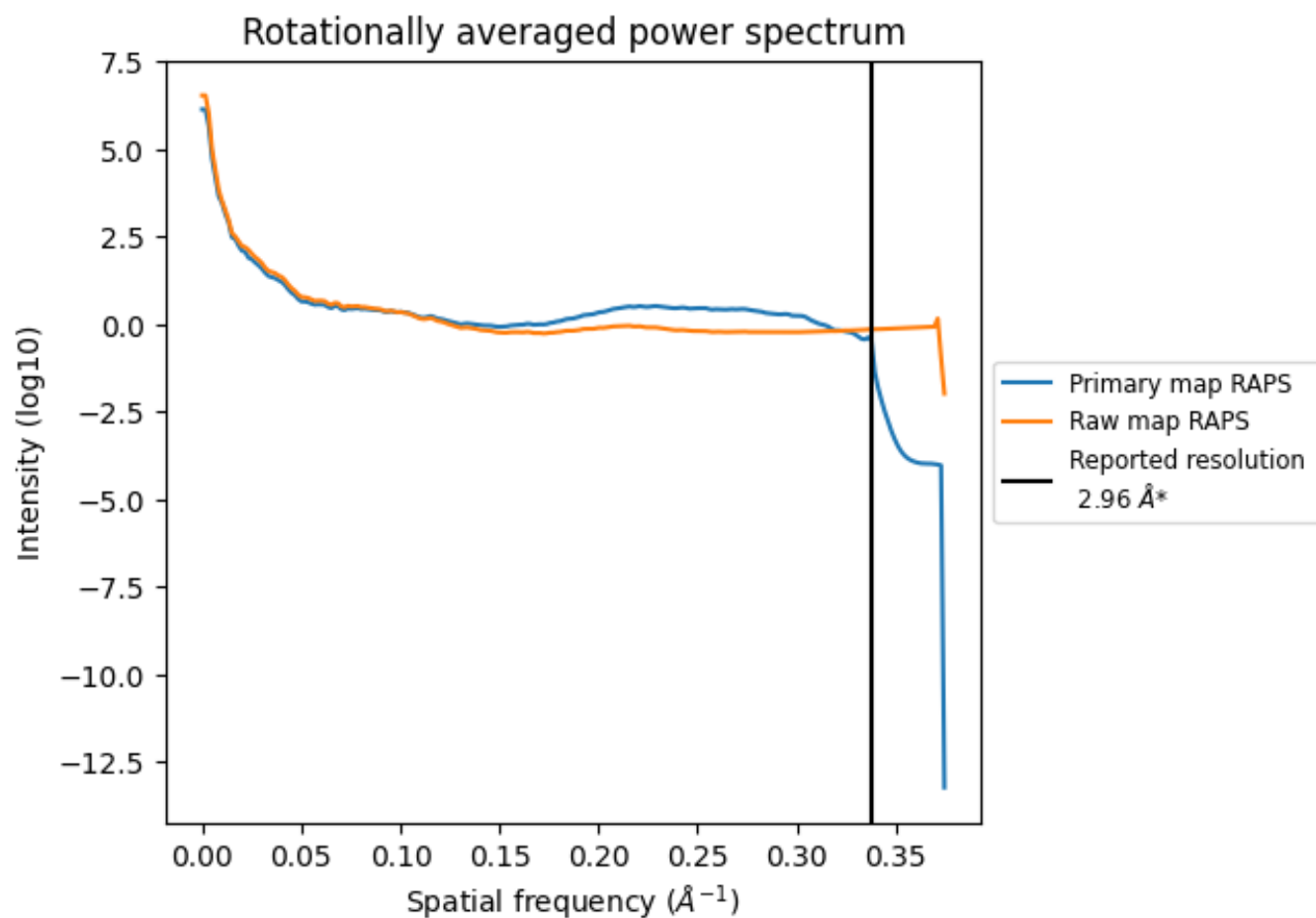
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1548 nm³; this corresponds to an approximate mass of 1398 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 ⓘ

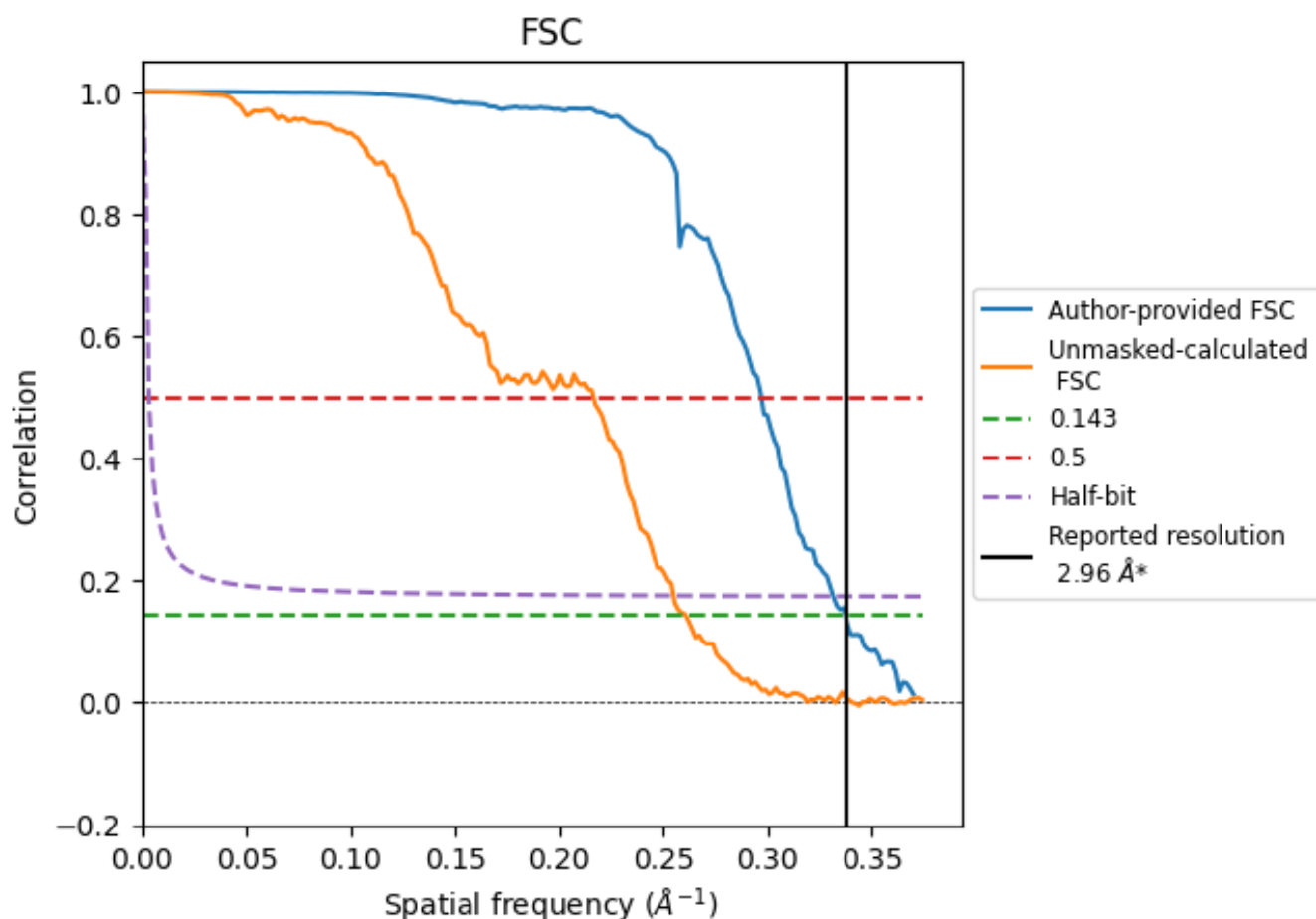


*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

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 0.338 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.36	3.01
Unmasked-calculated*	3.83	4.62	3.92

*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 3.83 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-49393 and PDB model 9NGU. Per-residue inclusion information can be found in section [3](#) on page [18](#).

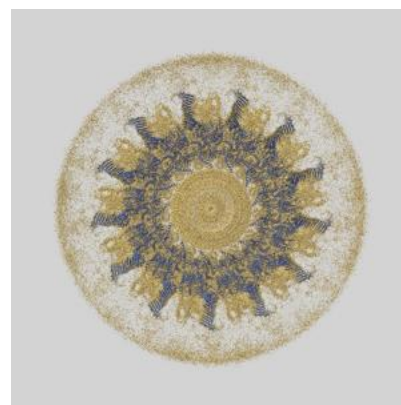
9.1 Map-model overlay [i](#)



X



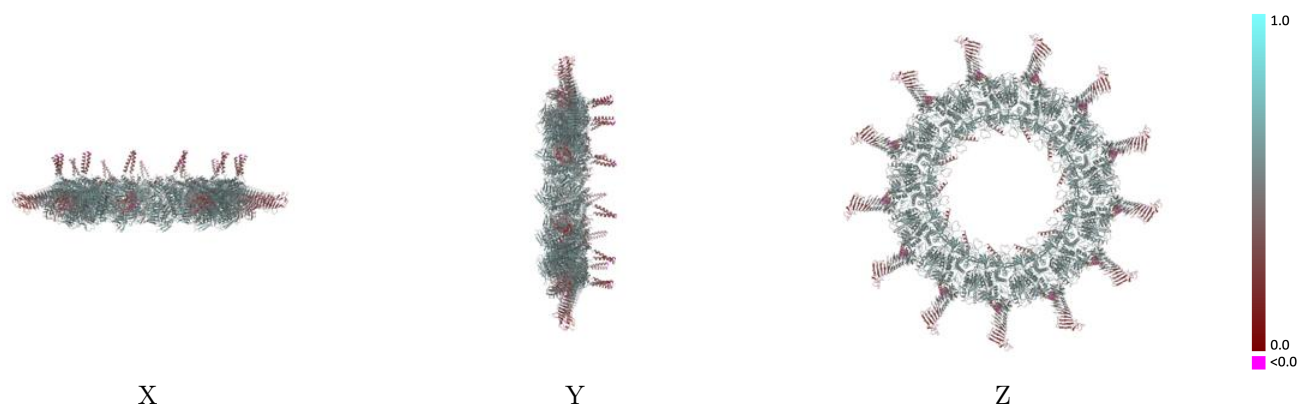
Y



Z

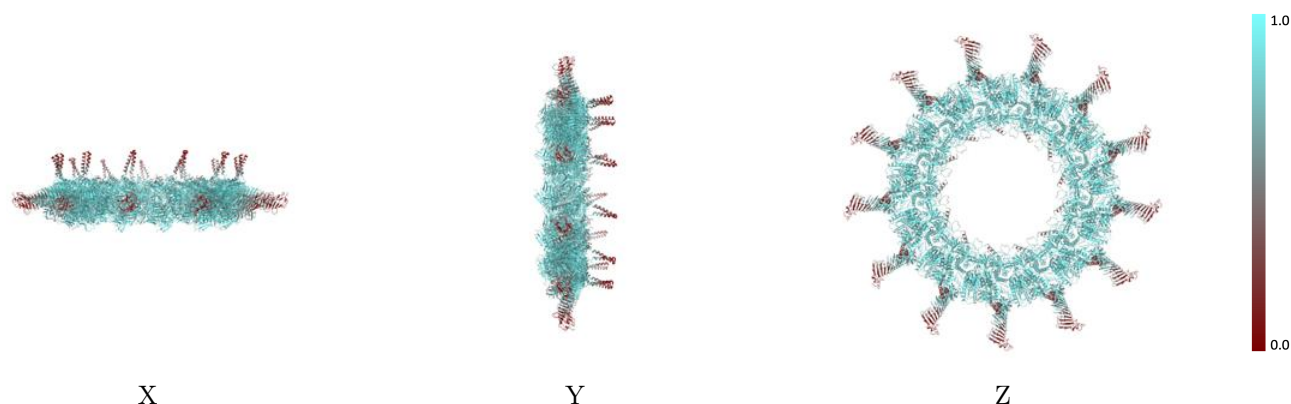
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



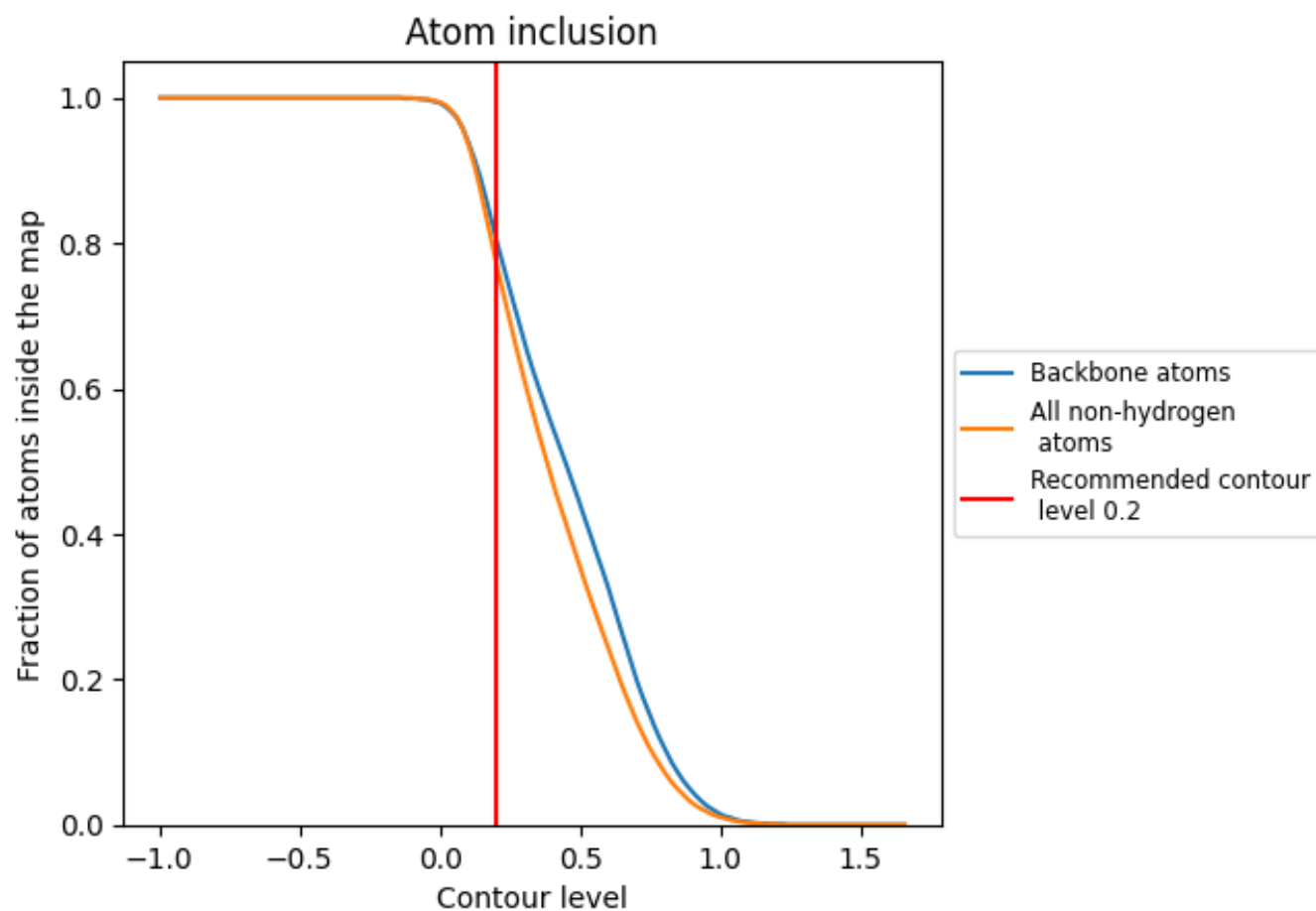
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7750	 0.5120
Aa	 0.8750	 0.5600
Ab	 0.8780	 0.5500
Ac	 0.5520	 0.4120
Ad	 0.8740	 0.5550
Ae	 0.8510	 0.5520
Af	 0.6700	 0.4700
Ag	 0.9370	 0.5980
Ah	 0.7860	 0.5120
Ai	 0.8350	 0.5430
Aj	 0.7040	 0.4820
Ak	 0.8790	 0.5610
Al	 0.8840	 0.5530
Am	 0.5560	 0.4100
An	 0.8720	 0.5540
Ao	 0.8660	 0.5490
Ap	 0.6560	 0.4660
Aq	 0.9260	 0.5920
Ar	 0.7770	 0.5100
As	 0.8350	 0.5400
At	 0.7060	 0.4760
Au	 0.8850	 0.5630
Av	 0.8750	 0.5510
Aw	 0.5490	 0.4080
Ax	 0.8880	 0.5560
Ay	 0.8550	 0.5510
Az	 0.6760	 0.4690
Ba	 0.9310	 0.5910
Bb	 0.7830	 0.5090
Bc	 0.8310	 0.5400
Bd	 0.6980	 0.4780
Be	 0.8750	 0.5610
Bf	 0.8790	 0.5520
Bg	 0.5490	 0.4080
Bh	 0.8760	 0.5510



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Chain	Atom inclusion	Q-score
Bi	 0.8600	 0.5550
Bj	 0.6760	 0.4670
Bk	 0.9250	 0.5940
Bl	 0.7840	 0.5130
Bm	 0.8340	 0.5430
Bn	 0.7090	 0.4800
Bo	 0.8710	 0.5610
Bp	 0.8890	 0.5520
Bq	 0.5460	 0.4090
Br	 0.8720	 0.5520
Bs	 0.8590	 0.5540
Bt	 0.6650	 0.4700
Bu	 0.9310	 0.5900
Bv	 0.7800	 0.5080
Bw	 0.8340	 0.5410
Bx	 0.6980	 0.4820
By	 0.8770	 0.5620
Bz	 0.8820	 0.5520
Ca	 0.5520	 0.4050
Cb	 0.8770	 0.5540
Cc	 0.8570	 0.5520
Cd	 0.6700	 0.4720
Ce	 0.9290	 0.5910
Cf	 0.7750	 0.5080
Cg	 0.8340	 0.5410
Ch	 0.6950	 0.4740
Ci	 0.8790	 0.5580
Cj	 0.8900	 0.5500
Ck	 0.5520	 0.4080
Cl	 0.8740	 0.5540
Cm	 0.8610	 0.5480
Cn	 0.6650	 0.4710
Co	 0.9250	 0.5910
Cp	 0.7850	 0.5110
Cq	 0.8340	 0.5420
Cr	 0.6890	 0.4790
Cs	 0.8800	 0.5580
Ct	 0.8860	 0.5520
Cu	 0.5490	 0.4060
Cv	 0.8770	 0.5500
Cw	 0.8630	 0.5500
Cx	 0.6560	 0.4710

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Chain	Atom inclusion	Q-score
Cy	 0.9160	 0.5900
Cz	 0.7810	 0.5120
Da	 0.8310	 0.5400
Db	 0.7110	 0.4750
Dc	 0.8720	 0.5580
Dd	 0.8820	 0.5490
De	 0.5480	 0.4120
Df	 0.8760	 0.5570
Dg	 0.8540	 0.5490
Dh	 0.6670	 0.4690
Di	 0.9250	 0.5930
Dj	 0.7760	 0.5100
Dk	 0.8360	 0.5440
Dl	 0.7000	 0.4740
Dm	 0.8770	 0.5610
Dn	 0.8730	 0.5510
Do	 0.5520	 0.4100
Dp	 0.8810	 0.5510
Dq	 0.8620	 0.5530
Dr	 0.6560	 0.4700
Ds	 0.9320	 0.5900
Dt	 0.7830	 0.5080
Du	 0.8310	 0.5400
Dv	 0.6890	 0.4810
Dw	 0.8750	 0.5580
Dx	 0.8860	 0.5540
Dy	 0.5550	 0.4140
Dz	 0.8810	 0.5530
Ea	 0.8610	 0.5510
Eb	 0.6580	 0.4690
Ec	 0.9310	 0.5950
Ed	 0.7760	 0.5100
Ee	 0.8310	 0.5410
Ef	 0.7060	 0.4740
Eg	 0.8900	 0.5580
Eh	 0.8730	 0.5510
Ei	 0.5530	 0.4120
Ej	 0.8790	 0.5510
Ek	 0.8570	 0.5540
El	 0.6630	 0.4690
Em	 0.9250	 0.5930
En	 0.7780	 0.5100

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Chain	Atom inclusion	Q-score
Eo	 0.8370	 0.5400
Ep	 0.6890	 0.4760
Eq	 0.8770	 0.5620
Er	 0.8760	 0.5510
Es	 0.5550	 0.4130
Et	 0.8740	 0.5530
Eu	 0.8650	 0.5540
Ev	 0.6610	 0.4680
Ew	 0.9250	 0.5940
Ex	 0.7800	 0.5110
Ey	 0.8350	 0.5430
Ez	 0.6950	 0.4780