



## wwPDB EM Validation Summary Report ⓘ

Nov 4, 2025 – 11:31 AM EST

PDB ID : 9NH0 / pdb\_00009nh0  
EMDB ID : EMD-49398  
Title : In situ cryo-EM structure of PR and DotA-IcmX of the Legionella Dot/Icm T4SS machine at C1 symmetry  
Authors : Yue, J.; Liu, J.  
Deposited on : 2025-02-23  
Resolution : 4.63 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

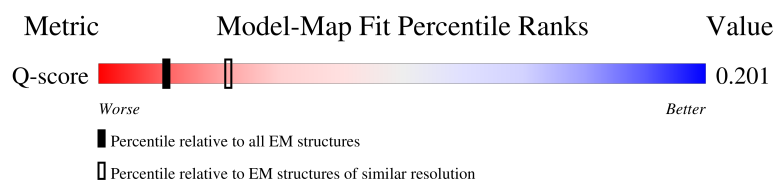
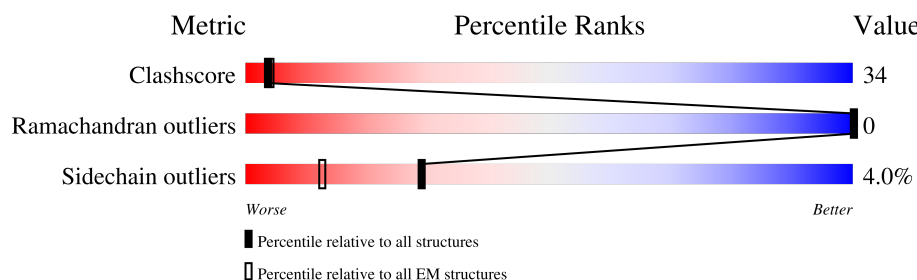
EMDB validation analysis : 0.0.1.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.63 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	2068 ( 4.13 - 5.13 )

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  $\geq 3$ , 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	16	<div> <div>100%</div> <div> <div>62%</div> <div>38%</div> </div> </div>
1	Ag	16	<div> <div>100%</div> <div> <div>50%</div> <div>50%</div> </div> </div>
1	Am	16	<div> <div>100%</div> <div> <div>31%</div> <div>62%</div> <div>6%</div> </div> </div>
1	As	16	<div> <div>100%</div> <div> <div>69%</div> <div>31%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	Ay	16	<div> <div>100%</div> <div>56% 44%</div> </div>
1	Be	16	<div> <div>100%</div> <div>69% 31%</div> </div>
1	Bk	16	<div> <div>100%</div> <div>38% 62%</div> </div>
1	Bq	16	<div> <div>100%</div> <div>62% 38%</div> </div>
1	Bw	16	<div> <div>100%</div> <div>69% 31%</div> </div>
1	Cc	16	<div> <div>100%</div> <div>38% 62%</div> </div>
1	Ci	16	<div> <div>100%</div> <div>50% 38% 12%</div> </div>
1	Co	16	<div> <div>100%</div> <div>56% 44%</div> </div>
1	Cu	16	<div> <div>100%</div> <div>50% 50%</div> </div>
1	Da	16	<div> <div>100%</div> <div>56% 44%</div> </div>
1	Dg	16	<div> <div>100%</div> <div>56% 38% 6%</div> </div>
1	Dm	16	<div> <div>100%</div> <div>56% 38% 6%</div> </div>
1	Ds	16	<div> <div>100%</div> <div>50% 44% 6%</div> </div>
1	Dy	16	<div> <div>100%</div> <div>69% 31%</div> </div>
2	Ab	9	<div> <div>78%</div> <div>56% 44%</div> </div>
2	Ah	9	<div> <div>89%</div> <div>56% 44%</div> </div>
2	An	9	<div> <div>100%</div> <div>67% 33%</div> </div>
2	At	9	<div> <div>100%</div> <div>44% 56%</div> </div>
2	Az	9	<div> <div>100%</div> <div>56% 44%</div> </div>
2	Bf	9	<div> <div>100%</div> <div>44% 56%</div> </div>
2	Bl	9	<div> <div>100%</div> <div>44% 56%</div> </div>
2	Br	9	<div> <div>100%</div> <div>56% 44%</div> </div>
2	Bx	9	<div> <div>89%</div> <div>56% 44%</div> </div>
2	Cd	9	<div> <div>100%</div> <div>56% 44%</div> </div>
2	Cj	9	<div> <div>100%</div> <div>56% 44%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Cp	9	
2	Cv	9	
2	Db	9	
2	Dh	9	
2	Dn	9	
2	Dt	9	
2	Dz	9	
3	Ac	16	
3	Ai	16	
3	Ao	16	
3	Au	16	
3	Ba	16	
3	Bg	16	
3	Bm	16	
3	Bs	16	
3	By	16	
3	Ce	16	
3	Ck	16	
3	Cq	16	
3	Cw	16	
3	Dc	16	
3	Di	16	
3	Do	16	
3	Du	16	
3	Ea	16	

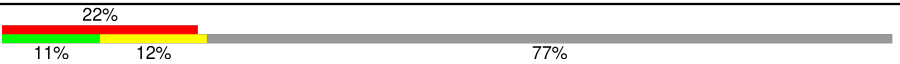


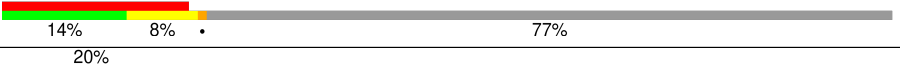



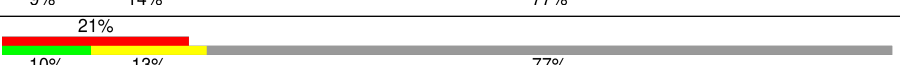
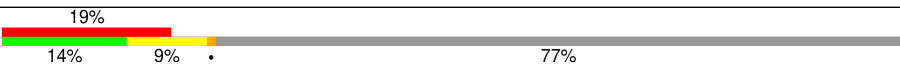

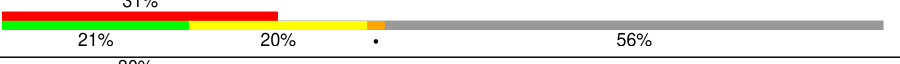




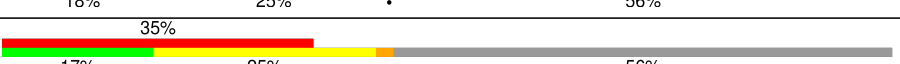









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Mol	Chain	Length	Quality of chain
4	Ad	5	
4	Aj	5	
4	Ap	5	
4	Av	5	
4	Bb	5	
4	Bh	5	
4	Bn	5	
4	Bt	5	
4	Bz	5	
4	Cf	5	
4	Cl	5	
4	Cr	5	
4	Cx	5	
4	Dd	5	
4	Dj	5	
4	Dp	5	
4	Dv	5	
4	Eb	5	
5	Ae	269	
5	Ak	269	
5	Aq	269	
5	Aw	269	
5	Bc	269	
5	Bi	269	
5	Bo	269	

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Mol	Chain	Length	Quality of chain
5	Bu	269	
5	Ca	269	
5	Cg	269	
5	Cm	269	
5	Cs	269	
5	Cy	269	
5	De	269	
5	Dk	269	
5	Dq	269	
5	Dw	269	
5	Ec	269	
6	Af	361	
6	Al	361	
6	Ar	361	
6	Ax	361	
6	Bd	361	
6	Bj	361	
6	Bp	361	
6	Bv	361	
6	Cb	361	
6	Ch	361	
6	Cn	361	
6	Ct	361	
6	Cz	361	
6	Df	361	

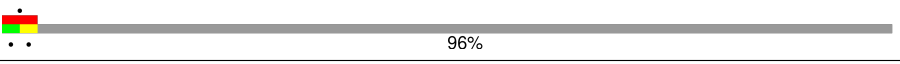
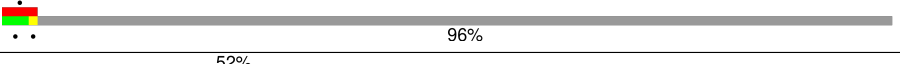










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Mol	Chain	Length	Quality of chain
6	Dl	361	
6	Dr	361	
6	Dx	361	
6	Ed	361	
7	Ee	1048	
7	Ef	1048	
7	Eg	1048	
7	Eh	1048	
7	Ei	1048	
7	Ej	1048	
7	Ek	1048	
7	El	1048	
7	Em	1048	
7	En	1048	
7	Eo	1048	
7	Ep	1048	
7	Eq	1048	
7	Er	1048	
7	Es	1048	
7	Et	1048	
7	Eu	1048	
7	Ev	1048	
7	Fg	1048	
7	Fh	1048	
7	Fi	1048	

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Mol	Chain	Length	Quality of chain
7	Fj	1048	
7	Fk	1048	
8	Ew	466	
8	Ex	466	
8	Ey	466	
8	Ez	466	
8	Fa	466	
9	Fb	1048	
9	Fc	1048	
9	Fd	1048	
9	Fe	1048	
9	Ff	1048	



## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 94015 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 unknown peptide E.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Aa	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ag	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Am	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	As	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ay	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Be	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bk	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bq	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Bw	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Cc	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ci	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Co	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Cu	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Da	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Dg	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Dm	16	Total	C	N	O	S	0	0
			117	71	20	25	1		
1	Ds	16	Total	C	N	O	S	0	0
			117	71	20	25	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	Dy	16	Total	C	N	O	S	0	0
			117	71	20	25	1		

- Molecule 2 is a protein called unknown peptide F.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Ab	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Ah	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	An	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	At	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Az	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Bf	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Bl	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Br	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Bx	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cd	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cj	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cp	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Cv	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Db	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dh	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dn	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dt	9	Total	C	N	O	S	0	0
			61	35	12	12	2		
2	Dz	9	Total	C	N	O	S	0	0
			61	35	12	12	2		

- Molecule 3 is a protein called unknown peptide G.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Ac	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ai	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ao	16	Total	C	N	O	0	0
			125	78	21	26		
3	Au	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ba	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bg	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bm	16	Total	C	N	O	0	0
			125	78	21	26		
3	Bs	16	Total	C	N	O	0	0
			125	78	21	26		
3	By	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ce	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ck	16	Total	C	N	O	0	0
			125	78	21	26		
3	Cq	16	Total	C	N	O	0	0
			125	78	21	26		
3	Cw	16	Total	C	N	O	0	0
			125	78	21	26		
3	Dc	16	Total	C	N	O	0	0
			125	78	21	26		
3	Di	16	Total	C	N	O	0	0
			125	78	21	26		
3	Do	16	Total	C	N	O	0	0
			125	78	21	26		
3	Du	16	Total	C	N	O	0	0
			125	78	21	26		
3	Ea	16	Total	C	N	O	0	0
			125	78	21	26		

- Molecule 4 is a protein called unknown peptide H.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Ad	5	Total	C	N	O	0	0
			36	23	5	8		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Aj	5	Total	C	N	O	0	0
			36	23	5	8		
4	Ap	5	Total	C	N	O	0	0
			36	23	5	8		
4	Av	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bb	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bh	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bn	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bt	5	Total	C	N	O	0	0
			36	23	5	8		
4	Bz	5	Total	C	N	O	0	0
			36	23	5	8		
4	Cf	5	Total	C	N	O	0	0
			36	23	5	8		
4	Cl	5	Total	C	N	O	0	0
			36	23	5	8		
4	Cr	5	Total	C	N	O	0	0
			36	23	5	8		
4	Cx	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dd	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dj	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dp	5	Total	C	N	O	0	0
			36	23	5	8		
4	Dv	5	Total	C	N	O	0	0
			36	23	5	8		
4	Eb	5	Total	C	N	O	0	0
			36	23	5	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Ae	63	Total	C	N	O	S	0	0
			484	308	84	91	1		
5	Ak	63	Total	C	N	O	S	0	0
			484	308	84	91	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	Aq	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Aw	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bc	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bi	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bo	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Bu	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Ca	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cg	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cm	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cs	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Cy	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	De	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dk	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dq	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Dw	63	Total 484	C 308	N 84	O 91	S 1	0	0
5	Ec	63	Total 484	C 308	N 84	O 91	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Af	160	Total 1238	C 795	N 207	O 233	S 3	0	0
6	Al	160	Total 1238	C 795	N 207	O 233	S 3	0	0
6	Ar	160	Total 1238	C 795	N 207	O 233	S 3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Ax	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Bd	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Bj	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Bp	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Bv	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Cb	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Ch	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Cn	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Ct	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Cz	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Df	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Dl	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Dr	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Dx	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		
6	Ed	160	Total	C	N	O	S	0	0
			1238	795	207	233	3		

- Molecule 7 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ee	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Ef	59	Total	C	N	O	S	0	0
			472	287	81	103	1		
7	Eg	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Eh	48	Total	C	N	O	S	0	0
			397	244	68	84	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	Ei	49	Total	C	N	O	S	0	0
			402	247	69	85	1		
7	Ej	58	Total	C	N	O	S	0	0
			464	283	80	100	1		
7	Ek	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	El	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Em	46	Total	C	N	O	S	0	0
			381	232	66	82	1		
7	En	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Eo	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Ep	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Eq	57	Total	C	N	O	S	0	0
			459	280	79	99	1		
7	Er	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Es	56	Total	C	N	O	S	0	0
			454	277	78	98	1		
7	Et	48	Total	C	N	O	S	0	0
			397	244	68	84	1		
7	Eu	59	Total	C	N	O	S	0	0
			472	287	81	103	1		
7	Ev	34	Total	C	N	O	S	0	0
			276	168	47	60	1		
7	Fg	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
7	Fh	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
7	Fi	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
7	Fj	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
7	Fk	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

- Molecule 8 is a protein called IcmX (IcmY).

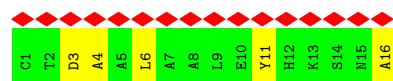
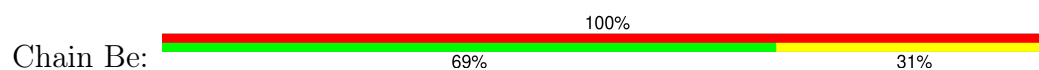
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Ew	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
8	Ex	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
8	Ey	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
8	Ez	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		
8	Fa	417	Total	C	N	O	S	0	0
			3213	2013	542	646	12		

- Molecule 9 is a protein called DotA.

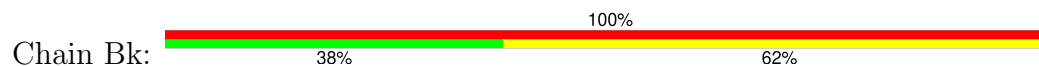
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Fb	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fc	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fd	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fe	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Ff	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		







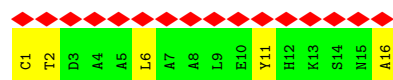
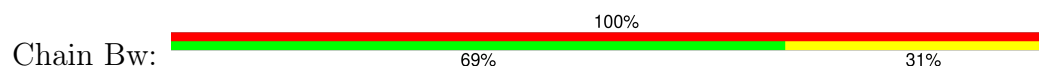
- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



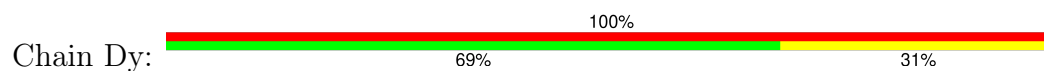
- Molecule 1: unknown peptide E



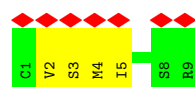
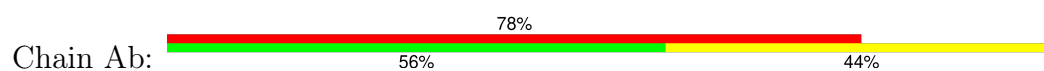
- Molecule 1: unknown peptide E



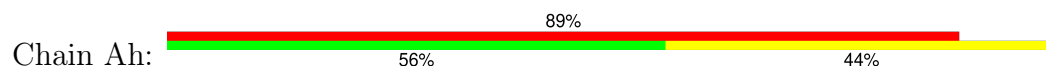
- Molecule 1: unknown peptide E



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



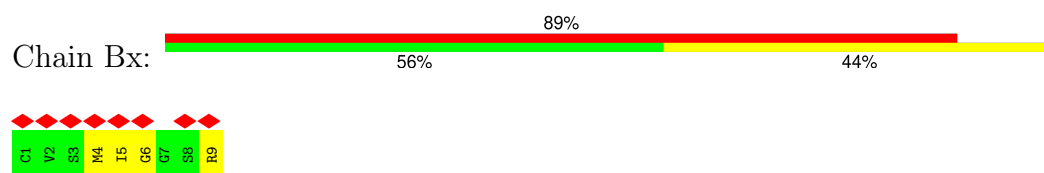
- Molecule 2: unknown peptide F



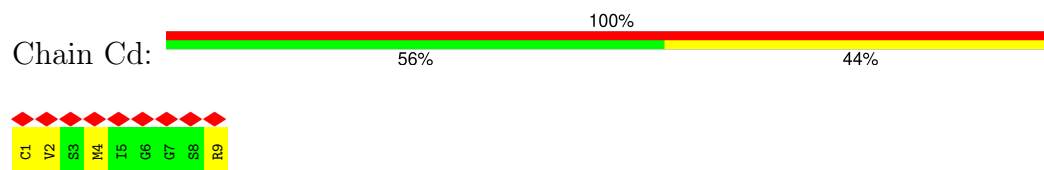
- Molecule 2: unknown peptide F



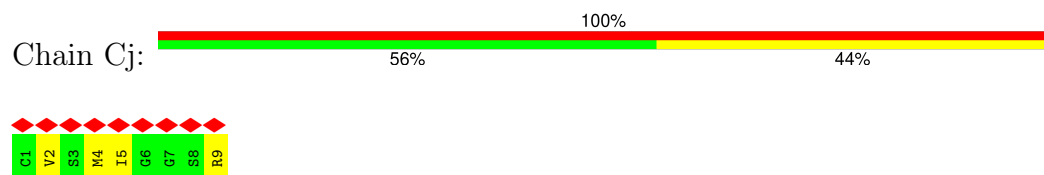
- Molecule 2: unknown peptide F



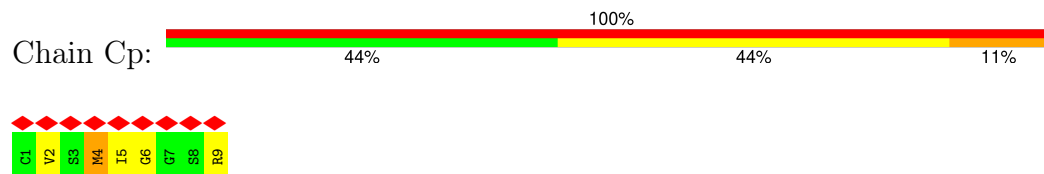
- Molecule 2: unknown peptide F



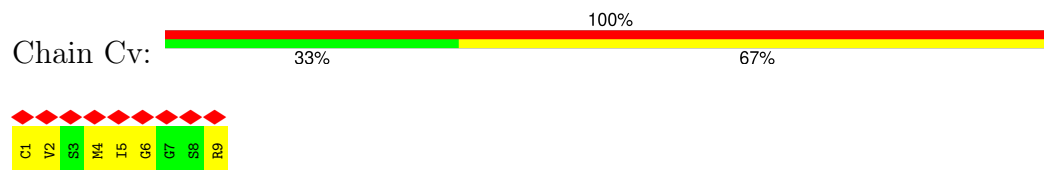
- Molecule 2: unknown peptide F



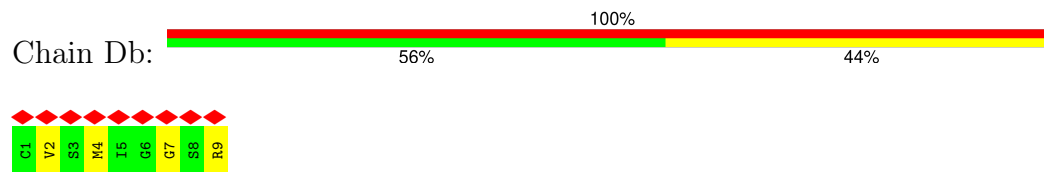
- Molecule 2: unknown peptide F



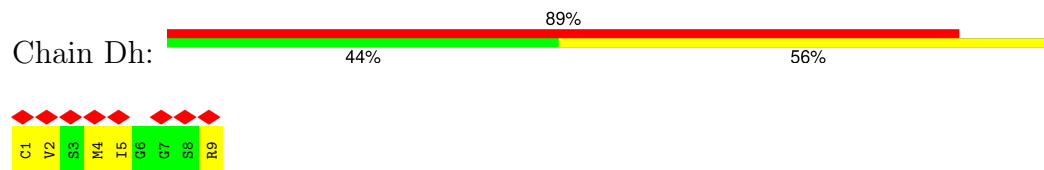
- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



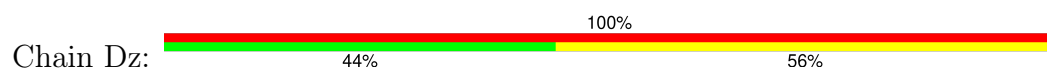
- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 3: unknown peptide G



- Molecule 3: unknown peptide G



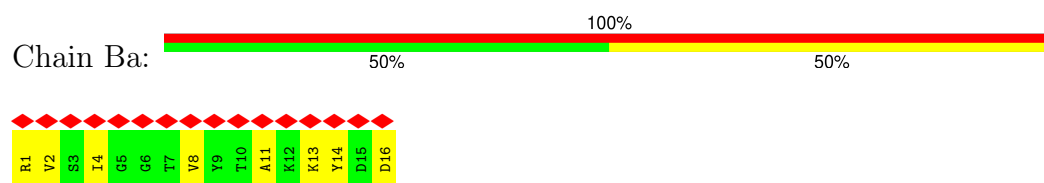
- Molecule 3: unknown peptide G



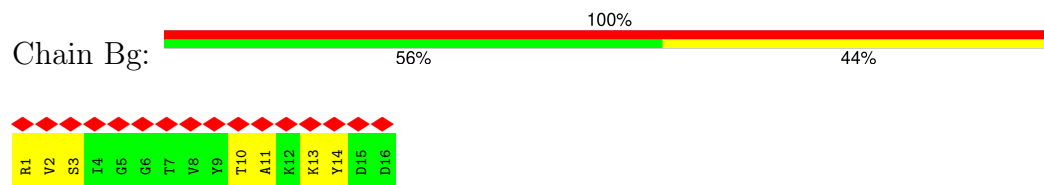
- Molecule 3: unknown peptide G



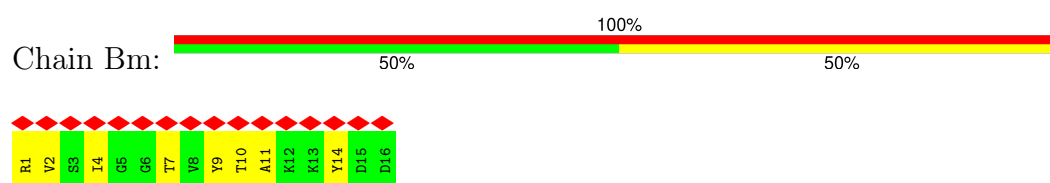
- Molecule 3: unknown peptide G



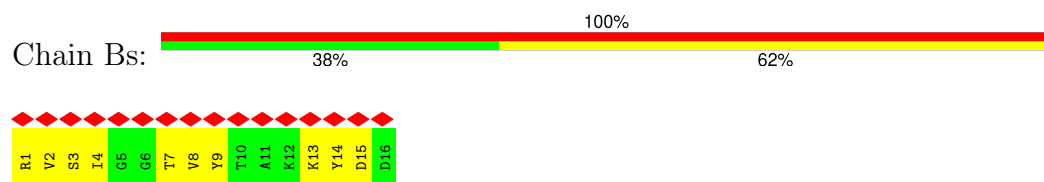
- Molecule 3: unknown peptide G



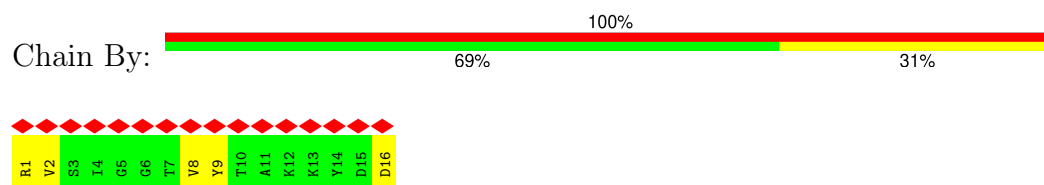
- Molecule 3: unknown peptide G



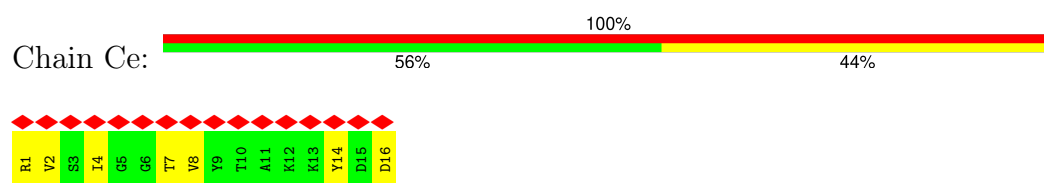
- Molecule 3: unknown peptide G



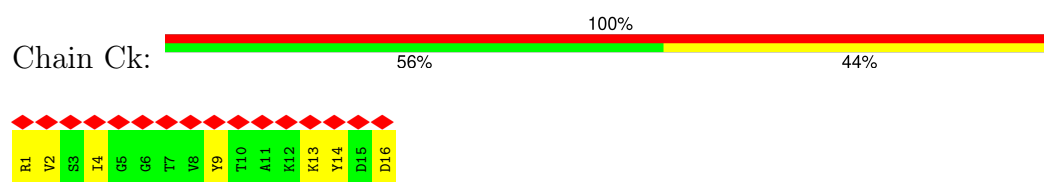
- Molecule 3: unknown peptide G



- Molecule 3: unknown peptide G



- Molecule 3: unknown peptide G



## ● Molecule 3: unknown peptide G



## ● Molecule 3: unknown peptide G



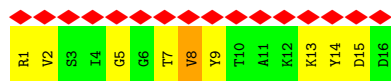
## ● Molecule 3: unknown peptide G



## ● Molecule 3: unknown peptide G



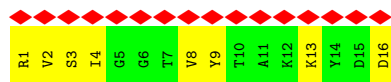
## ● Molecule 3: unknown peptide G



## ● Molecule 3: unknown peptide G



## ● Molecule 3: unknown peptide G

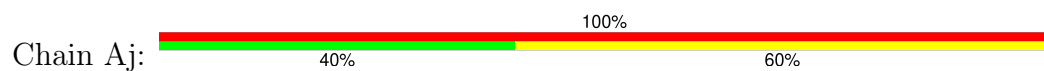




- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



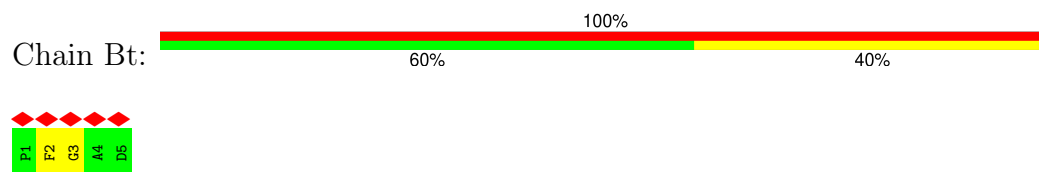
- Molecule 4: unknown peptide H



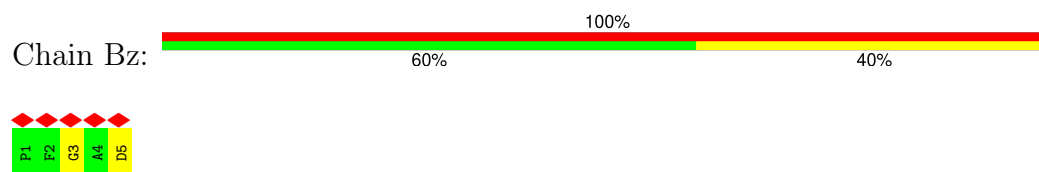
- Molecule 4: unknown peptide H



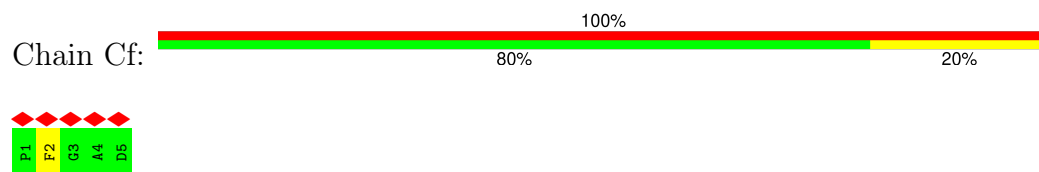
- Molecule 4: unknown peptide H



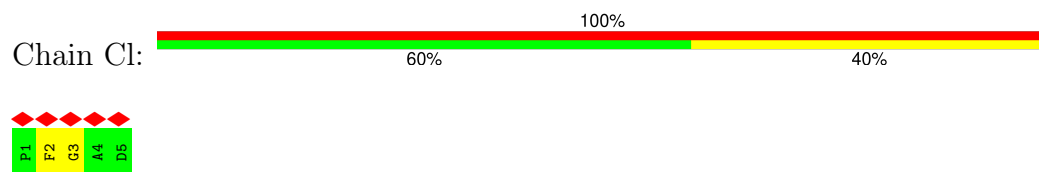
- Molecule 4: unknown peptide H



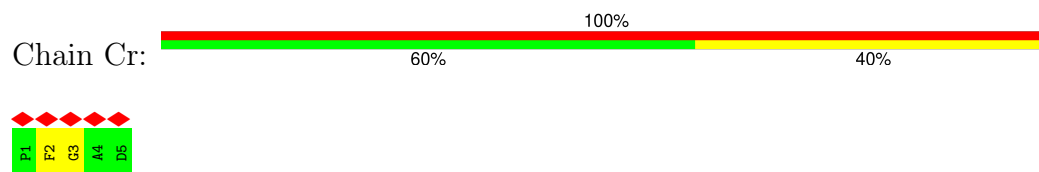
- Molecule 4: unknown peptide H



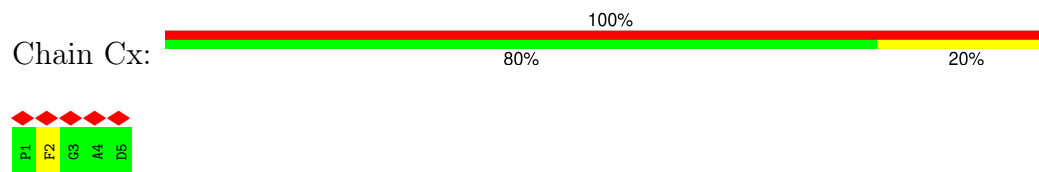
- Molecule 4: unknown peptide H



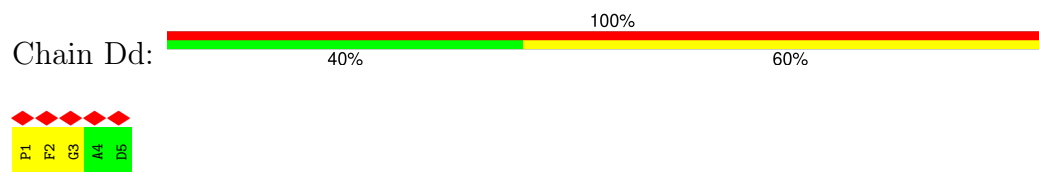
- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H

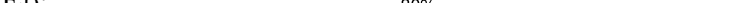


- Chain Dp: 



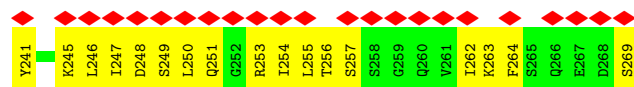
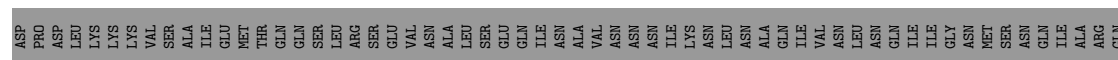
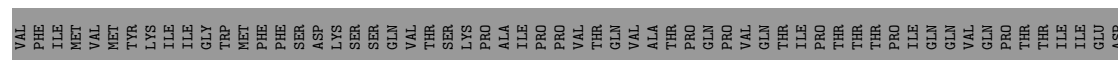
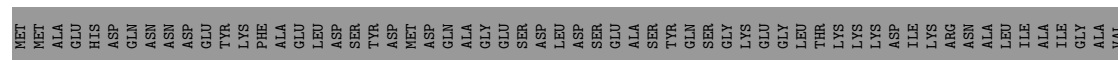
- Chain Dv: 



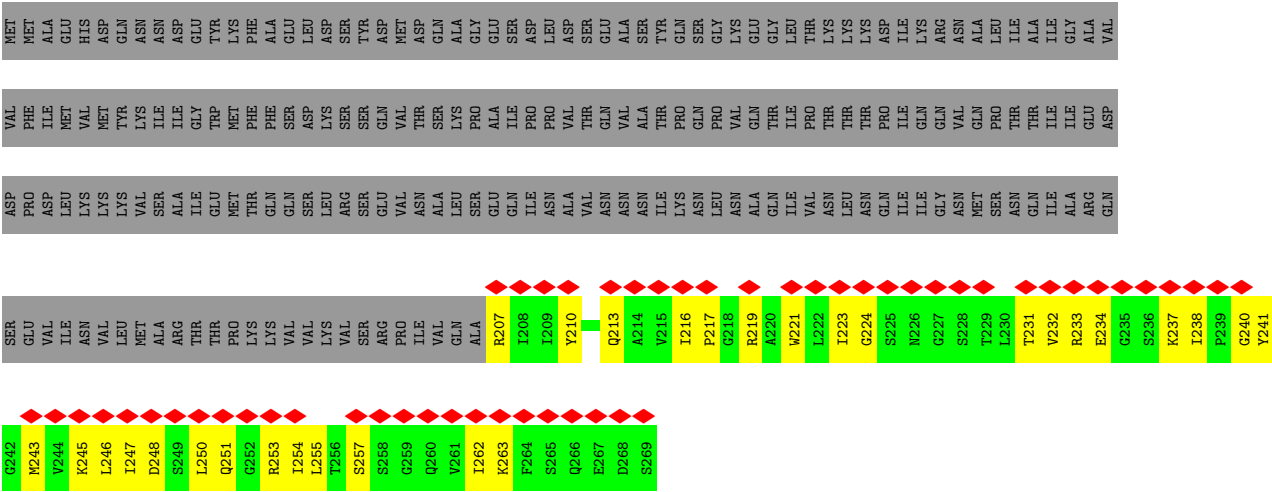
- Chain Eb: 



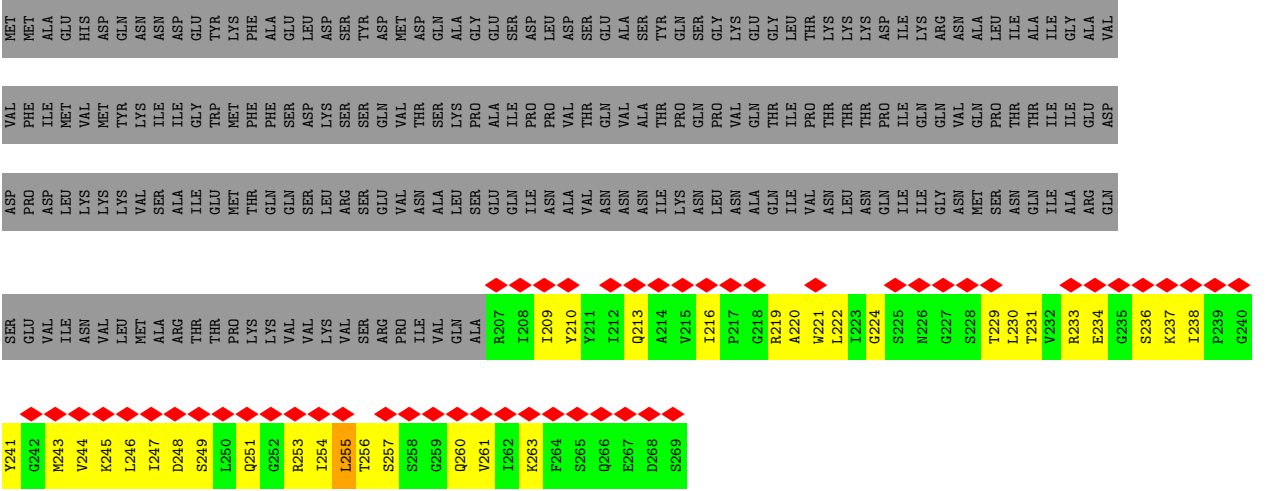
- Chain Ae: 19% 11% 12% 77%



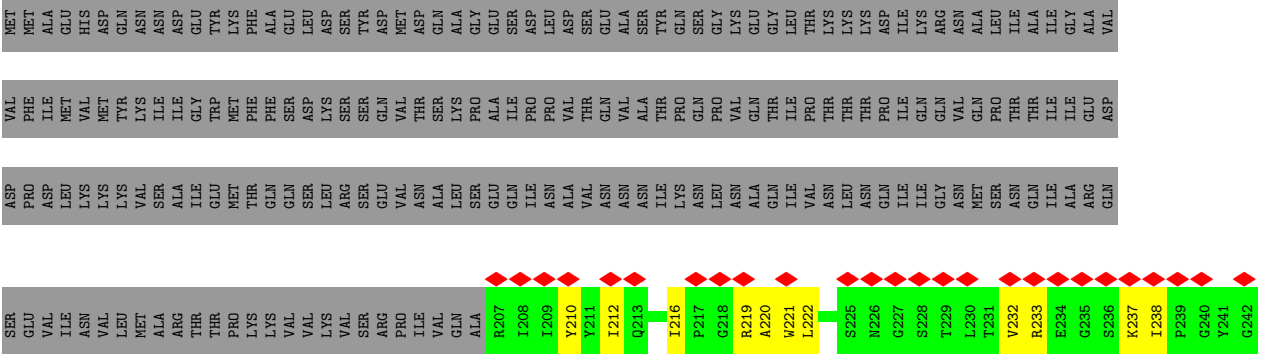
- Chain Ak: 20% 12% 11% 77%

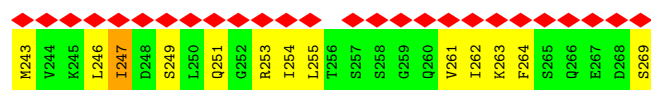


• Molecule 5: IcmG (DotF)

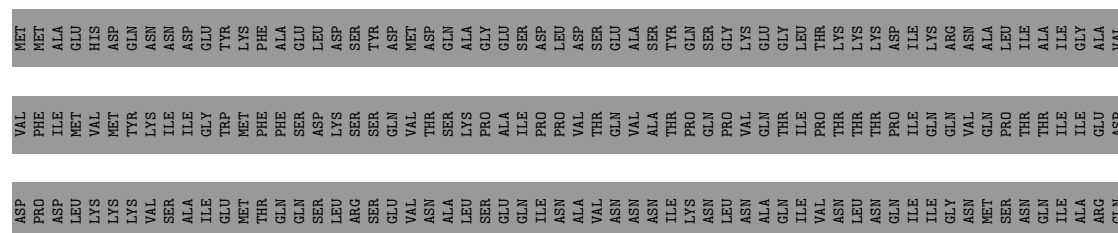


• Molecule 5: IcmG (DotF)

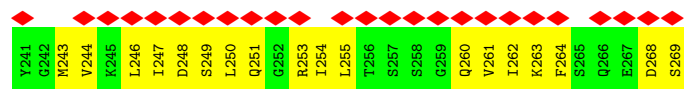
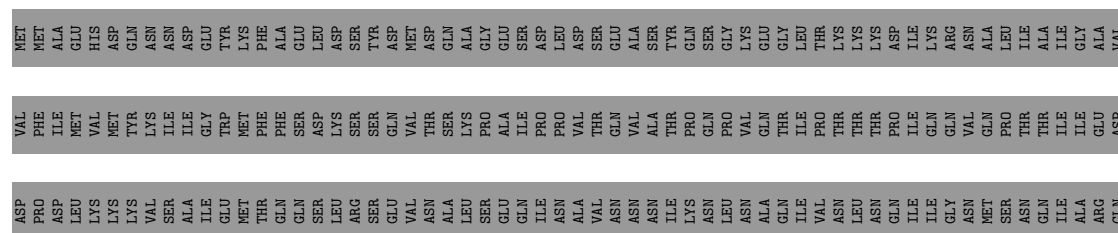




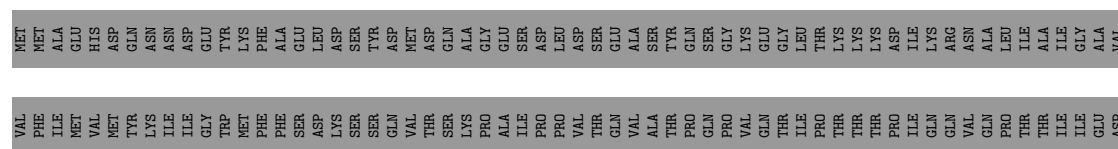
## • Molecule 5: IcmG (DotF)

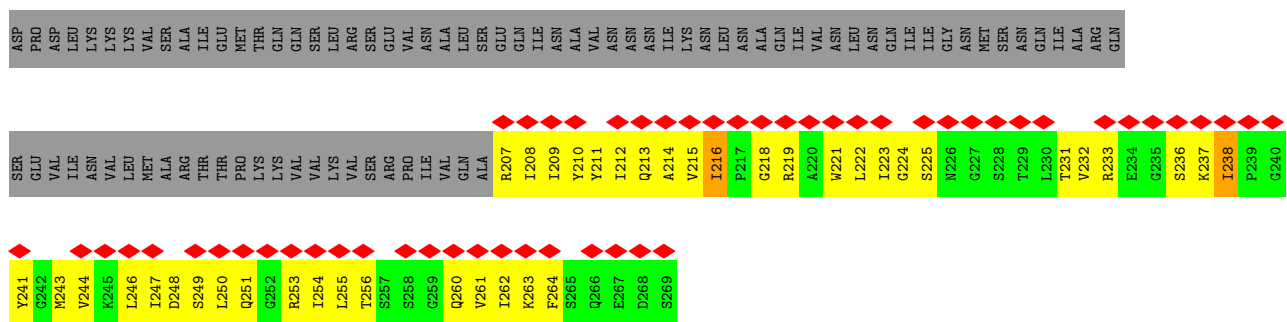


## • Molecule 5: IcmG (DotF)

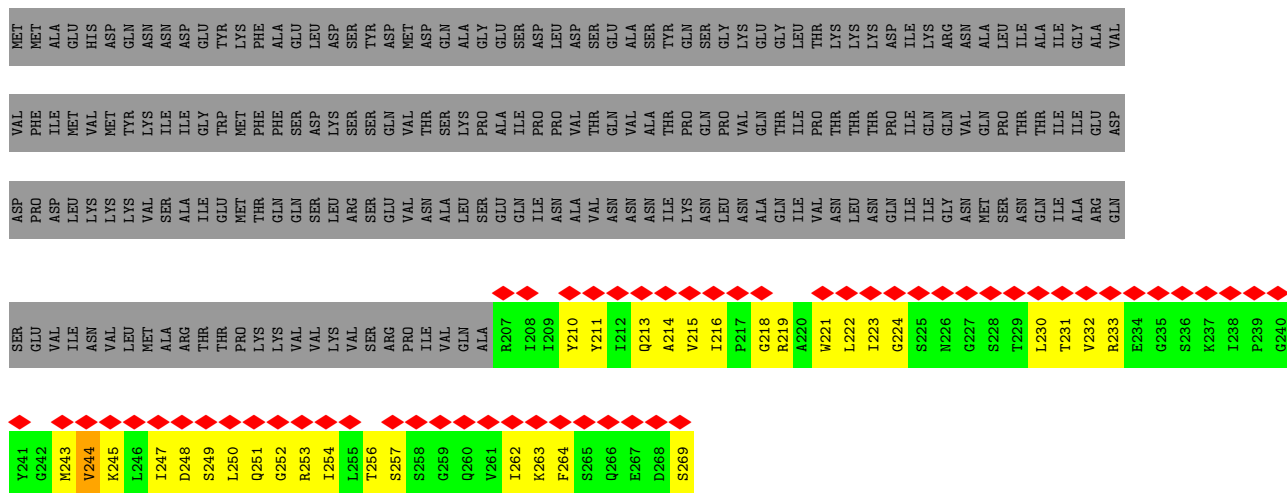


## • Molecule 5: IcmG (DotF)

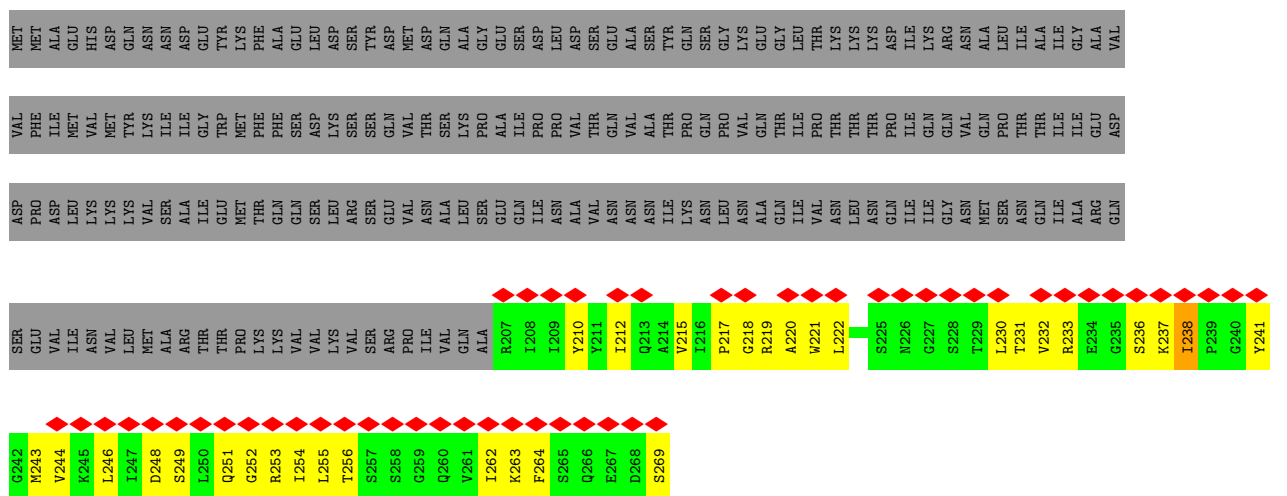




- Molecule 5: IcmG (DotF)



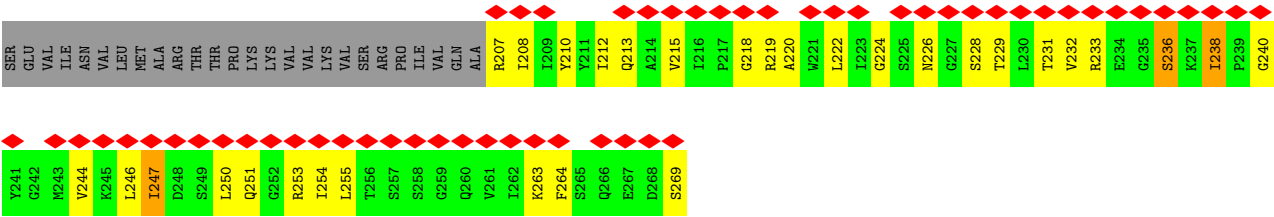
- Molecule 5: IcmG (DotF)



- Molecule 5: IcmG (DotF)



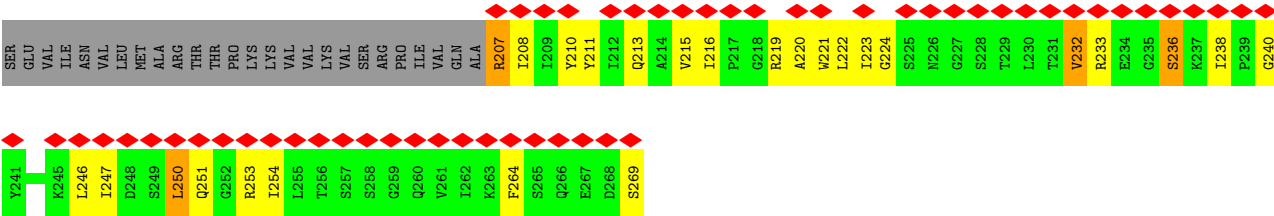
MET	MET	ASP
MET	ALA	PRO
GLU	ILE	GLU
ASP	LEU	ASP
HIS	VAL	LYS
ASP	MET	LYS
GLN	TYR	VAL
ASN	LYS	VAL
ASN	LYS	VAL
ASP	ILE	SER
GLU	ALA	ALA
TRP	GLY	THR
TYR	TRP	GLU
GLY	MET	THR
PHE	PHE	THR
ALA	PHE	GLN
GLU	SER	GLN
LEU	ASP	SER
ASP	LYS	LEU
SER	SER	ARG
TYR	SER	SER
ASP	GLN	GLU
MET	VAL	ASP
ASP	THR	ILE
GLN	SER	ALA
ALA	LYS	LEU
GLY	PRO	SER
GLU	ALA	GLU
ILE	ILE	GLN
ASP	PRO	ILE
LEU	PRO	ILE
ASP	VAL	ALA
SER	THR	ASN
GLU	ALA	ASN
GLY	THR	ILE
LEU	PRO	LYS
THR	ILE	ASN
THR	THR	LEU
LYS	THR	GLN
LYS	THR	GLN
ASP	PRO	GLN
ILE	ILE	ILE
LYS	ILE	ILE
ARG	GLN	GLY
ASN	VAL	ASN
ALA	GLN	MET
ALA	PRO	SER
LEU	PRO	LEU
ILE	THR	ILE
ALA	THR	GLN
ALA	ILE	ILE
GLY	GLU	ALA
VAL	ASP	GLN



● Molecule 5: IcmG (DotF)



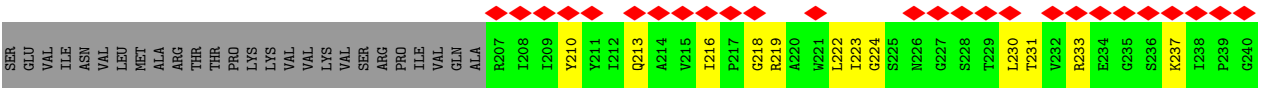
MET	MET	ASP
ALA	ILE	PRO
GLU	MET	LEU
HIS	VAL	LYS
ASP	MET	LYS
GLN	TYR	VAL
ASN	LYS	VAL
ASN	ILE	SER
ASP	ILE	ALA
GLU	TRP	GLU
THR	MET	THR
TYR	PHE	GLN
PHE	PHE	LEU
ALA	ASP	SER
LEU	ASP	ARG
LYS	SER	SER
LYS	SER	SER
THR	ASP	GLU
GLN	VAL	VAL
VAL	THR	ASN
ASP	THR	ASN
ILE	SER	ALA
VAL	LYS	LEU
GLN	PRO	SER
ALA	ILE	GLN
GLY	ILE	GLU
GLU	ILE	ILE
SER	PRO	ILE
GLY	THR	THR
LYS	THR	VAL
LYS	THR	ASN
ASP	PRO	ILE
ILE	ILE	GLY
LYS	ARG	GLN
ARG	VAL	GLY
ASN	GLN	ILE
ALA	VAL	THR
ALA	PRO	THR
LEU	PRO	ILE
ILE	THR	ILE
THR	THR	GLY
ALA	THR	ALA
VAL	ASP	VAL



● Molecule 5: IcmG (DotF)

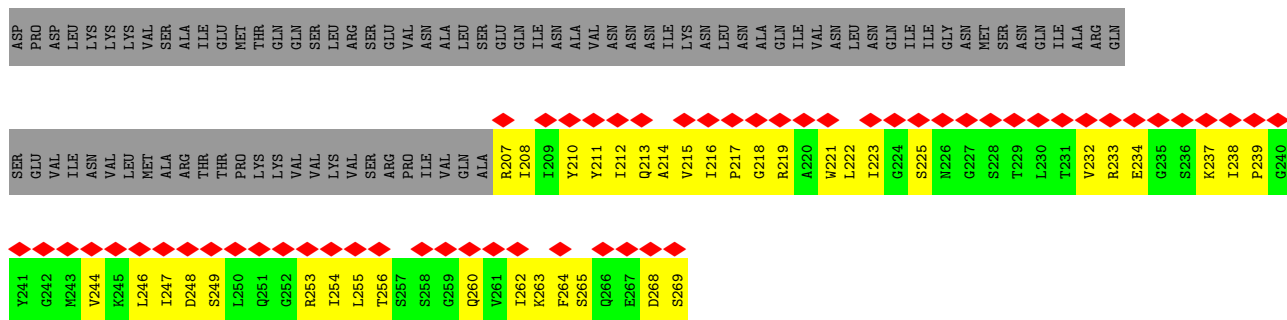


MET	MET	ASP
ALA	ILE	PRO
GLU	MET	LEU
HIS	VAL	LYS
ASP	MET	LYS
GLN	TYR	VAL
ASN	LYS	VAL
ASN	ILE	SER
ASP	ILE	ALA
GLU	TRP	GLU
THR	MET	THR
TYR	PHE	GLN
PHE	PHE	LEU
ALA	ASP	SER
LEU	ASP	ARG
LYS	SER	SER
LYS	SER	SER
THR	ASP	GLU
GLN	VAL	VAL
VAL	THR	ASN
ASP	THR	ASN
ILE	SER	ALA
VAL	LYS	LEU
GLN	PRO	SER
ALA	ILE	GLN
GLY	ILE	GLU
GLU	ILE	ILE
SER	PRO	ILE
GLY	THR	THR
LYS	THR	VAL
LYS	THR	ASN
ASP	PRO	ILE
ILE	ILE	GLY
LYS	ARG	GLN
ARG	VAL	GLY
ASN	GLN	ILE
ALA	VAL	THR
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ILE	THR	ILE
THR	THR	GLY
ALA	THR	ALA
VAL	ASP	VAL

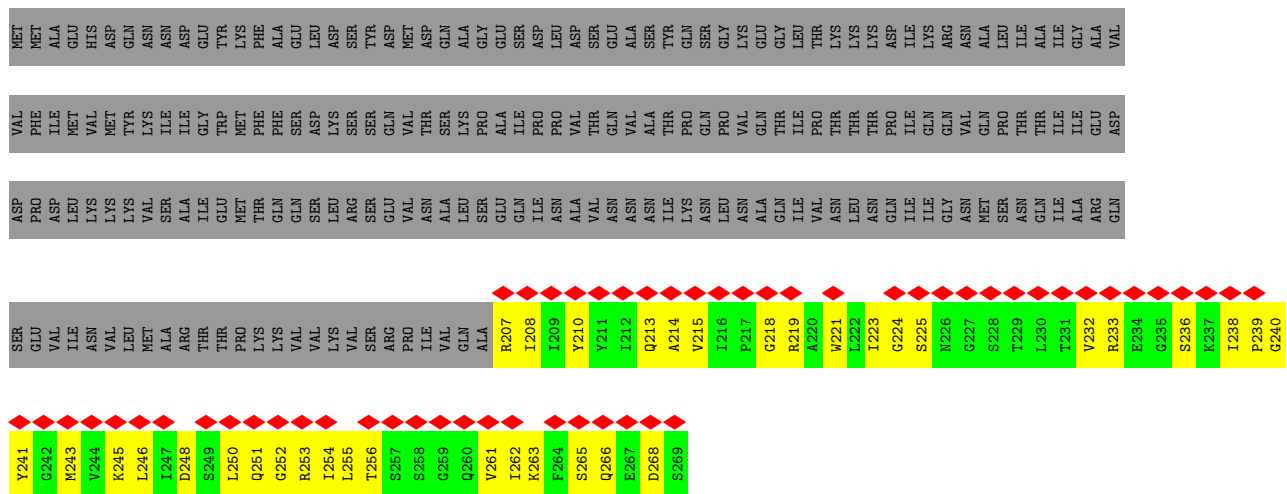




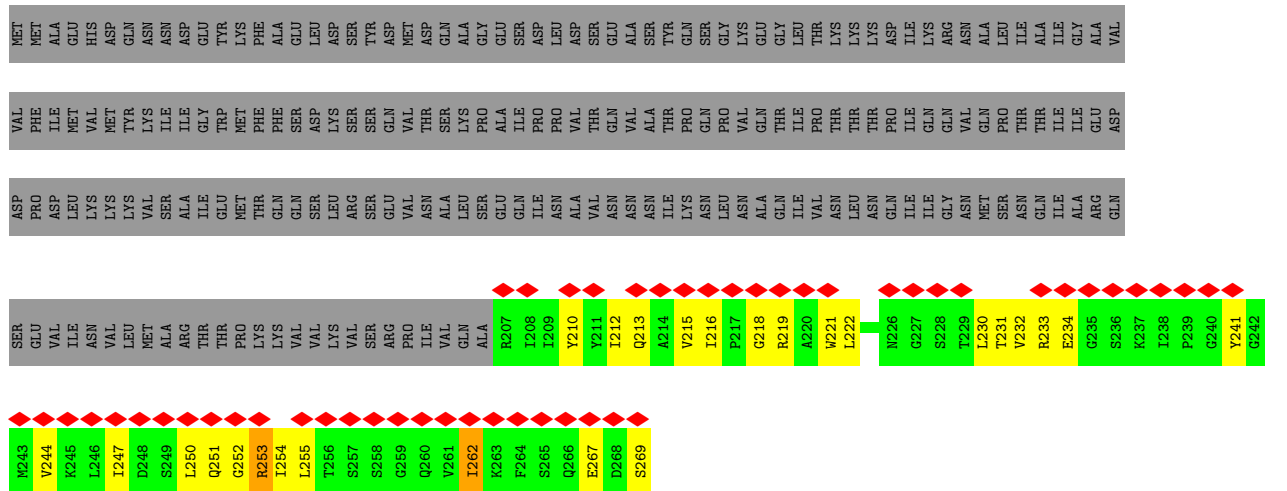




- Molecule 5: IcmG (DotF)



- Molecule 5: IcmG (DotF)

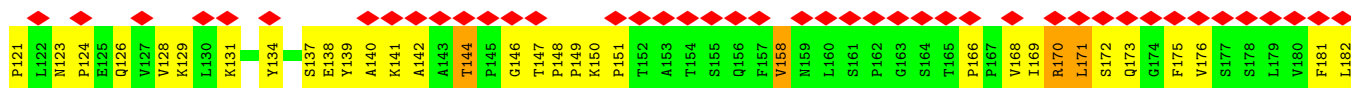


- Molecule 5: IcmG (DotF)

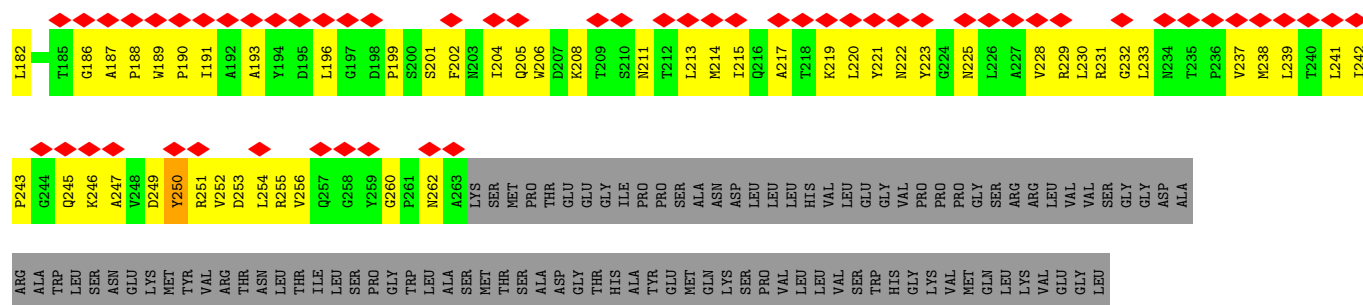


[illegible]

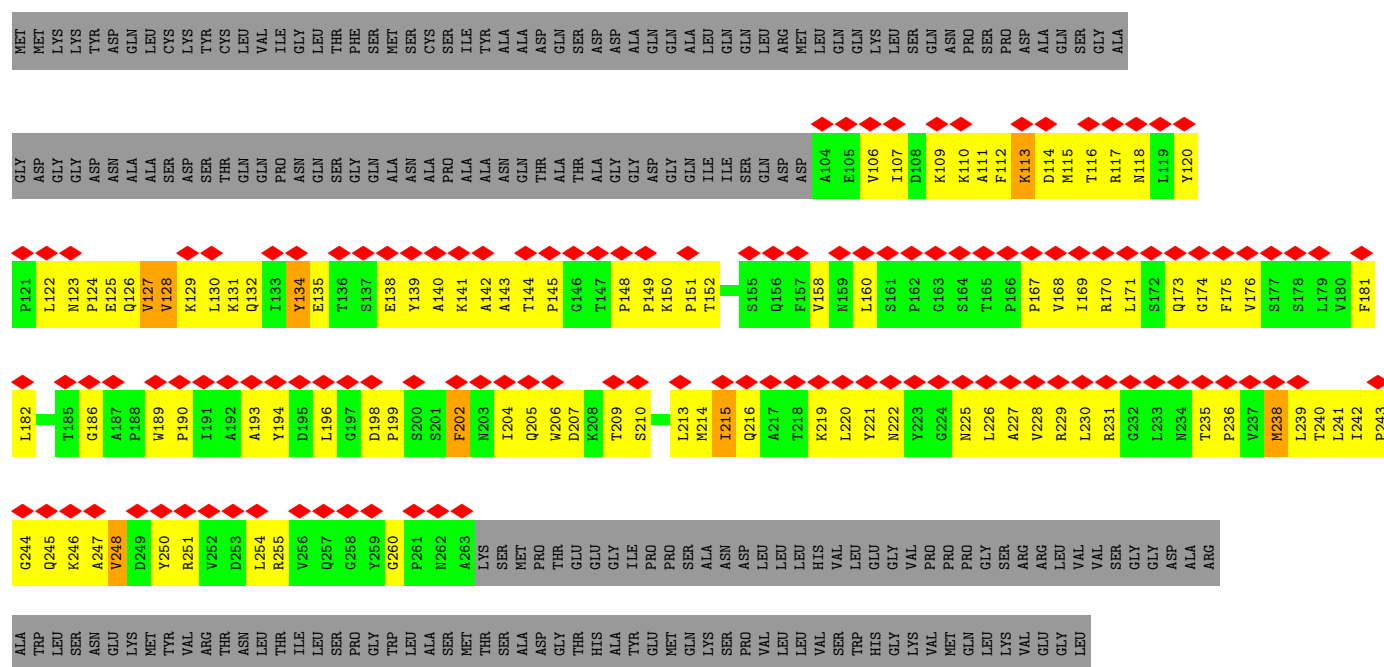
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E104	E105	V106	I107	D108	K109	K110	A111	F112	K113	D114	M115	T116	R117	N118	L119	Y120																																			



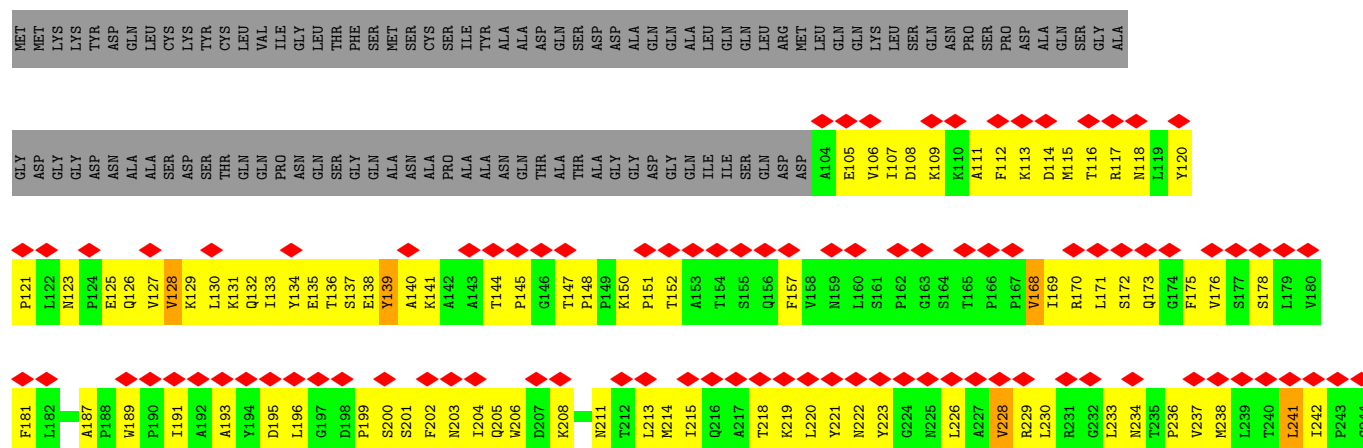




• Molecule 6: IcmK (DotH)

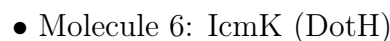
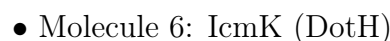


• Molecule 6: IcmK (DotH)

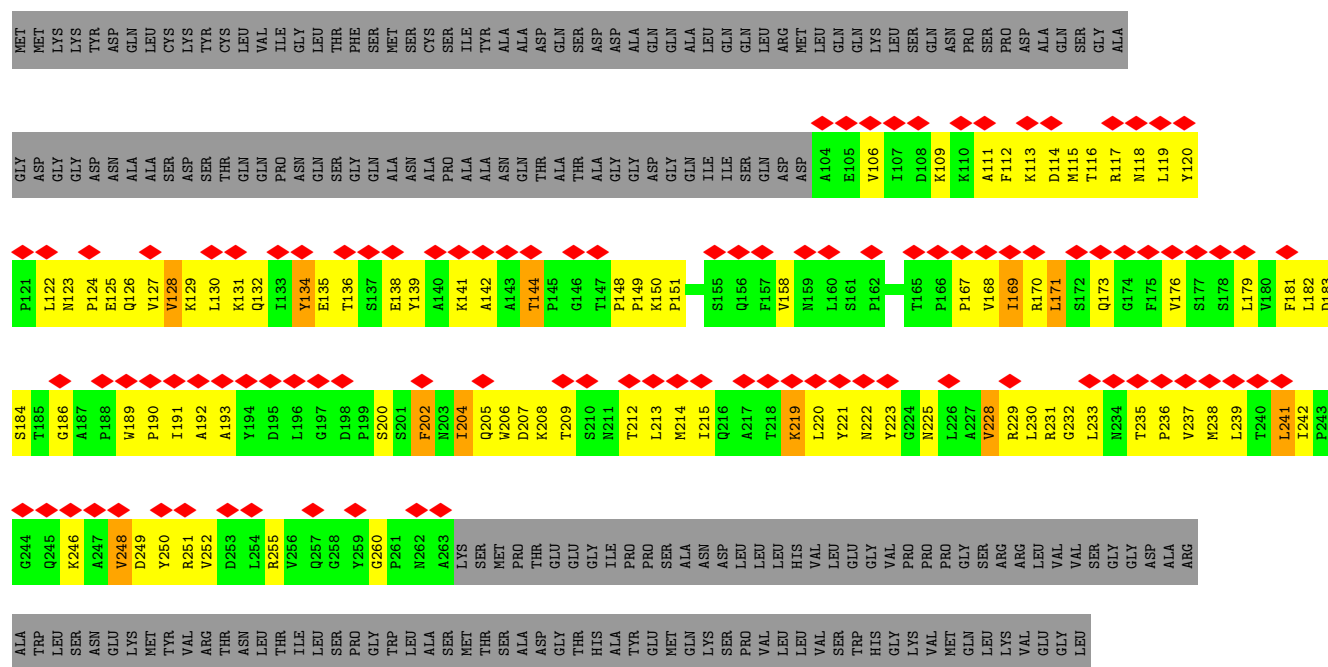
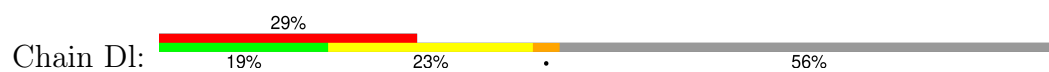




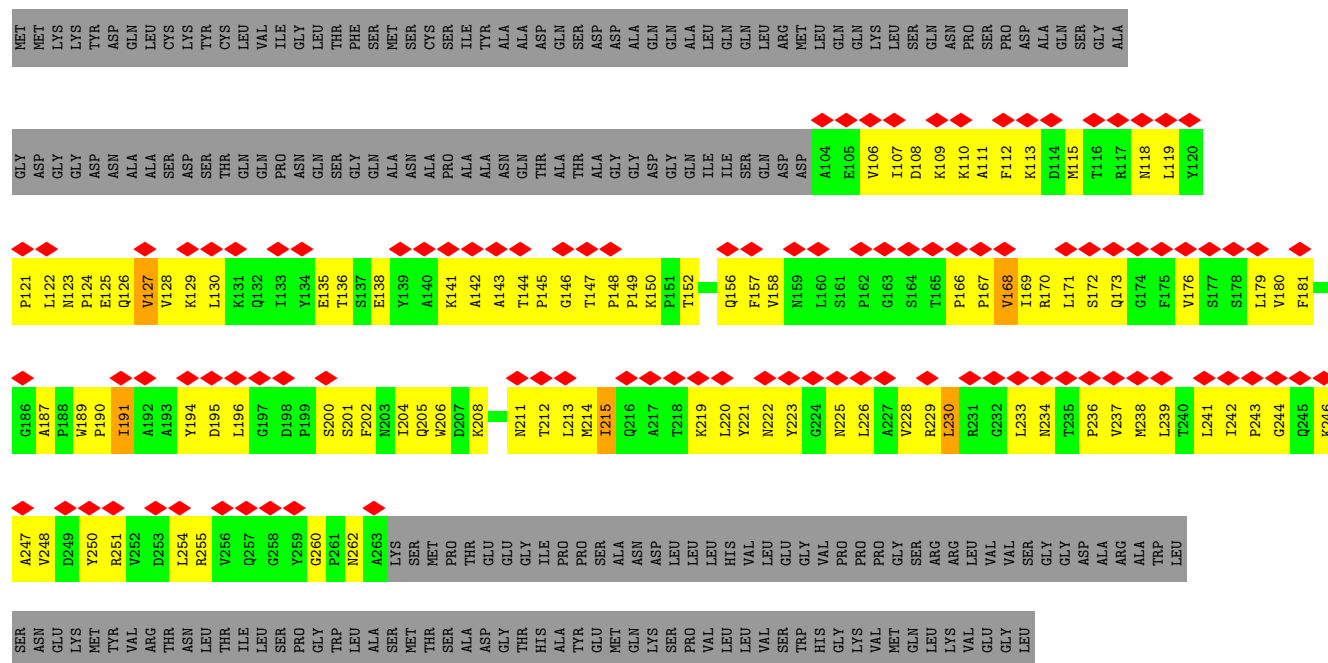






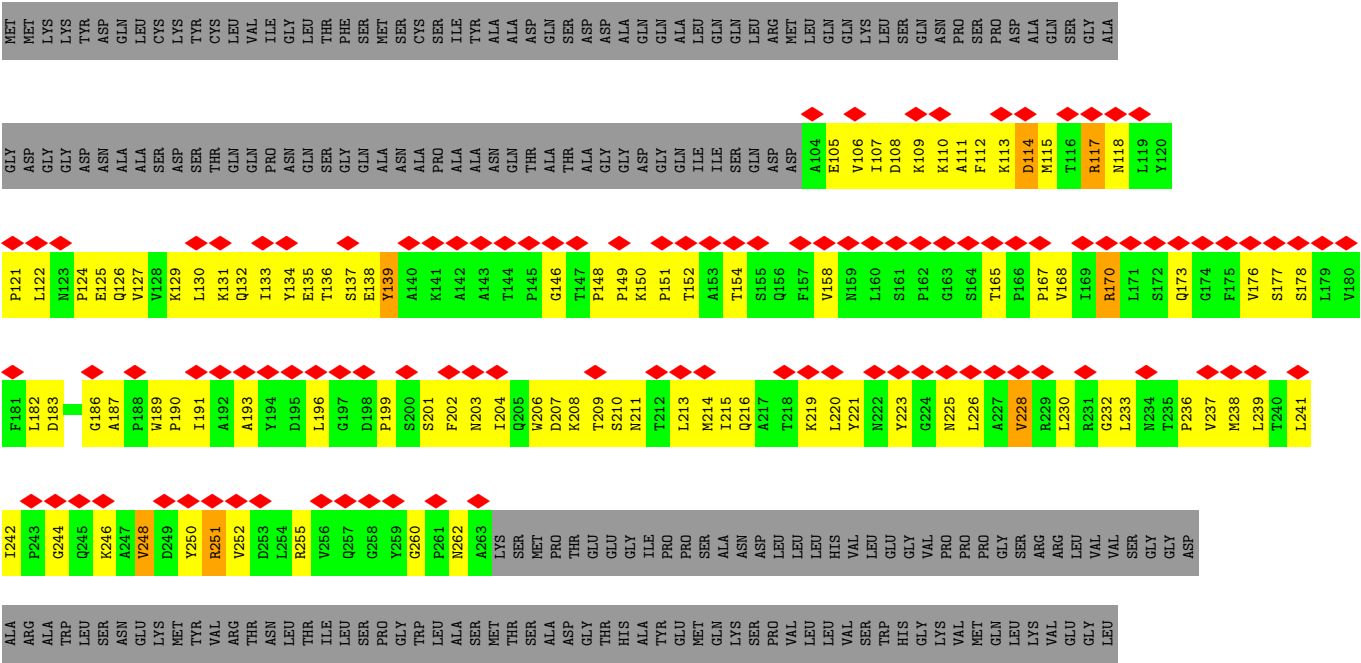


• Molecule 6: IcmK (DotH)

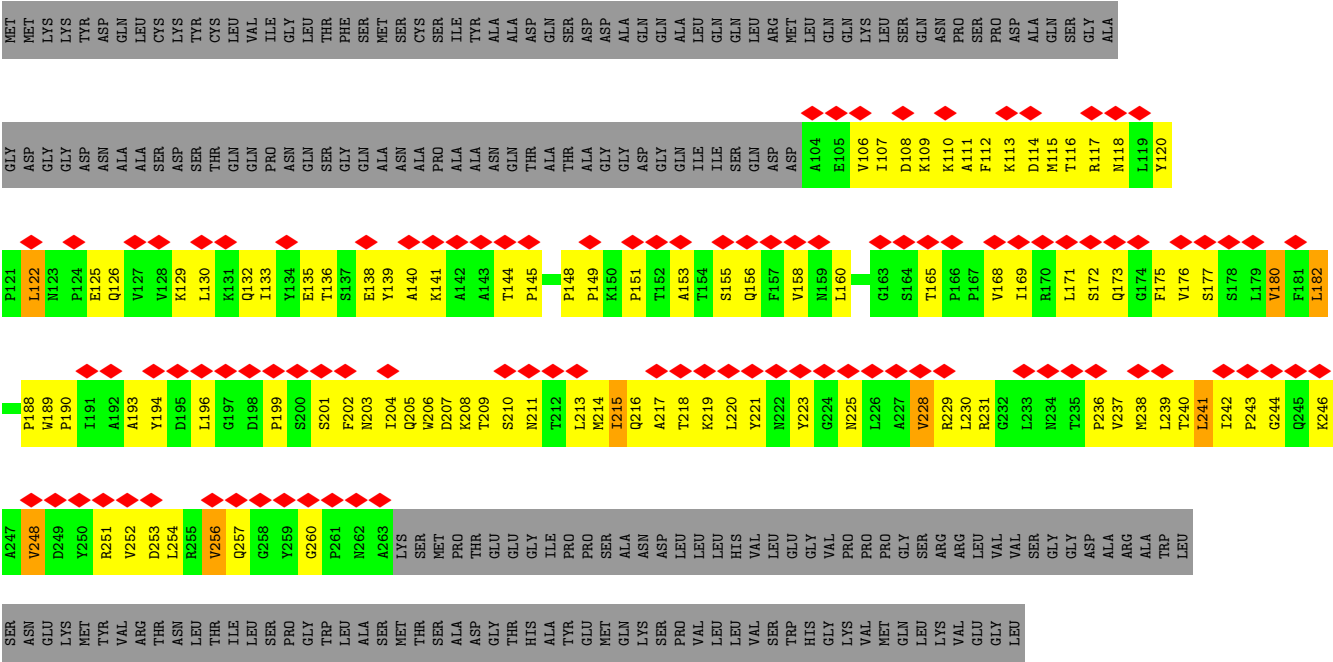


• Molecule 6: IcmK (DotH)

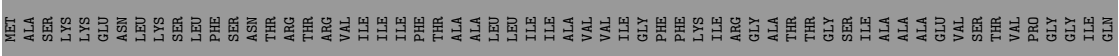




• Molecule 6: IcmK (DotH)



• Molecule 7: IcmE (DotG)



- Molecule 7: IcmE (DotG)

[illegible]

- Molecule 7: IcmE (DotG)



MET	ALA	SER	LYS	GLU	ASN	LEU	SER	PHE	THR	ARG	THR	ARG	VAL	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ALA	VAL	VAL	ILE	ILE	GLY	PHE	PHE	LYS	ILE	ILE	ARG	GLY	GLY	ALA	THR	THR	GLY	SER	SER	ILE	ALA	ALA	ALA	GLU	VAL	VAL	THR	PRO	GLY	GLY	ILE
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- Molecule 7: IcmE (DotG)

Chain Ei:  95%

[illegible]

- Molecule 7: IcmE (DotG)

Chain Ej:  94%

MET	ALA	SER	LYS	GLU	ASN	LEU	LYS	SER	PHE	SER	THR	THR	ARG	ARG	VAL	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ALA	VAL	VAL	ILE	ILE	GLY	PHE	PHE	LYS	ILE	ILE	ARG	GLY	ARG	ALA	ALA	THR	THR	GLY	SER	SER	ILE	ALA	ALA	GLU	GLU	VAL	VAL	THR	THR	VAL	PRO	GLY	GLY	ILE	ILE	GLN
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- Molecule 7: IcmE (DotG)

[illegible]





- Molecule 7: IcmE (DotG)



MET	ALA	SER	LYS	GLU	ASN	LYS	SER	LEU	PHE	SER	THR	ARG	THR	ARG	VAL	ILE	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ILE	ALA	VAL	VAL	VAL	ILE	ILE	GLY	PHE	PHE	LYS	LYS	ILE	ARG	GLY	ALA	THR	THR	SER	ILE	ALA	ALA	ALA	GLU	VAL	SER	THR	VAL	PRO	GLY	GLY	ILE
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- Molecule 7: IcmE (DotG)



MET	ALA	SER	LYS	GLU	ASN	LEU	LYS	SER	PHE	SER	THR	ARG	THR	ARG	VAL	ILE	ILE	PHE	THR	ALA	ALA	VAL	VAL	ILE	ILE	PHE	THR	ALA	LEU	LEU	ILE	ILE	ILE	ALA	VAL	VAL	ILE	ILE	GLY	GLY	ALA	THR	THR	GLY	SER	SER	ILE	ILE	ALA	ALA	GLU	GLU	VAL	VAL	SER	THR	THR	VAL	PRO	PRO	GLY	GLY	ILE	ILE	TYP
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- Molecule 7: IcmE (DotG)



MET	ALA	SER	LYS	GLU	ASN	LEU	PHE	SER	THR	ARG	THR	ARG	VAL	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ILE	ILE	GLY	PHE	PHE	LYS	ILE	ILE	ARG	GLY	ALA	THR	THR	GLY	SER	ILE	ALA	ALA	ALA	GLU	VAL	SER	THR	VAL	PRO	GLY	GLY	ILE	TRP
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- Molecule 7: IcmE (DotG)

Chain Es:  95%

[illegible]



MET	ALA	SER	LYS	GLU	ASN	LYS	SER	LEU	PHE	SER	THR	ARG	ARG	VAL	ILE	ILE	PHE	THR	ALA	ALA	LEU	LEU	ILE	ILE	ALA	VAL	VAL	VAL	GLY	PHE	PHE	LYS	ILE	ILE	ARG	GLY	ALA	THR	THR	GLY	SER	SER	ILE	ILE	ALA	ALA	GLU	GLU	VAL	VAL	SER	THR	THR	VAL	PRO	PRO	GLY	GLY	ILE	ILE	TYP
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- Molecule 7: IcmE (DotG)



M1	A2	S3	K4	K5	E6	N7	L8	K9	S10	L11	F12	S13	N14	T15	R16	T17	R18	V19	I20	I21	I22	F23	T24	A25	A26	L27	L28	I29	I30	A31	V32	V33	I34	G35	F36	F37	K38	I39	R40	G41	A42	T43	THR	GLY	GLY	SER	ILE	ALA	ALA	ALA	ALA	GLU	VAL	SER	THR	VAL	PRO	GLY	GLY	ILE	ILE
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- Molecule 7: IcmE (DotG)

Chain Fh:  96%



- Molecule 7: IcmE (DotG)

Chain Fi:  96%





- Molecule 7: IcmE (DotG)

Chain Fk:  96%

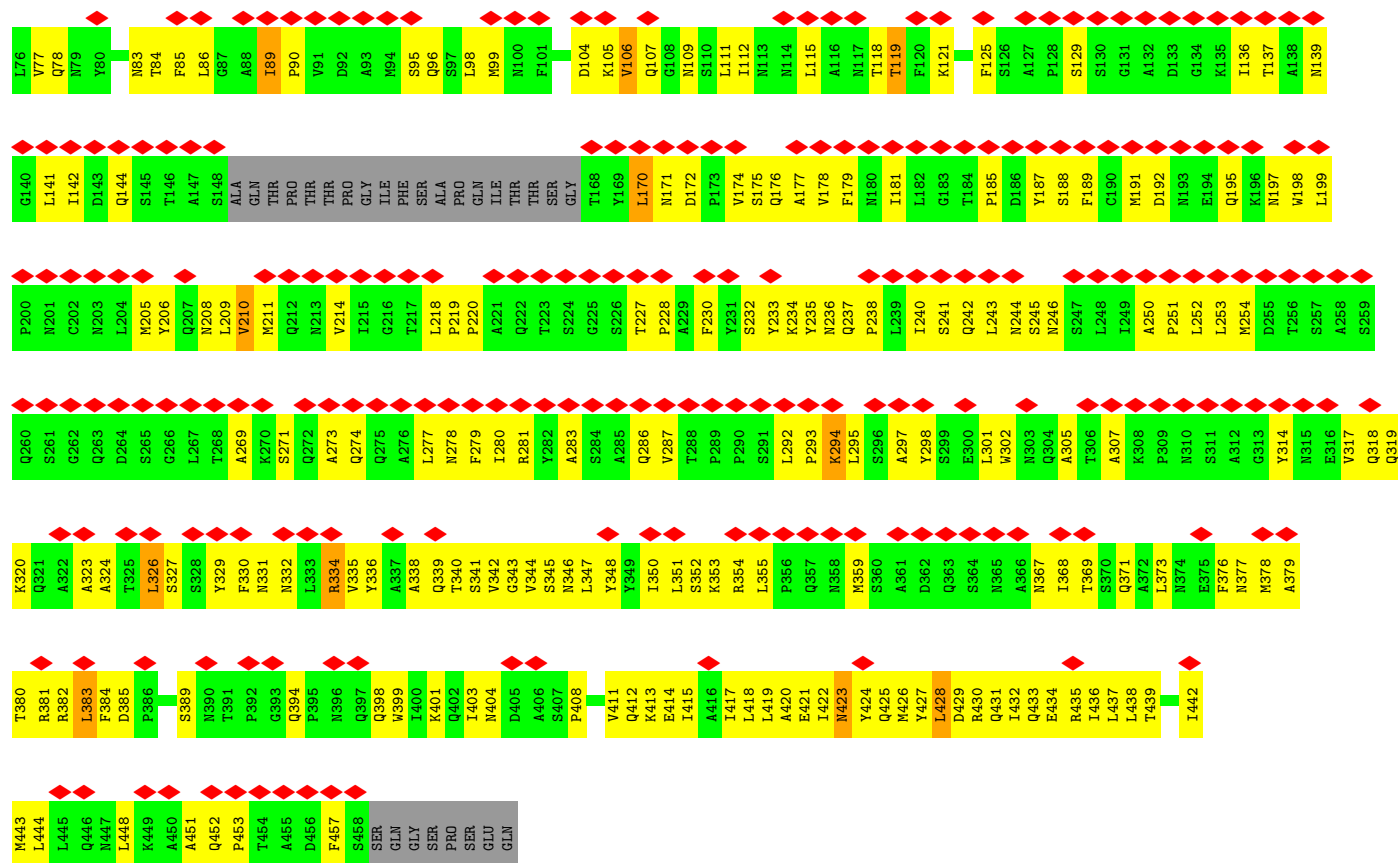




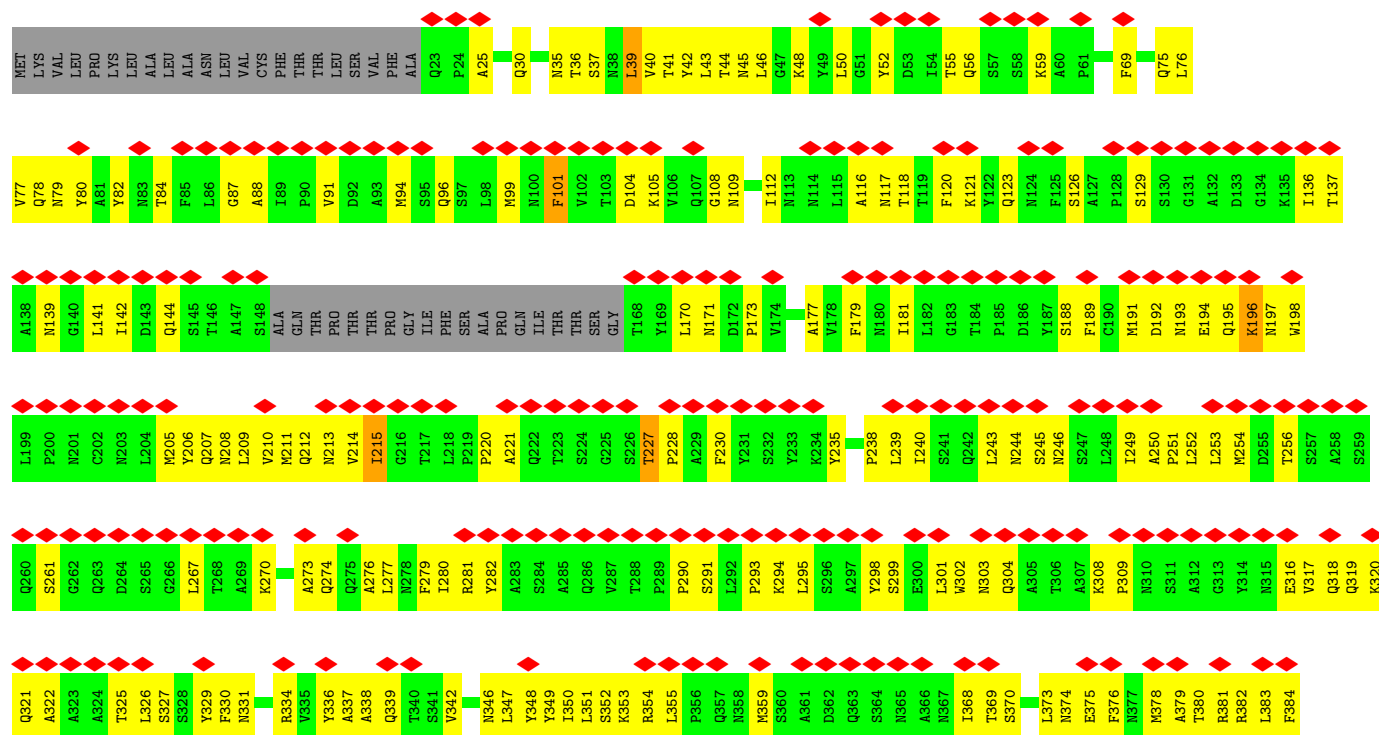
- Molecule 8: IcmX (IcmY)

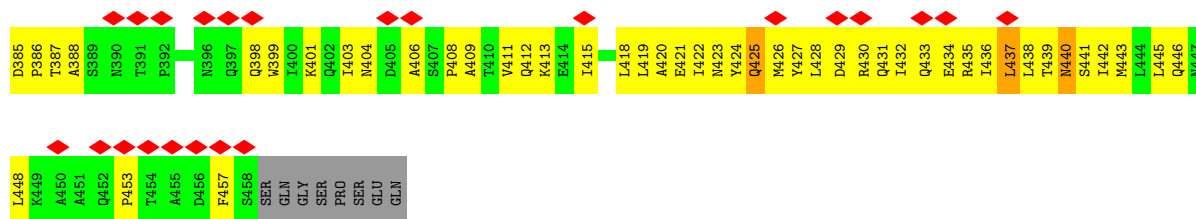
Response	Percentage
Very bad	52%
Bad	43%
Not bad	44%
Very good	11%



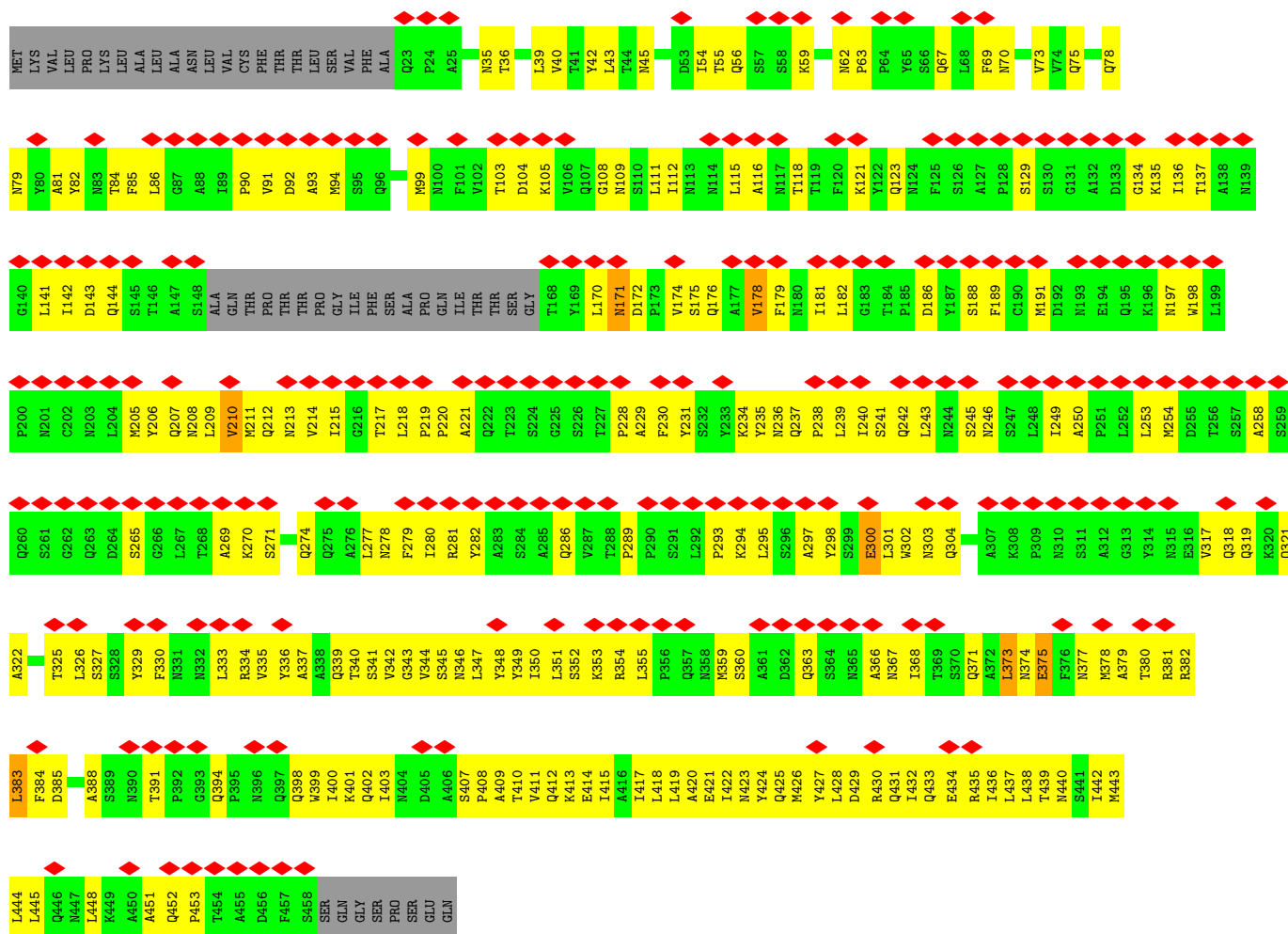
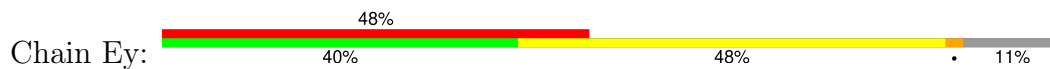


### • Molecule 8: IcmX (IcmY)

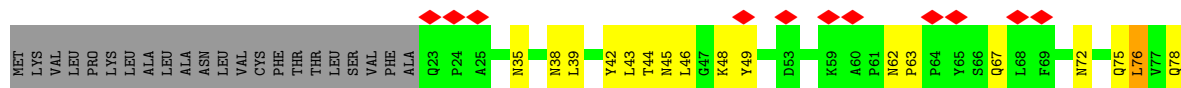
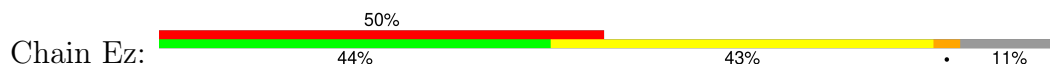


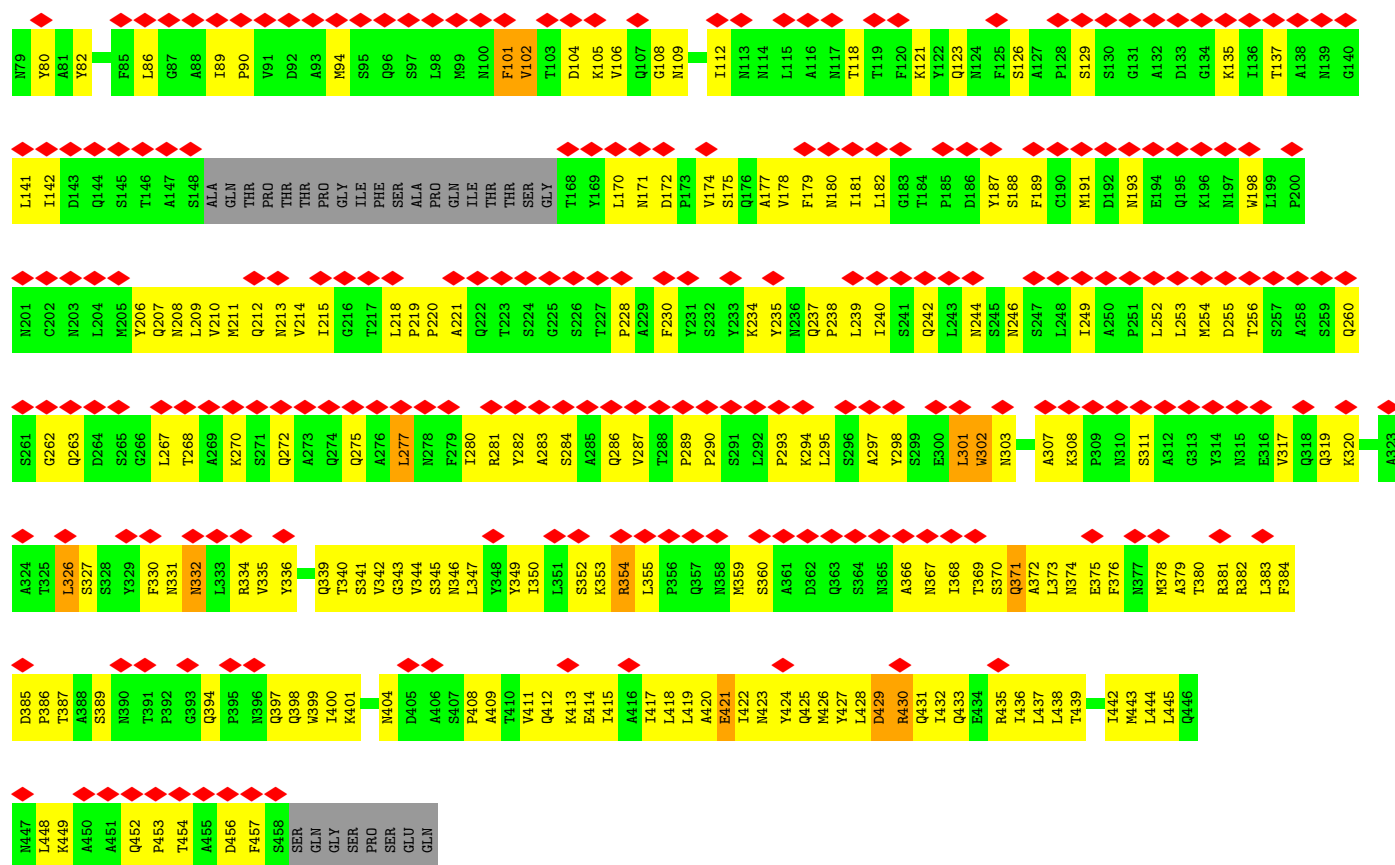


• Molecule 8: IcmX (IcmY)

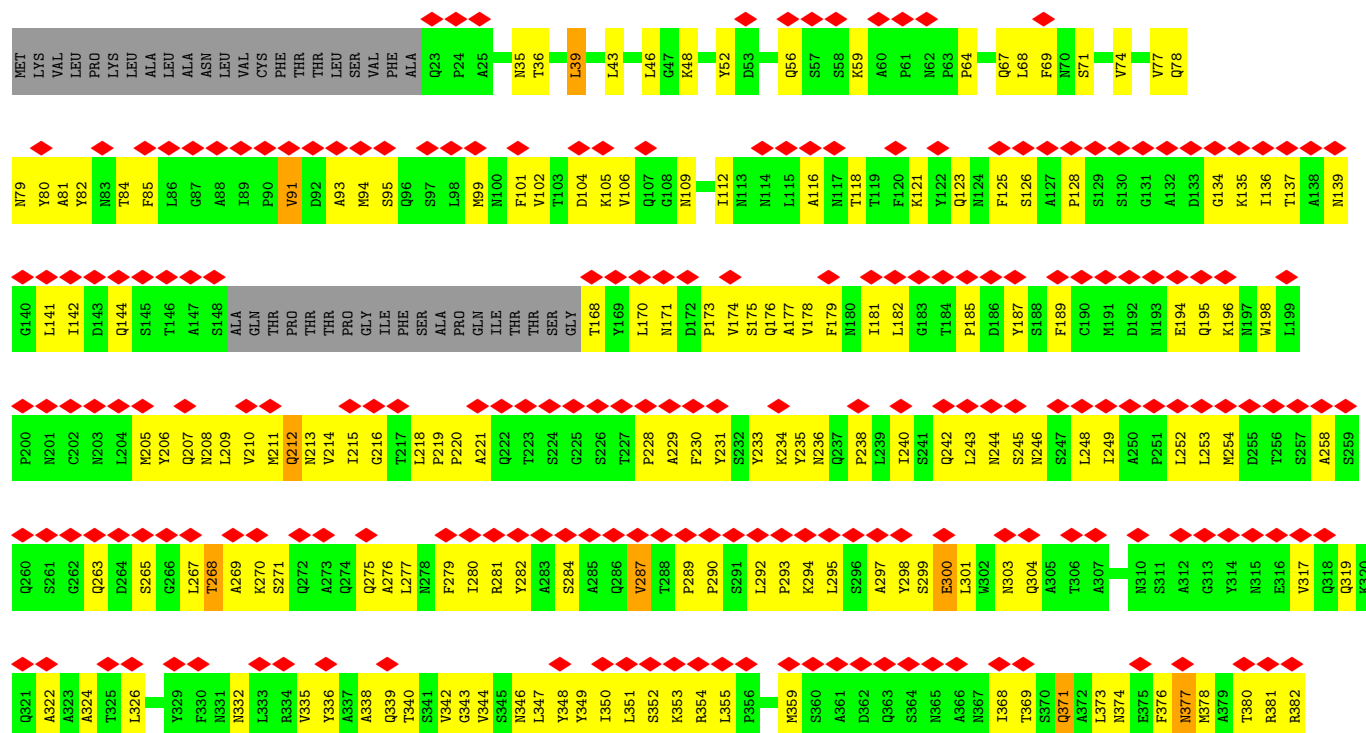


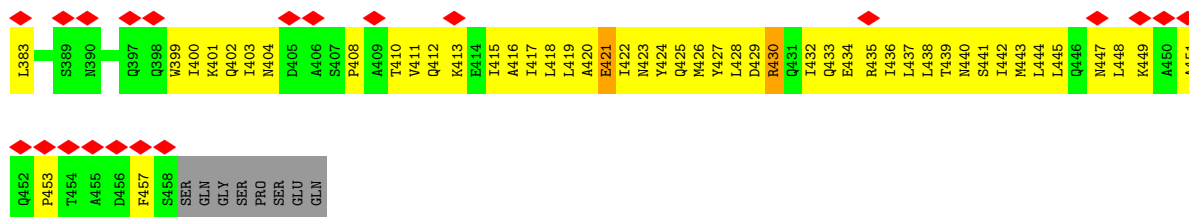
• Molecule 8: IcmX (IcmY)



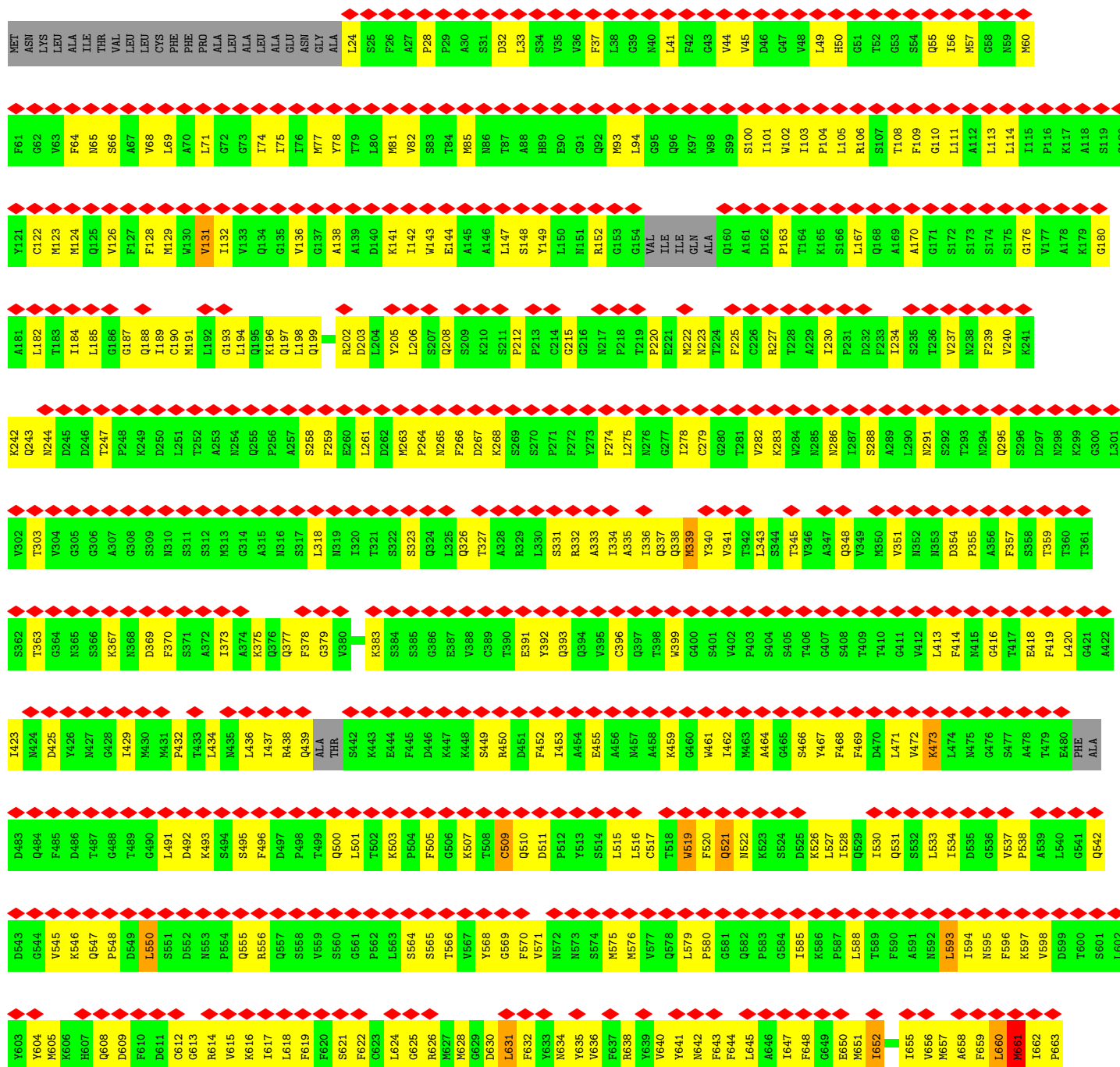
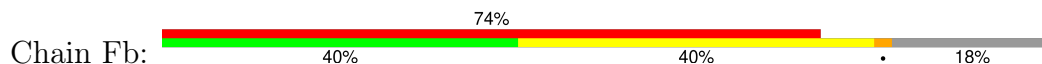


• Molecule 8: IcmX (IcmY)





## • Molecule 9: DotA



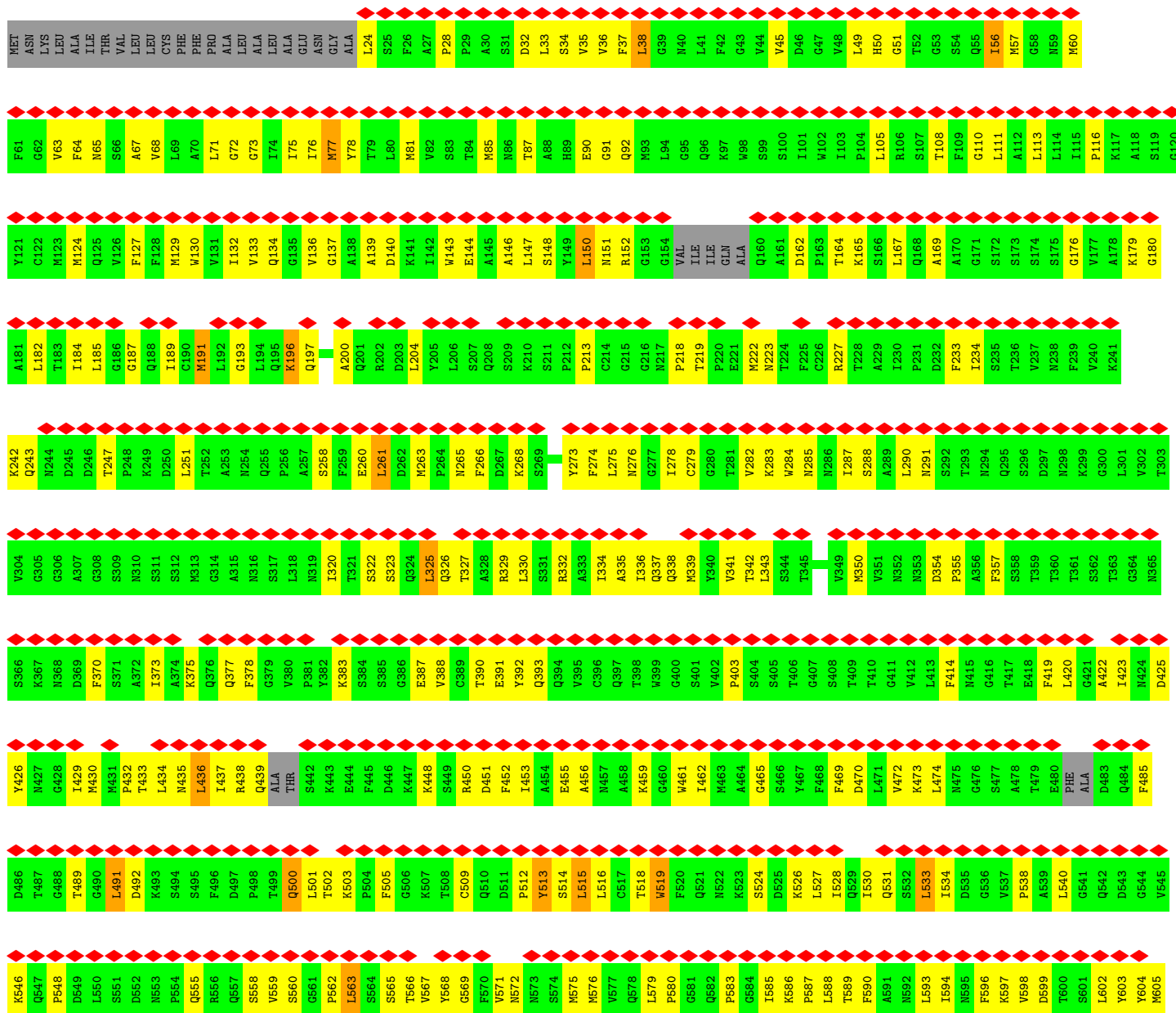
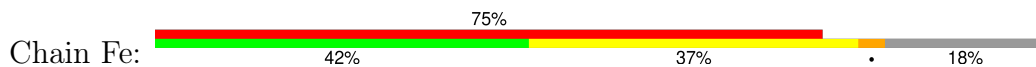




ASP	GLN	GLY	ILE	GLU	THR	TRP	GLU	LYS	GLY	THR	SER	SER	ASN	ASP	ALA	LYS	ARG	PHE	PHE	GLN	SER	ALA	GLY	GLY	ASN	TRP	THR	THR	GLY	ALA	LYS	MET	ASP	THR	SER	GLN	TRP	ASP	ASN	ASN	PHE	LYS	GLN	ASP	LYS	LEU	THR	GLY	ASP	TYR	GLN	SER	THR	ALA	LEU	GLU	GLY	G901	G902	G903	G904	W905	A906
T787	H788	P789	E790	G791	N792	E793	A794	F795	G796	K797	G798	E799	F800	A801	I802	M803	L804	L805	V806	M807	V808	F809	L810	R811	Y812	I813	F814	Y815	L816	I817	G818	Y819	I820	F821	T822	L823	G824	L825	S826	Y827	L828	W829	L830	G831	VAL	G832	W833	G834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L844	G845	SER			
L727	I728	M729	K730	A731	M732	P733	L734	L735	M736	A737	W738	I739	G740	T741	M742	V743	S744	I745	G746	F747	W748	T749	A750	Y751	Y752	I753	F754	Y755	L756	P757	R758	M759	I760	F761	T762	F763	G764	S765	F766	A767	W768	L769	G770	A771	I772	W773	E774	A775	M776	W777	A778	A779	P780	I781	Y782	A783	L784	G785	V786				
H607	Q608	D609	F610	D611	G612	G613	R614	V615	R616	I617	L618	F619	F620	S621	P681	G682	I683	M684	P685	I686	V687	M628	G629	D630	L631	F632	Y633	N634	G635	V636	F637	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	N651	I652	N653	S654	L655	V656	M657	A658	L660	R661	I662	P663	L664	G665	G666				
M667	K668	D669	I670	F671	I672	V673	G674	V675	D676	T677	L678	T679	Q680	P681	G682	I683	M684	P685	I686	V687	A688	L689	N689	Y691	M692	G693	S813	T694	M695	Y696	P697	N698	F699	S700	G701	T702	L703	W704	L705	T706	L707	L708	W709	M710	VAL	W713	S714	S715	L716	I717	F718	L719	F720	G721	I722	F723	I724	F725	A726				
L727	I728	M729	K730	A731	M732	P733	L734	L735	M736	A737	W738	I739	G740	T741	M742	V743	S744	I745	G746	F747	W748	T749	A750	Y751	Y752	I753	F754	Y755	L756	P757	R758	M759	I760	F761	T762	F763	G764	S765	F766	A767	W768	L769	G770	A771	I772	W773	E774	A775	M776	W777	A778	A779	P780	I781	Y782	A783	L784	G785	V786				
T787	H788	P789	E790	G791	N792	E793	A794	F795	G796	K797	G798	E799	F800	A801	I802	M803	L804	L805	V806	M807	V808	F809	L810	R811	Y812	I813	F814	Y815	L816	I817	G818	Y819	I820	F821	T822	L823	G824	L825	S826	Y827	L828	W829	L830	G831	VAL	G832	W833	G834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L844	G845	SER			
Y121	C122	M123	M124	Q125	V126	F127	I128	M129	M130	V131	I132	V133	Q134	G135	V136	G137	A138	A139	D140	K141	I142	W143	E144	A145	A146	L147	S148	Y149	L150	N151	R152	G153	G154	VAL	ILE	ILE	GLN	Q160	A161	D162	P163	T164	K165	S166	L167	Q168	A169	A170	G171	S172	S173	S174	S175	G176	V177	A178	K179	G180					
A181	L182	T183	I184	L185	G186	G187	Q188	I189	C190	M191	L192	G193	L194	Q195	K196	Q199	R202	D203	L204	Y205	L206	D267	K268	S269	S270	P271	L147	F272	Y273	G215	G216	N217	P218	T219	P220	E221	M222	N223	T224	F225	C226	R227	T228	A229	I230	P231	D232	F233	I234	S235	T236	V237	N238	F239	V240	K241	G242	Q243	N244				
D245	D246	T247	P248	K249	D250	L251	T252	N254	A253	Q255	P256	A257	S258	F259	E260	L261	D262	M263	P264	N265	F266	D267	K268	S269	S270	P271	F272	Y273	F274	L275	N276	G277	I278	C279	G280	T281	N282	K283	W284	N285	N286	I287	S288	A289	L290	N291	S292	T293	N294	Q295	S296	D297	N298	G300	L301	V302	T303	V304					
G305	G306	A307	G308	S309	N310	S311	S312	M313	G314	A315	N316	S317	L318	N319	I320	T321	S322	S323	Q324	L325	Q326	T327	A328	R329	L330	S331	R332	A333	I334	A335	I336	Q337	Q338	M339	Y340	P341	T342	L343	S344	A347	M350	V351	N352	N353	D354	P355	A356	F357	S358	T359	T360	T361	S362	T363	G364	N365	S366						
K367	N368	D369	F370	S371	A372	I373	A374	K375	Q376	Q377	F378	G379	V380	P381	Y382	K383	S384	S385	G386	E387	V388	C389	T390	E391	Y392	Q393	Q394	V395	C396	Q397	T398	W399	G400	S401	V402	P403	S404	S405	T406	G407	S408	T409	F410	G411	V412	L413	F414	N415	G416	T417	E418	F419	L420	G421	A422	L423	N424	D425	Y426				
N427	G428	I429	M430	M431	D432	T433	L434	N435	A436	I437	R438	Q439	ALA	THR	S442	K443	E444	F445	D446	K447	K448	S449	R450	D451	F452	I453	A454	E455	A456	C457	A458	K459	G460	V461	I462	M463	A464	G465	S466	Y467	F468	F469	D470	L471	Y472	K473	N474	N475	G476	S477	A478	T479	PHE	ALA	D483	Q484	F485	D486					
T487	G488	T489	G490	L491	D492	K493	S494	S495	F496	D497	P498	T499	S500	L501	T502	K503	P504	F505	S506	K507	T508	C509	S510	D511	P512	Y513	S514	L515	L516	C517	T518	W519	F520	Q521	N522	K523	S524	D525	K526	L527	T528	Q529	T530	Q531	S532	L533	T534	D535	G536	V537	P538	A539	L540	G541	Q542	D543	G544	V545	K546				
Q547	P548	D549	L550	S551	D552	N553	P554	Q555	R556	Q557	S558	V559	S560	G561	P562	L563	S564	S565	T566	V567	Y568	G569	F570	V571	N572	N573	S574	M575	M576	V577	Q578	L579	Y641	G581	Q582	P583	G584	I585	S586	F587	L588	T589	F590	A591	N592	L593	T594	N595	F596	K597	V598	D599	T600	S601	L602	V603	V604	N605	V606				
H607	Q608	D609	F610	D611	G612	G613	R614	V615	R616	I617	L618	F619	F620	S621	P681	G682	I683	M684	P685	I686	V687	M628	G629	D630	L631	F632	Y633	N634	G635	V636	F637	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	N651	I652	N653	S654	L655	V656	M657	A658	L660	R661	I662	P663	L664	G665	G666				
M667	K668	D669	I670	F671	I672	V673	G674	V675	D676	T677	L678	T679	Q680	P681	G682	I683	M684	P685	I686	V687	A688	L689	N689	Y691	M692	G693	S813	T694	M695	Y696	P697	N698	F699	S700	G701	T702	L703	W704	L705	T706	L707	L708	W709	M710	VAL	W713	S714	S715	L716	I717	F718	L719	F720	G721	I722	F723	I724	F725	A726				
L727	I728	M729	K730	A731	M732	P733	L734	L735	M736	A737	W738	I739	G740	T741	M742	V743	S744	I745	G746	F747	W748	T749	A750	Y751	Y752	I753	F754	Y755	L756	P757	R758	M759	I760	F761	T762	F763	G764	S765	F766	A767	W768	L769	G770	A771	I772	W773	E774	A775	M776	W777	A778	A779	P780	I781	Y782	A783	L784	G785	V786				
T787	H788	P789	E790	G791	N792	E793	A794	F795	G796	K797	G798	E799	F800	A801	I802	M803	L804	L805	V806	M807	V808	F809	L810	R811	Y812	I813	F814	Y815	L816	I817	G818	Y819	I820	F821	T822	L823	G824	L825	S826	Y827	L828	W829	L830	G831	VAL	G832	W833	G834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L844	G845	SER			



- Molecule 9: DotA





SER	GLY	G904	L784	I724	L664	L602	Q542	ALA	A422	T361	L301
SER	ARG	W905	G785	F725	Q665	Y603	D543	D483	I423	S362	V302
PRO	VAL	A906	V786	A726	G666	Y604	G544	Q484	N424	T363	T303
THR	LYS	G907	T787	L727	M667	M605	V545	F485	Y426	G364	V304
GLY	ALA	W908	H788	I728	M668	K606	Q547	D486	G428	N365	G305
GLY	GLY	Y909	P789	W729	D669	H607	Q548	G488	T427	S366	G306
ALA	ALA	A910	E790	M730	I670	Q608	P548	T489	G428	A307	A307
THR	THR	F911	G791	A731	F671	D609	D549	T489	I429	N368	G308
GLY	GLY	F912	W792	M732	I672	F610	L550	G490	M430	D369	S309
GLY	LYS	F913	W793	P733	G674	D611	S551	L491	M431	F370	N310
ALA	LYS	E793	G675	L734	G674	C612	D552	D492	P432	S371	S311
GLY	THR	A794	V675	L735	V675	G613	N553	K493	T433	S312	S312
SER	SER	F795	Q676	W736	Q676	R614	P554	S494	L434	M313	M313
GLY	ASN	G796	T677	A737	T677	V615	Q555	S495	N435	G314	G314
GLY	ASP	K797	L678	W738	L678	K616	R556	F496	L436	A315	A315
THR	ALA	G798	T679	I739	T679	I617	Q557	D497	I437	N316	N316
SER	LYS	E799	Q680	G740	Q680	L618	S558	P498	R439	S317	S317
LEU	ARG	F800	P681	T741	P681	F619	V559	T499	Q439	G379	L318
GLY	PHE	M921	G682	W742	G682	W620	S560	Q500	ALA	V380	N319
ALA	PHE	I802	I683	H743	I683	S821	G561	L501	THR	P381	N319
LYS	GLN	M803	N684	S744	N684	F622	P562	T502	S442	I320	I320
GLN	ALA	I804	P685	L745	P685	C623	L563	K503	K443	T321	T321
GLY	ASN	L805	I686	I745	I686	L624	S564	K503	E444	S322	S322
LEU	TRP	W806	G687	G746	G687	G625	T566	P504	F445	S323	S323
GLY	TRP	N807	V687	F747	V687	R626	S565	F505	D446	Q324	Q324
LYS	THR	K928	A688	W748	A688	M627	T567	G506	K447	L325	L325
ALA	ALA	F809	I689	T749	I689	M628	Y568	K507	K448	Q326	Q326
PRO	MET	L810	A690	A750	A690	L631	G569	T508	V388	T327	T327
ALA	ASP	R811	N691	Y751	N691	F632	F570	C509	S449	A328	A328
GLN	THR	P812	G693	Y752	G693	Y633	N571	Q510	R450	R329	R329
LYS	GLN	S813	T694	L753	T694	M634	N572	D511	D451	L330	L330
ILE	TRP	L814	G695	P754	G695	Y635	N573	P512	F452	S331	S331
SER	ASP	M815	Y696	V755	Y696	Y636	N574	Y513	A454	R332	R332
ASN	ASN	I816	I697	V756	I697	F637	S574	S514	E455	A333	A333
ALA	PHE	T817	N698	L756	N698	R638	M575	L515	A456	I334	I334
LYS	LYS	G818	G699	P757	G699	Y639	M576	L516	C396	A335	A335
ASP	ASP	C819	F699	W758	F699	V640	V577	C517	N457	I336	I336
VAL	LEU	Y819	S700	M759	S700	Y641	Q578	T518	A458	Q337	Q337
SER	THR	I820	G701	L760	G701	F642	L579	W519	K459	Q338	Q338
GLY	GLY	A821	T702	F761	T702	N642	P580	F520	G460	M339	M339
ASP	ASP	E822	L703	T762	L703	F643	Q581	Q521	W461	Y340	Y340
TYR	TYR	I823	W704	F763	W704	F644	Q582	N522	I462	V341	V341
ASN	GLN	A824	T705	G764	T705	L645	P583	K523	M463	T342	T342
SER	SER	E825	T706	S765	T706	A646	G584	S524	A464	L343	L343
THR	THR	S826	L707	F766	L707	I647	I585	D525	G465	S344	S344
ALA	ALA	W827	L708	A767	L708	F648	K586	K526	S405	T345	T345
LEU	LEU	Y827	N709	W768	N709	M651	K586	L527	T406	V346	V346
GLY	GLY	W828	W710	L769	W710	I652	P587	L528	G407	A347	A347
THR	THR	C829	A711	I770	A711	S653	L588	Q529	S408	Q348	Q348
GLY	GLY	Y830	V713	A771	V713	G654	T589	I530	T409	V349	V349
GLY	GLY	W831	W714	W772	W714	I655	F590	Q531	T410	M350	M350
THR	THR	I832	S715	I773	S715	V656	A591	L471	G411	V351	V351
GLN	GLN	L833	L716	E774	L716	A658	N592	V472	V412	N352	N352
TRP	TRP	N834	I717	A775	I717	F659	L593	K473	L413	N353	N353
GLY	GLY	A835	P718	W776	P718	M660	I594	L474	F414	D354	D354
GLY	GLY	G836	L719	V777	L719	L660	N595	N475	M415	P355	P355
GLU	GLU	F837	L720	V777	L720	M661	F596	G476	G416	A356	A356
ALA	ALA	D838	F720	A778	F720	I662	K597	S477	T417	F357	F357
LYS	LYS	H839	G721	W779	G721	P663	V598	P538	E418	S358	S358
			I722		I722		D599	A539	T419	T359	T359
			F723		F723		T600	L540	E480	T360	T360
							S601	G541	PHE		

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37503	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	0.434	Depositor
Minimum map value	-0.283	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.16	Depositor
Map size ( $\text{\AA}$ )	640.8192, 640.8192, 640.8192	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2516, 1.2516, 1.2516	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	0.11	0/118	0.44	0/158
1	Ag	0.18	0/118	0.64	0/158
1	Am	0.14	0/118	0.40	0/158
1	As	0.15	0/118	0.38	0/158
1	Ay	0.12	0/118	0.44	0/158
1	Be	0.14	0/118	0.43	0/158
1	Bk	0.13	0/118	0.52	0/158
1	Bq	0.11	0/118	0.42	0/158
1	Bw	0.16	0/118	0.45	0/158
1	Cc	0.13	0/118	0.40	0/158
1	Ci	0.13	0/118	0.47	0/158
1	Co	0.16	0/118	0.69	0/158
1	Cu	0.09	0/118	0.37	0/158
1	Da	0.16	0/118	0.63	0/158
1	Dg	0.16	0/118	0.68	0/158
1	Dm	0.13	0/118	0.49	0/158
1	Ds	0.13	0/118	0.50	0/158
1	Dy	0.13	0/118	0.50	0/158
2	Ab	0.34	0/60	0.53	0/76
2	Ah	0.27	0/60	0.60	0/76
2	An	0.59	0/60	1.04	0/76
2	At	0.20	0/60	0.56	0/76
2	Az	0.23	0/60	0.56	0/76
2	Bf	0.21	0/60	0.44	0/76
2	Bl	0.31	0/60	0.81	0/76
2	Br	0.40	0/60	0.89	0/76
2	Bx	0.21	0/60	0.71	0/76
2	Cd	0.28	0/60	0.61	0/76
2	Cj	0.28	0/60	0.62	0/76
2	Cp	0.24	0/60	0.45	0/76
2	Cv	0.19	0/60	0.43	0/76
2	Db	0.24	0/60	0.63	0/76
2	Dh	0.45	0/60	0.69	0/76
2	Dn	0.30	0/60	0.61	0/76

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Dt	0.28	0/60	0.67	0/76
2	Dz	0.21	0/60	0.40	0/76
3	Ac	0.10	0/126	0.29	0/167
3	Ai	0.17	0/126	0.44	0/167
3	Ao	0.18	0/126	0.43	0/167
3	Au	0.13	0/126	0.36	0/167
3	Ba	0.13	0/126	0.37	0/167
3	Bg	0.13	0/126	0.33	0/167
3	Bm	0.17	0/126	0.49	0/167
3	Bs	0.15	0/126	0.34	0/167
3	By	0.12	0/126	0.36	0/167
3	Ce	0.13	0/126	0.39	0/167
3	Ck	0.13	0/126	0.38	0/167
3	Cq	0.15	0/126	0.47	0/167
3	Cw	0.13	0/126	0.39	0/167
3	Dc	0.13	0/126	0.40	0/167
3	Di	0.14	0/126	0.48	0/167
3	Do	0.12	0/126	0.33	0/167
3	Du	0.17	0/126	0.52	0/167
3	Ea	0.11	0/126	0.50	0/167
4	Ad	0.12	0/37	0.22	0/47
4	Aj	0.11	0/37	0.26	0/47
4	Ap	0.14	0/37	0.34	0/47
4	Av	0.09	0/37	0.19	0/47
4	Bb	0.20	0/37	0.39	0/47
4	Bh	0.11	0/37	0.23	0/47
4	Bn	0.11	0/37	0.25	0/47
4	Bt	0.12	0/37	0.31	0/47
4	Bz	0.14	0/37	0.27	0/47
4	Cf	0.17	0/37	0.40	0/47
4	Cl	0.09	0/37	0.20	0/47
4	Cr	0.08	0/37	0.18	0/47
4	Cx	0.12	0/37	0.22	0/47
4	Dd	0.20	0/37	0.45	0/47
4	Dj	0.09	0/37	0.22	0/47
4	Dp	0.08	0/37	0.23	0/47
4	Dv	0.12	0/37	0.18	0/47
4	Eb	0.13	0/37	0.30	0/47
5	Ae	0.20	0/491	0.58	0/660
5	Ak	0.21	0/491	0.59	0/660
5	Aq	0.17	0/491	0.46	0/660
5	Aw	0.20	0/491	0.54	0/660
5	Bc	0.23	0/491	0.61	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
5	Bi	0.18	0/491	0.57	0/660
5	Bo	0.24	0/491	0.63	0/660
5	Bu	0.18	0/491	0.52	0/660
5	Ca	0.18	0/491	0.53	0/660
5	Cg	0.20	0/491	0.45	0/660
5	Cm	0.23	0/491	0.67	0/660
5	Cs	0.25	0/491	0.68	0/660
5	Cy	0.19	0/491	0.48	0/660
5	De	0.22	0/491	0.62	0/660
5	Dk	0.21	0/491	0.60	0/660
5	Dq	0.19	0/491	0.61	0/660
5	Dw	0.18	0/491	0.47	0/660
5	Ec	0.16	0/491	0.46	0/660
6	Af	0.27	0/1269	0.74	7/1734 (0.4%)
6	Al	0.26	0/1269	0.63	0/1734
6	Ar	0.26	0/1269	0.67	0/1734
6	Ax	0.27	0/1269	0.64	3/1734 (0.2%)
6	Bd	0.23	0/1269	0.59	0/1734
6	Bj	0.24	0/1269	0.65	0/1734
6	Bp	0.27	0/1269	0.76	0/1734
6	Bv	0.28	0/1269	0.68	1/1734 (0.1%)
6	Cb	0.23	0/1269	0.64	1/1734 (0.1%)
6	Ch	0.25	0/1269	0.65	2/1734 (0.1%)
6	Cn	0.28	0/1269	0.71	4/1734 (0.2%)
6	Ct	0.25	0/1269	0.64	2/1734 (0.1%)
6	Cz	0.26	0/1269	0.68	1/1734 (0.1%)
6	Df	0.30	0/1269	0.75	4/1734 (0.2%)
6	Dl	0.27	0/1269	0.69	0/1734
6	Dr	0.30	0/1269	0.80	2/1734 (0.1%)
6	Dx	0.26	0/1269	0.82	6/1734 (0.3%)
6	Ed	0.26	0/1269	0.63	0/1734
7	Ee	0.25	0/278	0.71	0/377
7	Ef	0.25	0/475	0.83	0/642
7	Eg	0.32	0/278	0.98	0/377
7	Eh	0.26	0/400	0.75	0/540
7	Ei	0.29	0/405	0.97	1/547 (0.2%)
7	Ej	0.35	0/467	1.14	4/631 (0.6%)
7	Ek	0.26	0/278	0.75	0/377
7	El	0.28	0/278	0.86	0/377
7	Em	0.35	0/384	0.99	1/518 (0.2%)
7	En	0.29	0/278	0.96	2/377 (0.5%)
7	Eo	0.27	0/278	0.83	1/377 (0.3%)
7	Ep	0.31	0/278	0.79	0/377

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
7	Eq	0.30	0/462	1.04	3/624 (0.5%)
7	Er	0.36	0/278	1.07	3/377 (0.8%)
7	Es	0.28	0/457	0.88	0/617
7	Et	0.26	0/400	0.85	1/540 (0.2%)
7	Eu	0.28	0/475	0.90	2/642 (0.3%)
7	Ev	0.33	0/278	1.07	2/377 (0.5%)
7	Fg	0.25	0/337	0.74	0/451
7	Fh	0.19	0/337	0.72	1/451 (0.2%)
7	Fi	0.20	0/337	0.68	1/451 (0.2%)
7	Fj	0.19	0/337	0.68	0/451
7	Fk	0.17	0/337	0.49	0/451
8	Ew	0.25	0/3277	0.65	1/4473 (0.0%)
8	Ex	0.24	0/3277	0.64	1/4473 (0.0%)
8	Ey	0.26	0/3277	0.64	0/4473
8	Ez	0.25	0/3277	0.66	6/4473 (0.1%)
8	Fa	0.28	0/3277	0.70	3/4473 (0.1%)
9	Fb	0.23	0/6715	0.65	2/9115 (0.0%)
9	Fc	0.23	0/6715	0.61	4/9115 (0.0%)
9	Fd	0.23	0/6715	0.66	3/9115 (0.0%)
9	Fe	0.23	0/6715	0.65	5/9115 (0.1%)
9	Ff	0.23	0/6715	0.63	1/9115 (0.0%)
All	All	0.24	0/95890	0.66	81/130045 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	Al	0	1
6	Ar	0	1
6	Bp	0	1
6	Bv	0	1
6	Ch	0	1
6	Ct	0	1
6	Df	0	1
6	Dl	0	1
6	Dx	0	1
7	Ej	0	1
7	En	0	1
7	Eq	0	1
7	Er	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Fa	0	1
9	Fb	0	1
9	Fe	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 81 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Ej	802	LEU	CA-CB-CG	9.24	148.64	116.30
7	Et	801	MET	CB-CG-SD	8.93	139.50	112.70
6	Af	110	LYS	CA-CB-CG	8.64	131.37	114.10
6	Df	146	GLY	CA-C-N	-8.61	104.57	120.94
6	Df	146	GLY	C-N-CA	-8.61	104.57	120.94

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	Al	219	LYS	Peptide
6	Ar	219	LYS	Peptide
6	Bp	238	MET	Peptide
6	Bv	214	MET	Peptide
6	Ch	219	LYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	117	0	111	7	0
1	Ag	117	0	111	10	0
1	Am	117	0	111	16	0
1	As	117	0	111	6	0
1	Ay	117	0	111	9	0
1	Be	117	0	111	6	0
1	Bk	117	0	111	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Bq	117	0	111	9	0
1	Bw	117	0	111	6	0
1	Cc	117	0	111	10	0
1	Ci	117	0	111	12	0
1	Co	117	0	111	8	0
1	Cu	117	0	111	6	0
1	Da	117	0	111	7	0
1	Dg	117	0	111	9	0
1	Dm	117	0	111	10	0
1	Ds	117	0	111	8	0
1	Dy	117	0	111	5	0
2	Ab	61	0	65	9	0
2	Ah	61	0	65	8	0
2	An	61	0	65	12	0
2	At	61	0	65	7	0
2	Az	61	0	65	10	0
2	Bf	61	0	65	12	0
2	Bl	61	0	65	9	0
2	Br	61	0	65	11	0
2	Bx	61	0	65	6	0
2	Cd	61	0	65	9	0
2	Cj	61	0	65	4	0
2	Cp	61	0	65	7	0
2	Cv	61	0	65	10	0
2	Db	61	0	65	9	0
2	Dh	61	0	65	10	0
2	Dn	61	0	65	10	0
2	Dt	61	0	65	7	0
2	Dz	61	0	65	7	0
3	Ac	125	0	126	9	0
3	Ai	125	0	126	11	0
3	Ao	125	0	126	17	0
3	Au	125	0	126	9	0
3	Ba	125	0	126	9	0
3	Bg	125	0	126	9	0
3	Bm	125	0	126	14	0
3	Bs	125	0	126	15	0
3	By	125	0	126	6	0
3	Ce	125	0	126	9	0
3	Ck	125	0	126	13	0
3	Cq	125	0	126	10	0
3	Cw	125	0	126	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Dc	125	0	126	5	0
3	Di	125	0	126	8	0
3	Do	125	0	126	15	0
3	Du	125	0	126	13	0
3	Ea	125	0	126	9	0
4	Ad	36	0	30	2	0
4	Aj	36	0	30	4	0
4	Ap	36	0	30	5	0
4	Av	36	0	30	2	0
4	Bb	36	0	30	2	0
4	Bh	36	0	30	5	0
4	Bn	36	0	30	3	0
4	Bt	36	0	30	4	0
4	Bz	36	0	30	2	0
4	Cf	36	0	30	3	0
4	Cl	36	0	30	3	0
4	Cr	36	0	30	2	0
4	Cx	36	0	30	1	0
4	Dd	36	0	30	5	0
4	Dj	36	0	30	2	0
4	Dp	36	0	30	3	0
4	Dv	36	0	30	2	0
4	Eb	36	0	30	1	0
5	Ae	484	0	502	41	0
5	Ak	484	0	502	31	0
5	Aq	484	0	502	33	0
5	Aw	484	0	502	22	0
5	Bc	484	0	502	41	0
5	Bi	484	0	502	37	0
5	Bo	484	0	502	42	0
5	Bu	484	0	502	31	0
5	Ca	484	0	502	37	0
5	Cg	484	0	502	33	0
5	Cm	484	0	502	29	0
5	Cs	484	0	502	25	0
5	Cy	484	0	502	29	0
5	De	484	0	502	35	0
5	Dk	484	0	502	48	0
5	Dq	484	0	502	32	0
5	Dw	484	0	502	25	0
5	Ec	484	0	502	23	0
6	Af	1238	0	1252	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Al	1238	0	1252	113	0
6	Ar	1238	0	1252	143	0
6	Ax	1238	0	1252	110	0
6	Bd	1238	0	1252	120	0
6	Bj	1238	0	1252	125	0
6	Bp	1238	0	1252	133	0
6	Bv	1238	0	1252	120	0
6	Cb	1238	0	1252	113	0
6	Ch	1238	0	1252	109	0
6	Cn	1238	0	1252	119	0
6	Ct	1238	0	1252	117	0
6	Cz	1238	0	1252	129	0
6	Df	1238	0	1252	126	0
6	Dl	1238	0	1252	129	0
6	Dr	1238	0	1252	134	0
6	Dx	1238	0	1252	121	0
6	Ed	1238	0	1252	121	0
7	Ee	276	0	263	24	0
7	Ef	472	0	453	48	0
7	Eg	276	0	263	30	0
7	Eh	397	0	386	36	0
7	Ei	402	0	391	45	0
7	Ej	464	0	449	53	0
7	Ek	276	0	263	30	0
7	El	276	0	263	36	0
7	Em	381	0	364	56	0
7	En	276	0	263	42	0
7	Eo	276	0	263	40	0
7	Ep	276	0	263	32	0
7	Eq	459	0	444	54	0
7	Er	276	0	263	33	0
7	Es	454	0	439	53	0
7	Et	397	0	386	51	0
7	Eu	472	0	453	37	0
7	Ev	276	0	263	43	0
7	Fg	334	0	378	24	0
7	Fh	334	0	378	26	0
7	Fi	334	0	378	21	0
7	Fj	334	0	378	19	0
7	Fk	334	0	378	17	0
8	Ew	3213	0	3131	301	0
8	Ex	3213	0	3131	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Ey	3213	0	3131	328	0
8	Ez	3213	0	3131	296	0
8	Fa	3213	0	3131	291	0
9	Fb	6560	0	6545	450	0
9	Fc	6560	0	6545	458	0
9	Fd	6560	0	6545	450	0
9	Fe	6560	0	6545	420	0
9	Ff	6560	0	6545	422	0
All	All	94015	0	93950	6392	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 34.

The worst 5 of 6392 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:Ew:428:LEU:HB2	8:Fa:430:ARG:HH22	1.06	1.15
9:Fc:929:ALA:O	9:Fc:932:LEU:HB3	1.47	1.14
9:Ff:936:LEU:HA	9:Ff:939:LYS:HE3	1.32	1.12
8:Ey:254:MET:HE3	8:Ey:354:ARG:HB3	1.37	1.03
6:Df:115:MET:HE1	7:Ep:798:THR:HA	1.40	1.01

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	14/16 (88%)	14 (100%)	0	0	100	100
1	Ag	14/16 (88%)	14 (100%)	0	0	100	100
1	Am	14/16 (88%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	As	14/16 (88%)	14 (100%)	0	0	100	100
1	Ay	14/16 (88%)	14 (100%)	0	0	100	100
1	Be	14/16 (88%)	14 (100%)	0	0	100	100
1	Bk	14/16 (88%)	14 (100%)	0	0	100	100
1	Bq	14/16 (88%)	14 (100%)	0	0	100	100
1	Bw	14/16 (88%)	14 (100%)	0	0	100	100
1	Cc	14/16 (88%)	14 (100%)	0	0	100	100
1	Ci	14/16 (88%)	14 (100%)	0	0	100	100
1	Co	14/16 (88%)	14 (100%)	0	0	100	100
1	Cu	14/16 (88%)	14 (100%)	0	0	100	100
1	Da	14/16 (88%)	14 (100%)	0	0	100	100
1	Dg	14/16 (88%)	14 (100%)	0	0	100	100
1	Dm	14/16 (88%)	14 (100%)	0	0	100	100
1	Ds	14/16 (88%)	14 (100%)	0	0	100	100
1	Dy	14/16 (88%)	14 (100%)	0	0	100	100
2	Ab	7/9 (78%)	7 (100%)	0	0	100	100
2	Ah	7/9 (78%)	7 (100%)	0	0	100	100
2	An	7/9 (78%)	7 (100%)	0	0	100	100
2	At	7/9 (78%)	7 (100%)	0	0	100	100
2	Az	7/9 (78%)	7 (100%)	0	0	100	100
2	Bf	7/9 (78%)	7 (100%)	0	0	100	100
2	Bl	7/9 (78%)	7 (100%)	0	0	100	100
2	Br	7/9 (78%)	7 (100%)	0	0	100	100
2	Bx	7/9 (78%)	7 (100%)	0	0	100	100
2	Cd	7/9 (78%)	7 (100%)	0	0	100	100
2	Cj	7/9 (78%)	7 (100%)	0	0	100	100
2	Cp	7/9 (78%)	7 (100%)	0	0	100	100
2	Cv	7/9 (78%)	7 (100%)	0	0	100	100
2	Db	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	Dh	7/9 (78%)	7 (100%)	0	0	100	100
2	Dn	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Dt	7/9 (78%)	7 (100%)	0	0	100	100
2	Dz	7/9 (78%)	7 (100%)	0	0	100	100
3	Ac	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Ai	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Ao	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Au	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Ba	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Bg	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Bm	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Bs	14/16 (88%)	14 (100%)	0	0	100	100
3	By	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ce	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Ck	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Cq	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Cw	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Dc	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Di	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Do	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Du	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ea	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
4	Ad	3/5 (60%)	3 (100%)	0	0	100	100
4	Aj	3/5 (60%)	3 (100%)	0	0	100	100
4	Ap	3/5 (60%)	3 (100%)	0	0	100	100
4	Av	3/5 (60%)	3 (100%)	0	0	100	100
4	Bb	3/5 (60%)	3 (100%)	0	0	100	100
4	Bh	3/5 (60%)	3 (100%)	0	0	100	100
4	Bn	3/5 (60%)	3 (100%)	0	0	100	100
4	Bt	3/5 (60%)	3 (100%)	0	0	100	100
4	Bz	3/5 (60%)	3 (100%)	0	0	100	100
4	Cf	3/5 (60%)	3 (100%)	0	0	100	100
4	Cl	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Cr	3/5 (60%)	3 (100%)	0	0	100	100
4	Cx	3/5 (60%)	3 (100%)	0	0	100	100
4	Dd	3/5 (60%)	3 (100%)	0	0	100	100
4	Dj	3/5 (60%)	3 (100%)	0	0	100	100
4	Dp	3/5 (60%)	3 (100%)	0	0	100	100
4	Dv	3/5 (60%)	3 (100%)	0	0	100	100
4	Eb	3/5 (60%)	3 (100%)	0	0	100	100
5	Ae	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Ak	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Aq	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
5	Aw	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
5	Bc	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
5	Bi	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Bo	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Bu	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
5	Ca	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
5	Cg	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Cm	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Cs	61/269 (23%)	53 (87%)	8 (13%)	0	100	100
5	Cy	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
5	De	61/269 (23%)	55 (90%)	6 (10%)	0	100	100
5	Dk	61/269 (23%)	56 (92%)	5 (8%)	0	100	100
5	Dq	61/269 (23%)	57 (93%)	4 (7%)	0	100	100
5	Dw	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Ec	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
6	Af	158/361 (44%)	153 (97%)	5 (3%)	0	100	100
6	Al	158/361 (44%)	149 (94%)	9 (6%)	0	100	100
6	Ar	158/361 (44%)	151 (96%)	7 (4%)	0	100	100
6	Ax	158/361 (44%)	149 (94%)	9 (6%)	0	100	100
6	Bd	158/361 (44%)	152 (96%)	6 (4%)	0	100	100
6	Bj	158/361 (44%)	148 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Bp	158/361 (44%)	147 (93%)	11 (7%)	0	100	100
6	Bv	158/361 (44%)	150 (95%)	8 (5%)	0	100	100
6	Cb	158/361 (44%)	151 (96%)	7 (4%)	0	100	100
6	Ch	158/361 (44%)	151 (96%)	7 (4%)	0	100	100
6	Cn	158/361 (44%)	146 (92%)	12 (8%)	0	100	100
6	Ct	158/361 (44%)	147 (93%)	11 (7%)	0	100	100
6	Cz	158/361 (44%)	150 (95%)	8 (5%)	0	100	100
6	Df	158/361 (44%)	149 (94%)	9 (6%)	0	100	100
6	Dl	158/361 (44%)	152 (96%)	6 (4%)	0	100	100
6	Dr	158/361 (44%)	152 (96%)	6 (4%)	0	100	100
6	Dx	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
6	Ed	158/361 (44%)	149 (94%)	9 (6%)	0	100	100
7	Ee	32/1048 (3%)	32 (100%)	0	0	100	100
7	Ef	57/1048 (5%)	57 (100%)	0	0	100	100
7	Eg	32/1048 (3%)	32 (100%)	0	0	100	100
7	Eh	46/1048 (4%)	44 (96%)	2 (4%)	0	100	100
7	Ei	47/1048 (4%)	45 (96%)	2 (4%)	0	100	100
7	Ej	56/1048 (5%)	56 (100%)	0	0	100	100
7	Ek	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
7	El	32/1048 (3%)	32 (100%)	0	0	100	100
7	Em	44/1048 (4%)	43 (98%)	1 (2%)	0	100	100
7	En	32/1048 (3%)	32 (100%)	0	0	100	100
7	Eo	32/1048 (3%)	32 (100%)	0	0	100	100
7	Ep	32/1048 (3%)	32 (100%)	0	0	100	100
7	Eq	55/1048 (5%)	52 (94%)	3 (6%)	0	100	100
7	Er	32/1048 (3%)	31 (97%)	1 (3%)	0	100	100
7	Es	54/1048 (5%)	53 (98%)	1 (2%)	0	100	100
7	Et	46/1048 (4%)	44 (96%)	2 (4%)	0	100	100
7	Eu	57/1048 (5%)	56 (98%)	1 (2%)	0	100	100
7	Ev	32/1048 (3%)	30 (94%)	2 (6%)	0	100	100
7	Fg	41/1048 (4%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Fh	41/1048 (4%)	41 (100%)	0	0	100	100
7	Fi	41/1048 (4%)	40 (98%)	1 (2%)	0	100	100
7	Fj	41/1048 (4%)	41 (100%)	0	0	100	100
7	Fk	41/1048 (4%)	40 (98%)	1 (2%)	0	100	100
8	Ew	413/466 (89%)	396 (96%)	17 (4%)	0	100	100
8	Ex	413/466 (89%)	398 (96%)	15 (4%)	0	100	100
8	Ey	413/466 (89%)	394 (95%)	19 (5%)	0	100	100
8	Ez	413/466 (89%)	388 (94%)	25 (6%)	0	100	100
8	Fa	413/466 (89%)	394 (95%)	19 (5%)	0	100	100
9	Fb	847/1048 (81%)	810 (96%)	37 (4%)	0	100	100
9	Fc	847/1048 (81%)	805 (95%)	42 (5%)	0	100	100
9	Fd	847/1048 (81%)	799 (94%)	48 (6%)	0	100	100
9	Fe	847/1048 (81%)	793 (94%)	54 (6%)	0	100	100
9	Ff	847/1048 (81%)	794 (94%)	53 (6%)	0	100	100
All	All	11881/43842 (27%)	11290 (95%)	591 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	11/11 (100%)	11 (100%)	0	100	100
1	Ag	11/11 (100%)	11 (100%)	0	100	100
1	Am	11/11 (100%)	10 (91%)	1 (9%)	7	24
1	As	11/11 (100%)	11 (100%)	0	100	100
1	Ay	11/11 (100%)	11 (100%)	0	100	100
1	Be	11/11 (100%)	11 (100%)	0	100	100
1	Bk	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Bq	11/11 (100%)	11 (100%)	0	100	100
1	Bw	11/11 (100%)	11 (100%)	0	100	100
1	Cc	11/11 (100%)	10 (91%)	1 (9%)	7	24
1	Ci	11/11 (100%)	9 (82%)	2 (18%)	1	8
1	Co	11/11 (100%)	11 (100%)	0	100	100
1	Cu	11/11 (100%)	11 (100%)	0	100	100
1	Da	11/11 (100%)	11 (100%)	0	100	100
1	Dg	11/11 (100%)	10 (91%)	1 (9%)	7	24
1	Dm	11/11 (100%)	10 (91%)	1 (9%)	7	24
1	Ds	11/11 (100%)	10 (91%)	1 (9%)	7	24
1	Dy	11/11 (100%)	11 (100%)	0	100	100
2	Ab	7/7 (100%)	7 (100%)	0	100	100
2	Ah	7/7 (100%)	7 (100%)	0	100	100
2	An	7/7 (100%)	7 (100%)	0	100	100
2	At	7/7 (100%)	7 (100%)	0	100	100
2	Az	7/7 (100%)	7 (100%)	0	100	100
2	Bf	7/7 (100%)	7 (100%)	0	100	100
2	Bl	7/7 (100%)	7 (100%)	0	100	100
2	Br	7/7 (100%)	7 (100%)	0	100	100
2	Bx	7/7 (100%)	7 (100%)	0	100	100
2	Cd	7/7 (100%)	7 (100%)	0	100	100
2	Cj	7/7 (100%)	6 (86%)	1 (14%)	2	13
2	Cp	7/7 (100%)	6 (86%)	1 (14%)	2	13
2	Cv	7/7 (100%)	7 (100%)	0	100	100
2	Db	7/7 (100%)	7 (100%)	0	100	100
2	Dh	7/7 (100%)	7 (100%)	0	100	100
2	Dn	7/7 (100%)	7 (100%)	0	100	100
2	Dt	7/7 (100%)	7 (100%)	0	100	100
2	Dz	7/7 (100%)	7 (100%)	0	100	100
3	Ac	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Ai	13/13 (100%)	12 (92%)	1 (8%)	10	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ao	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Au	13/13 (100%)	13 (100%)	0	100	100
3	Ba	13/13 (100%)	13 (100%)	0	100	100
3	Bg	13/13 (100%)	13 (100%)	0	100	100
3	Bm	13/13 (100%)	13 (100%)	0	100	100
3	Bs	13/13 (100%)	13 (100%)	0	100	100
3	By	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Ce	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Ck	13/13 (100%)	13 (100%)	0	100	100
3	Cq	13/13 (100%)	13 (100%)	0	100	100
3	Cw	13/13 (100%)	13 (100%)	0	100	100
3	Dc	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Di	13/13 (100%)	12 (92%)	1 (8%)	10	30
3	Do	13/13 (100%)	11 (85%)	2 (15%)	2	12
3	Du	13/13 (100%)	13 (100%)	0	100	100
3	Ea	13/13 (100%)	12 (92%)	1 (8%)	10	30
4	Ad	3/3 (100%)	3 (100%)	0	100	100
4	Aj	3/3 (100%)	3 (100%)	0	100	100
4	Ap	3/3 (100%)	3 (100%)	0	100	100
4	Av	3/3 (100%)	3 (100%)	0	100	100
4	Bb	3/3 (100%)	3 (100%)	0	100	100
4	Bh	3/3 (100%)	3 (100%)	0	100	100
4	Bn	3/3 (100%)	3 (100%)	0	100	100
4	Bt	3/3 (100%)	3 (100%)	0	100	100
4	Bz	3/3 (100%)	3 (100%)	0	100	100
4	Cf	3/3 (100%)	3 (100%)	0	100	100
4	Cl	3/3 (100%)	3 (100%)	0	100	100
4	Cr	3/3 (100%)	3 (100%)	0	100	100
4	Cx	3/3 (100%)	3 (100%)	0	100	100
4	Dd	3/3 (100%)	3 (100%)	0	100	100
4	Dj	3/3 (100%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Dp	3/3 (100%)	3 (100%)	0	100	100
4	Dv	3/3 (100%)	3 (100%)	0	100	100
4	Eb	3/3 (100%)	3 (100%)	0	100	100
5	Ae	53/237 (22%)	52 (98%)	1 (2%)	52	70
5	Ak	53/237 (22%)	52 (98%)	1 (2%)	52	70
5	Aq	53/237 (22%)	50 (94%)	3 (6%)	17	39
5	Aw	53/237 (22%)	51 (96%)	2 (4%)	28	49
5	Bc	53/237 (22%)	50 (94%)	3 (6%)	17	39
5	Bi	53/237 (22%)	52 (98%)	1 (2%)	52	70
5	Bo	53/237 (22%)	49 (92%)	4 (8%)	11	30
5	Bu	53/237 (22%)	51 (96%)	2 (4%)	28	49
5	Ca	53/237 (22%)	52 (98%)	1 (2%)	52	70
5	Cg	53/237 (22%)	49 (92%)	4 (8%)	11	30
5	Cm	53/237 (22%)	47 (89%)	6 (11%)	4	18
5	Cs	53/237 (22%)	53 (100%)	0	100	100
5	Cy	53/237 (22%)	51 (96%)	2 (4%)	28	49
5	De	53/237 (22%)	51 (96%)	2 (4%)	28	49
5	Dk	53/237 (22%)	53 (100%)	0	100	100
5	Dq	53/237 (22%)	53 (100%)	0	100	100
5	Dw	53/237 (22%)	50 (94%)	3 (6%)	17	39
5	Ec	53/237 (22%)	53 (100%)	0	100	100
6	Af	137/300 (46%)	127 (93%)	10 (7%)	11	31
6	Al	137/300 (46%)	131 (96%)	6 (4%)	24	46
6	Ar	137/300 (46%)	135 (98%)	2 (2%)	60	75
6	Ax	137/300 (46%)	128 (93%)	9 (7%)	14	35
6	Bd	137/300 (46%)	132 (96%)	5 (4%)	30	51
6	Bj	137/300 (46%)	132 (96%)	5 (4%)	30	51
6	Bp	137/300 (46%)	128 (93%)	9 (7%)	14	35
6	Bv	137/300 (46%)	130 (95%)	7 (5%)	20	42
6	Cb	137/300 (46%)	128 (93%)	9 (7%)	14	35
6	Ch	137/300 (46%)	130 (95%)	7 (5%)	20	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Cn	137/300 (46%)	127 (93%)	10 (7%)	11	31
6	Ct	137/300 (46%)	135 (98%)	2 (2%)	60	75
6	Cz	137/300 (46%)	130 (95%)	7 (5%)	20	42
6	Df	137/300 (46%)	128 (93%)	9 (7%)	14	35
6	Dl	137/300 (46%)	125 (91%)	12 (9%)	8	25
6	Dr	137/300 (46%)	128 (93%)	9 (7%)	14	35
6	Dx	137/300 (46%)	131 (96%)	6 (4%)	24	46
6	Ed	137/300 (46%)	127 (93%)	10 (7%)	11	31
7	Ee	31/765 (4%)	29 (94%)	2 (6%)	14	35
7	Ef	51/765 (7%)	48 (94%)	3 (6%)	16	38
7	Eg	31/765 (4%)	31 (100%)	0	100	100
7	Eh	44/765 (6%)	44 (100%)	0	100	100
7	Ei	44/765 (6%)	39 (89%)	5 (11%)	4	17
7	Ej	50/765 (6%)	48 (96%)	2 (4%)	27	48
7	Ek	31/765 (4%)	31 (100%)	0	100	100
7	El	31/765 (4%)	31 (100%)	0	100	100
7	Em	42/765 (6%)	38 (90%)	4 (10%)	7	22
7	En	31/765 (4%)	29 (94%)	2 (6%)	14	35
7	Eo	31/765 (4%)	30 (97%)	1 (3%)	34	54
7	Ep	31/765 (4%)	31 (100%)	0	100	100
7	Eq	50/765 (6%)	48 (96%)	2 (4%)	27	48
7	Er	31/765 (4%)	31 (100%)	0	100	100
7	Es	50/765 (6%)	44 (88%)	6 (12%)	4	17
7	Et	44/765 (6%)	42 (96%)	2 (4%)	23	46
7	Eu	51/765 (7%)	50 (98%)	1 (2%)	50	68
7	Ev	31/765 (4%)	31 (100%)	0	100	100
7	Fg	36/765 (5%)	36 (100%)	0	100	100
7	Fh	36/765 (5%)	36 (100%)	0	100	100
7	Fi	36/765 (5%)	36 (100%)	0	100	100
7	Fj	36/765 (5%)	34 (94%)	2 (6%)	17	39
7	Fk	36/765 (5%)	34 (94%)	2 (6%)	17	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ew	360/401 (90%)	350 (97%)	10 (3%)	38	58
8	Ex	360/401 (90%)	349 (97%)	11 (3%)	35	55
8	Ey	360/401 (90%)	352 (98%)	8 (2%)	47	65
8	Ez	360/401 (90%)	348 (97%)	12 (3%)	33	54
8	Fa	360/401 (90%)	353 (98%)	7 (2%)	52	70
9	Fb	715/858 (83%)	691 (97%)	24 (3%)	32	53
9	Fc	715/858 (83%)	682 (95%)	33 (5%)	23	45
9	Fd	715/858 (83%)	693 (97%)	22 (3%)	35	55
9	Fe	715/858 (83%)	676 (94%)	39 (6%)	18	40
9	Ff	715/858 (83%)	688 (96%)	27 (4%)	28	49
All	All	10292/34168 (30%)	9877 (96%)	415 (4%)	29	48

5 of 415 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Ex	197	ASN
9	Fb	774	GLU
9	Ff	603	TYR
8	Ex	440	ASN
8	Fa	95	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 194 such sidechains are listed below:

Mol	Chain	Res	Type
8	Ex	447	ASN
8	Fa	212	GLN
8	Ey	246	ASN
8	Ez	139	ASN
8	Fa	433	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no 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.



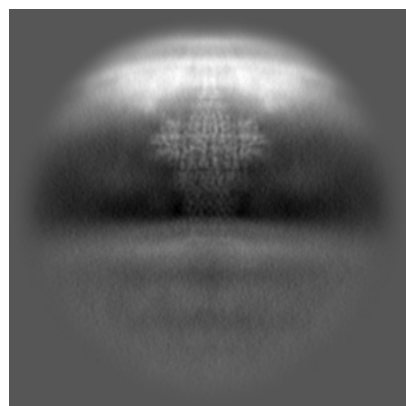
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49398. These allow visual inspection of the internal detail of the map and identification of artifacts.

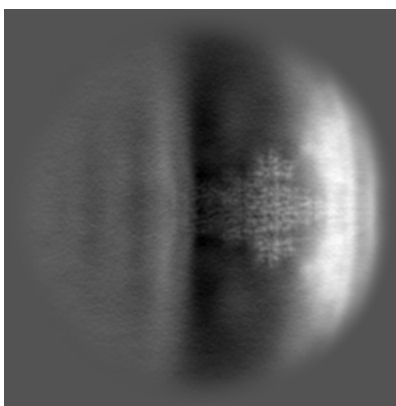
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

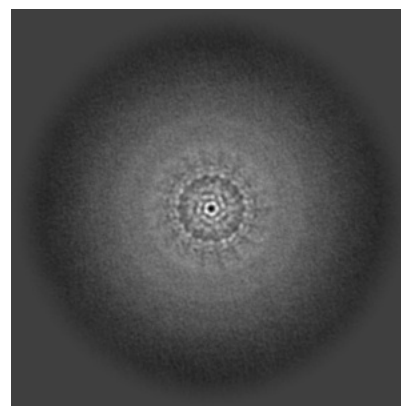
#### 6.1.1 Primary map



X

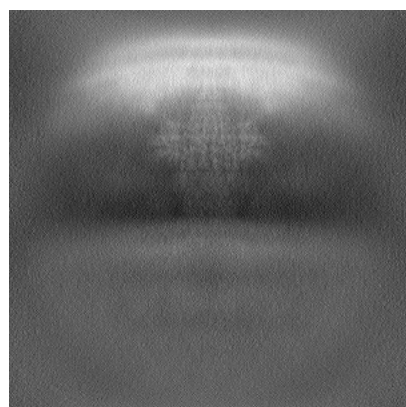


Y

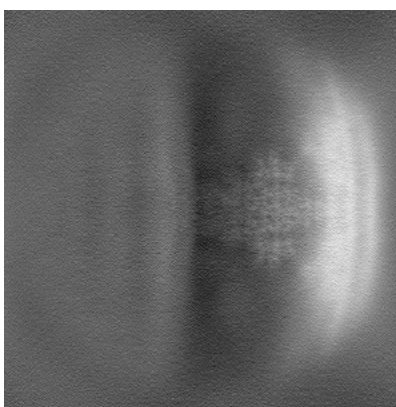


Z

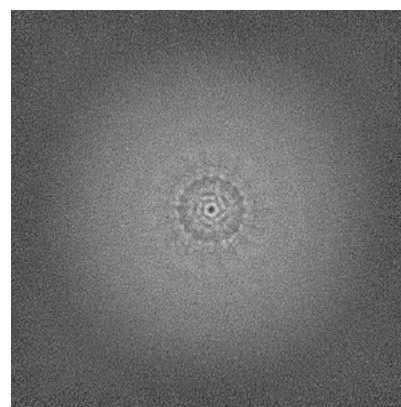
#### 6.1.2 Raw map



X



Y

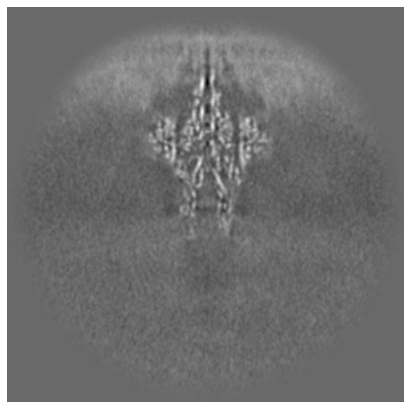


Z

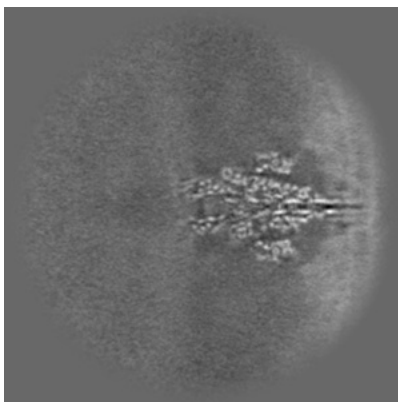
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

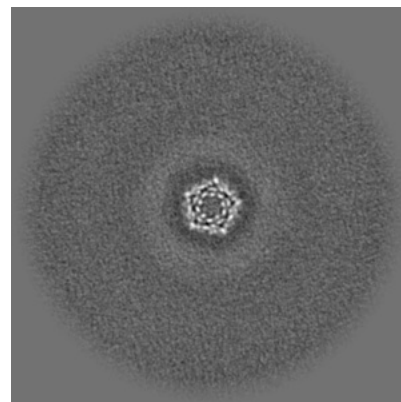
### 6.2.1 Primary map



X Index: 256

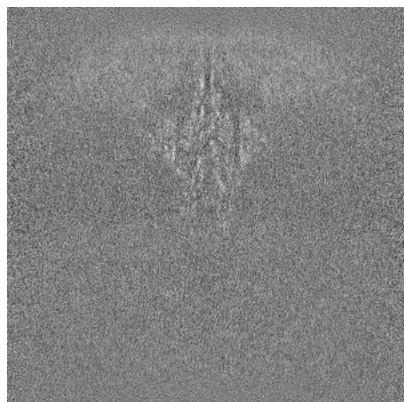


Y Index: 256

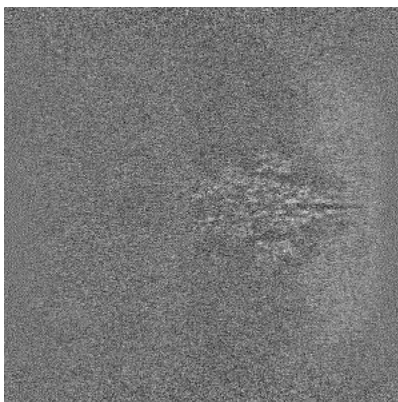


Z Index: 256

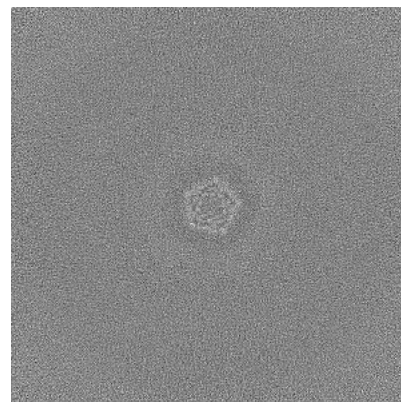
### 6.2.2 Raw map



X Index: 256



Y Index: 256

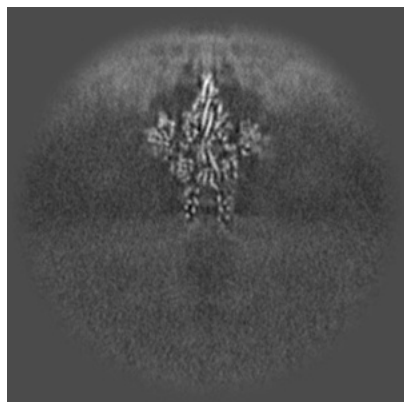


Z Index: 256

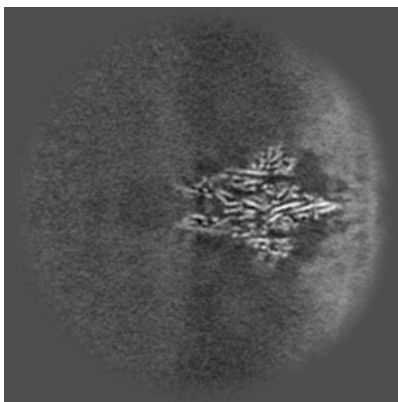
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

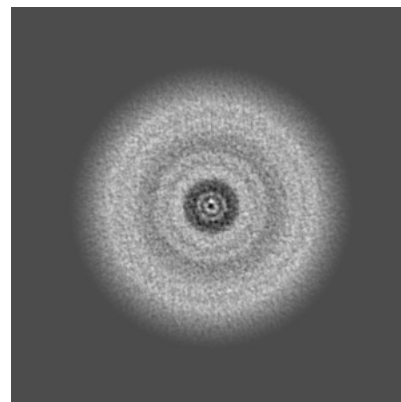
### 6.3.1 Primary map



X Index: 250

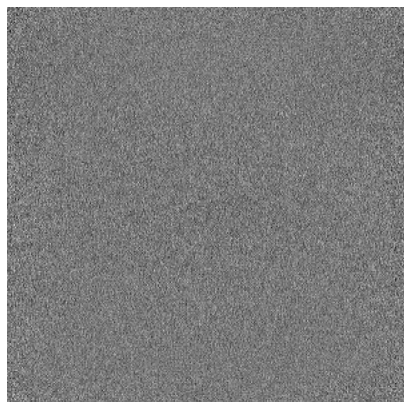


Y Index: 263

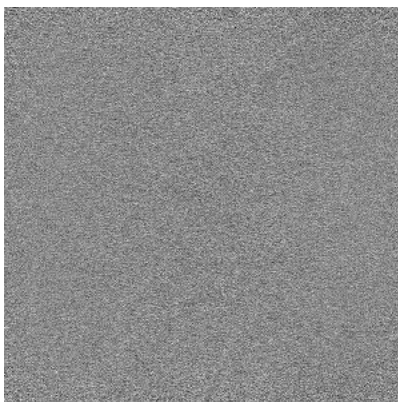


Z Index: 430

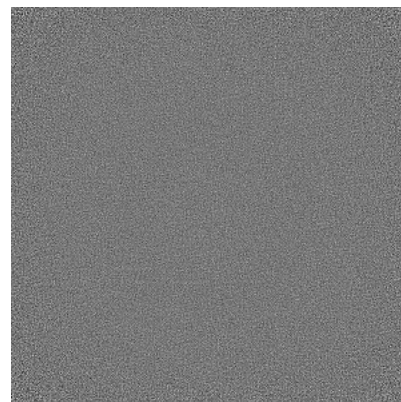
### 6.3.2 Raw map



X Index: 0



Y Index: 0



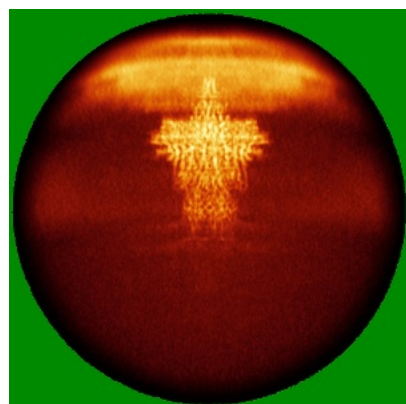
Z Index: 511

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

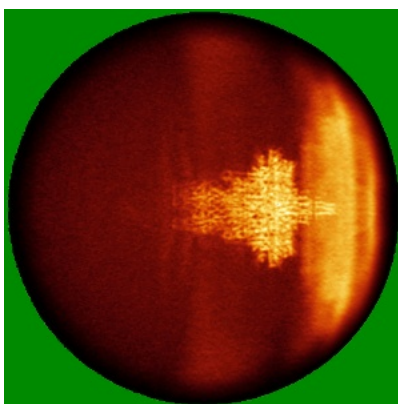


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

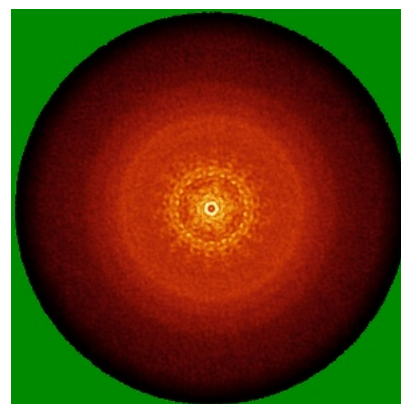
### 6.4.1 Primary map



X

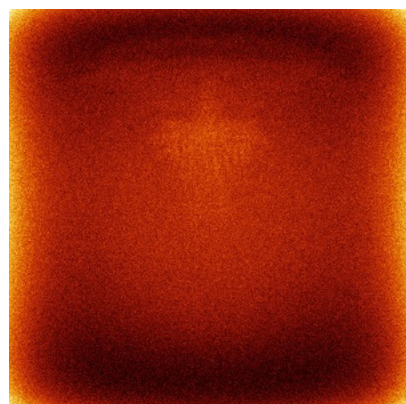


Y

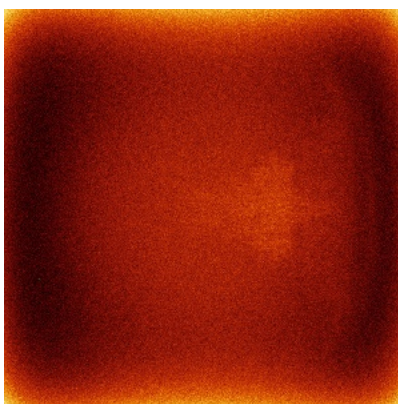


Z

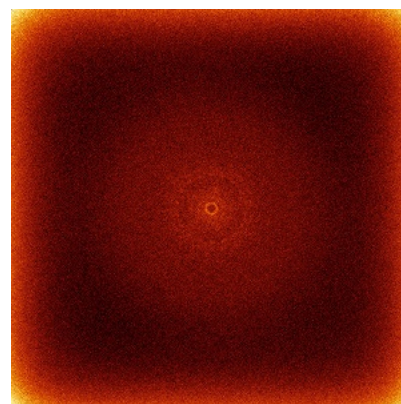
### 6.4.2 Raw map



X



Y

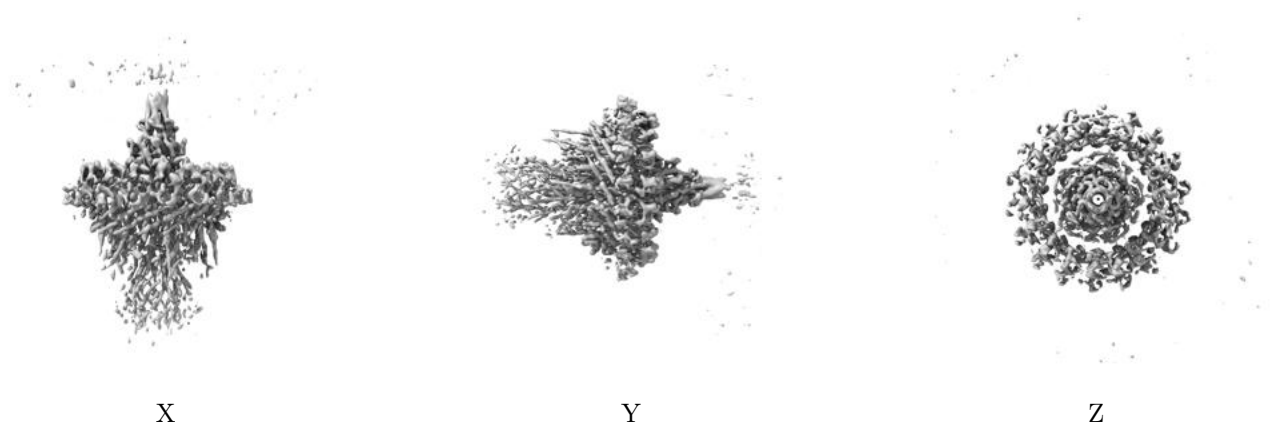


Z

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.

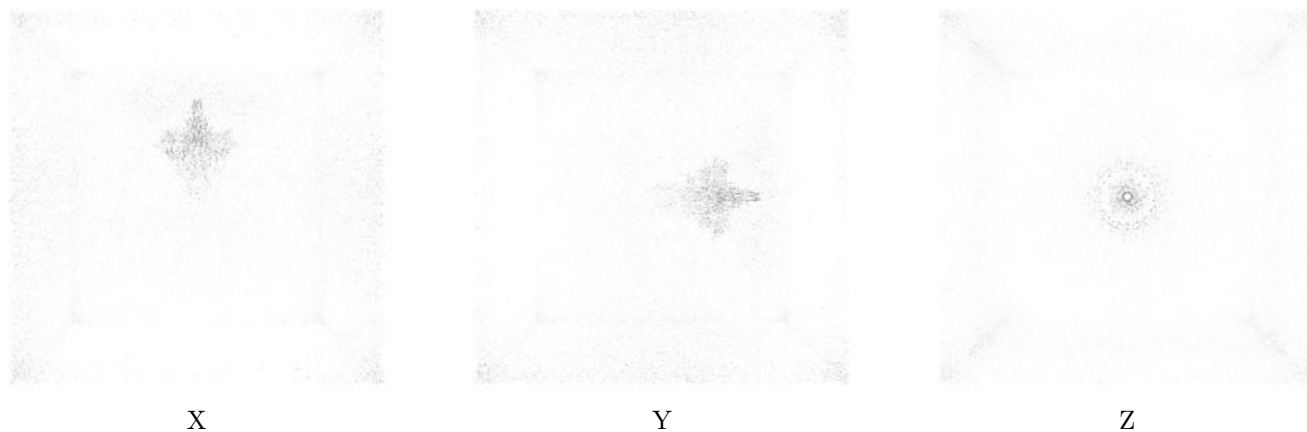
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

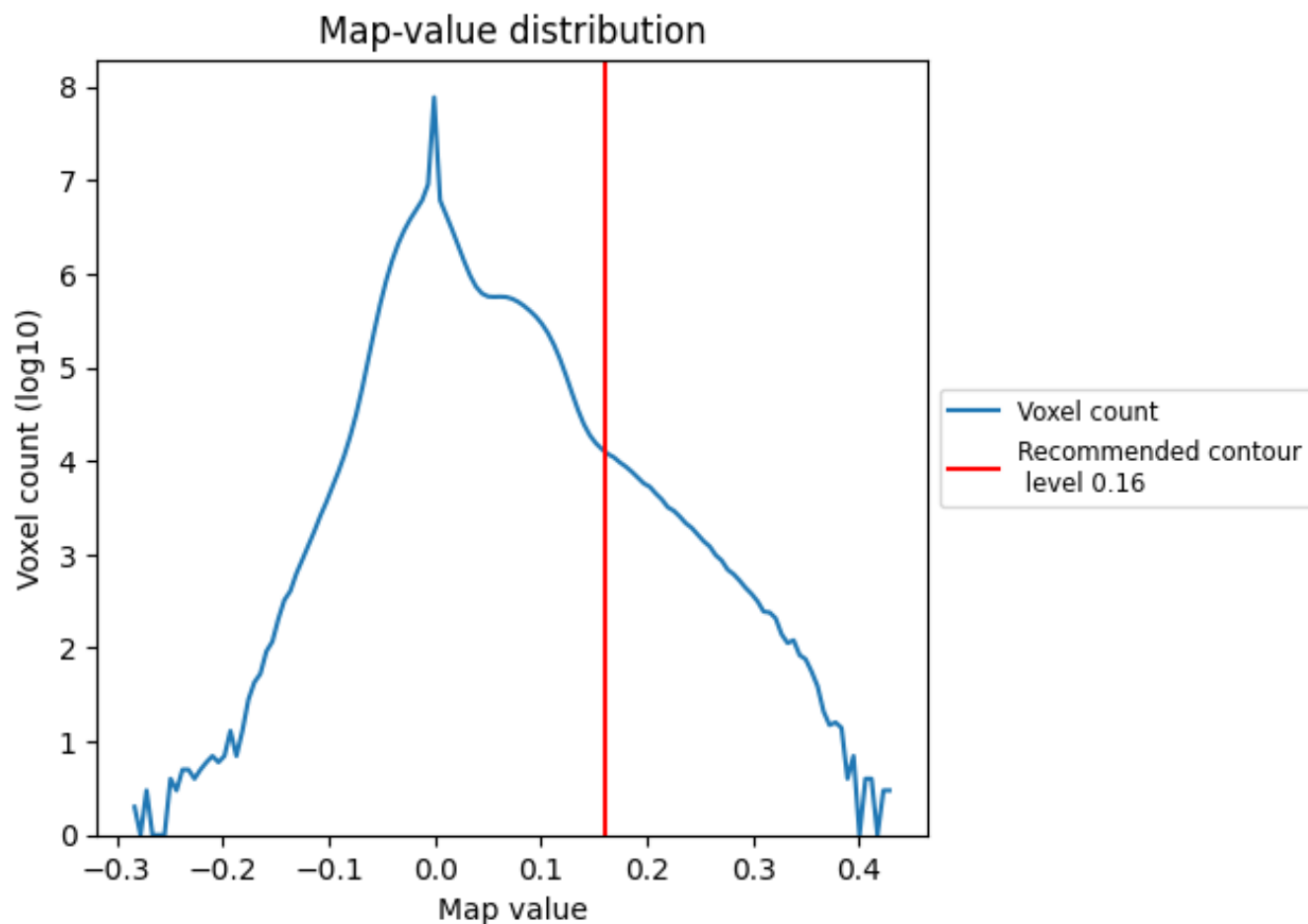
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

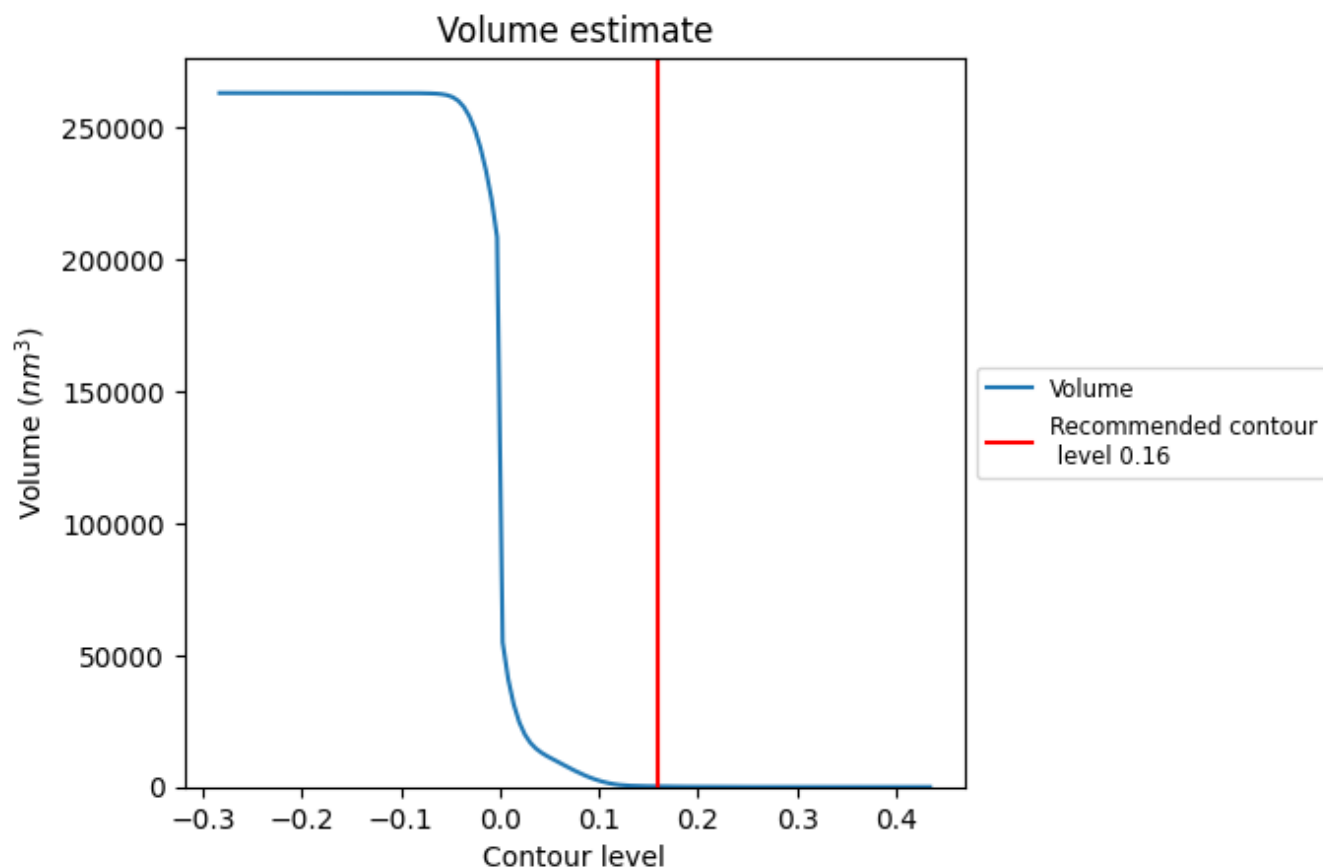
This section contains the results of statistical analysis of the map.

### 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.

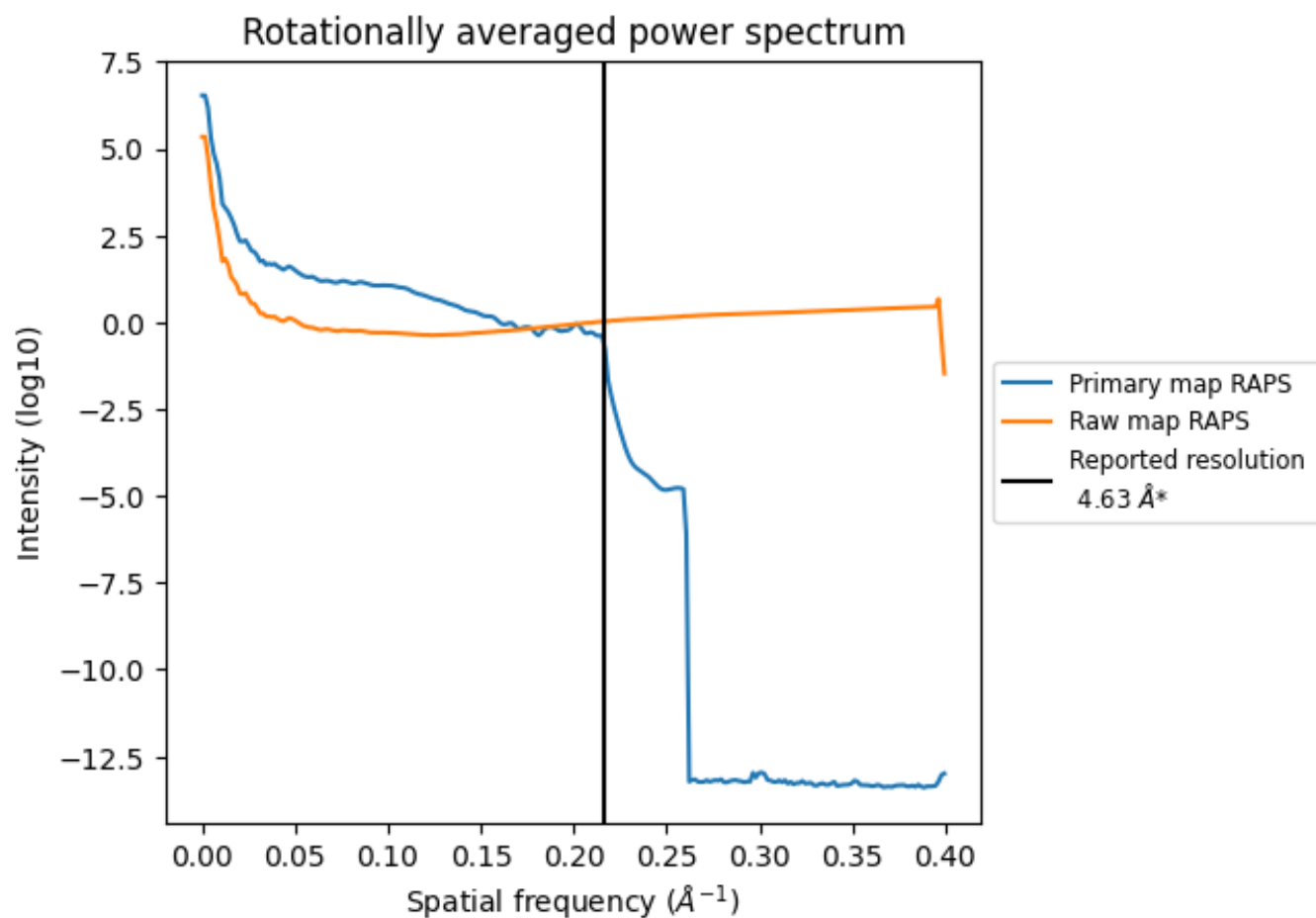
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm<sup>3</sup>; this corresponds to an approximate mass of 187 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 ⓘ



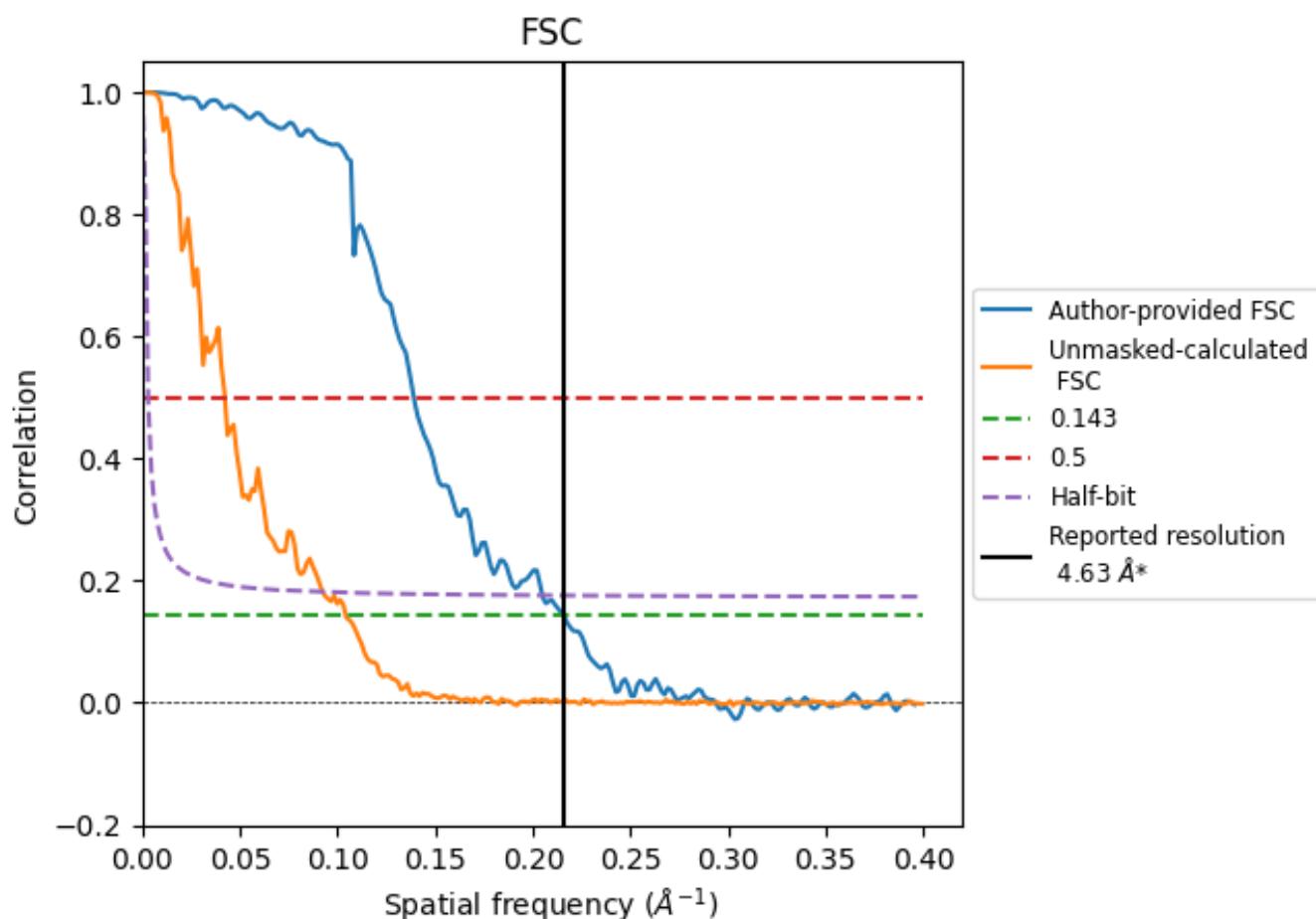
\*Reported resolution corresponds to spatial frequency of 0.216 Å<sup>-1</sup>



## 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 0.216 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

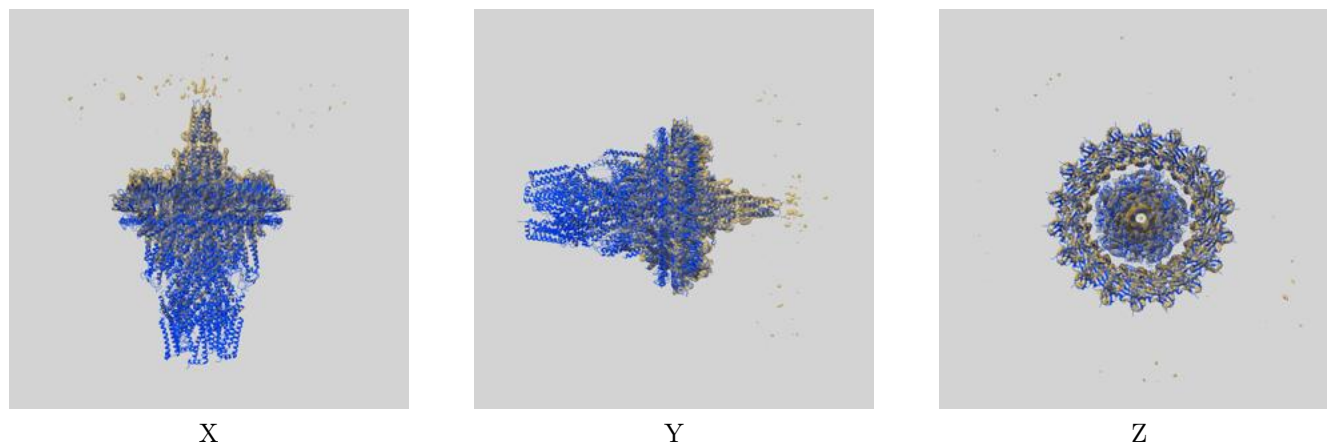
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	7.19	4.88
Unmasked-calculated*	9.59	23.64	10.82

\*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 9.59 differs from the reported value 4.63 by more than 10 %

## 9 Map-model fit [i](#)

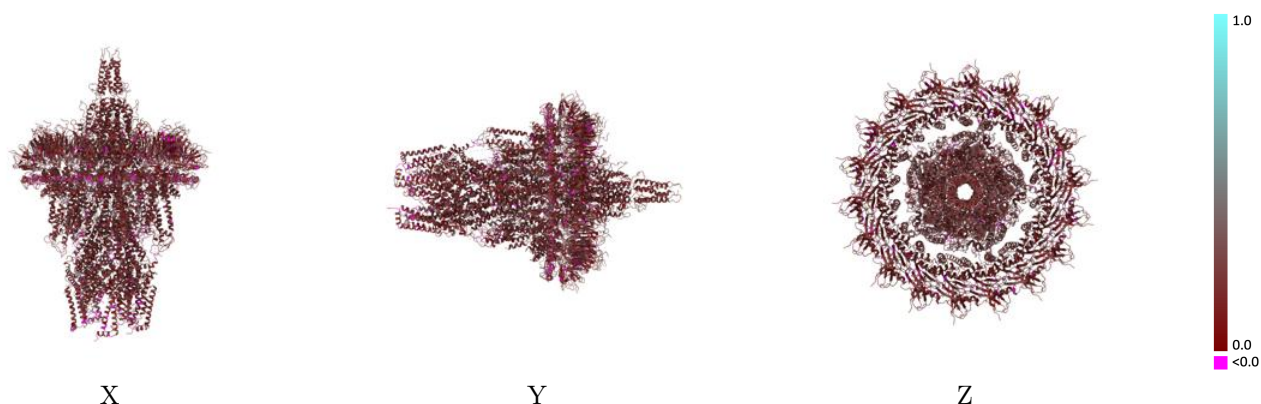
This section contains information regarding the fit between EMDB map EMD-49398 and PDB model 9NH0. Per-residue inclusion information can be found in section [3](#) on page [17](#).

### 9.1 Map-model overlay [i](#)



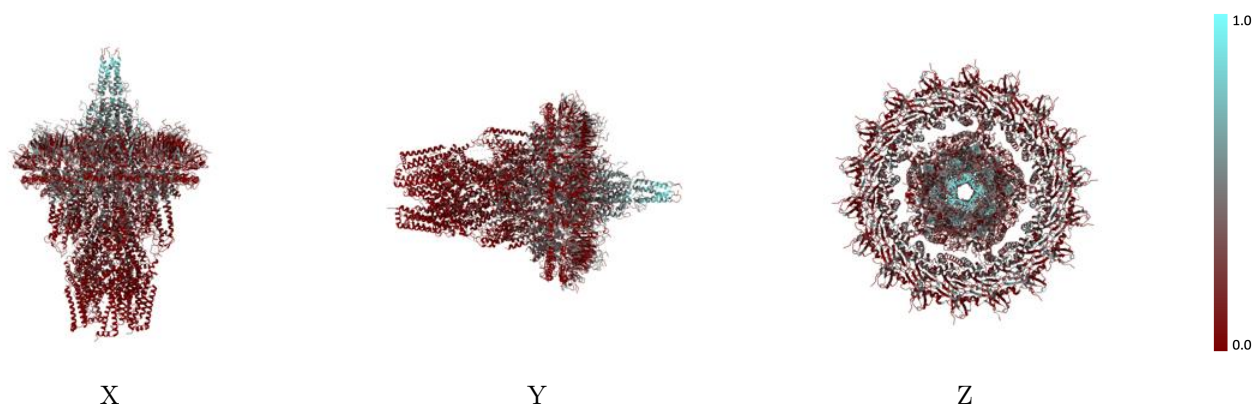
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



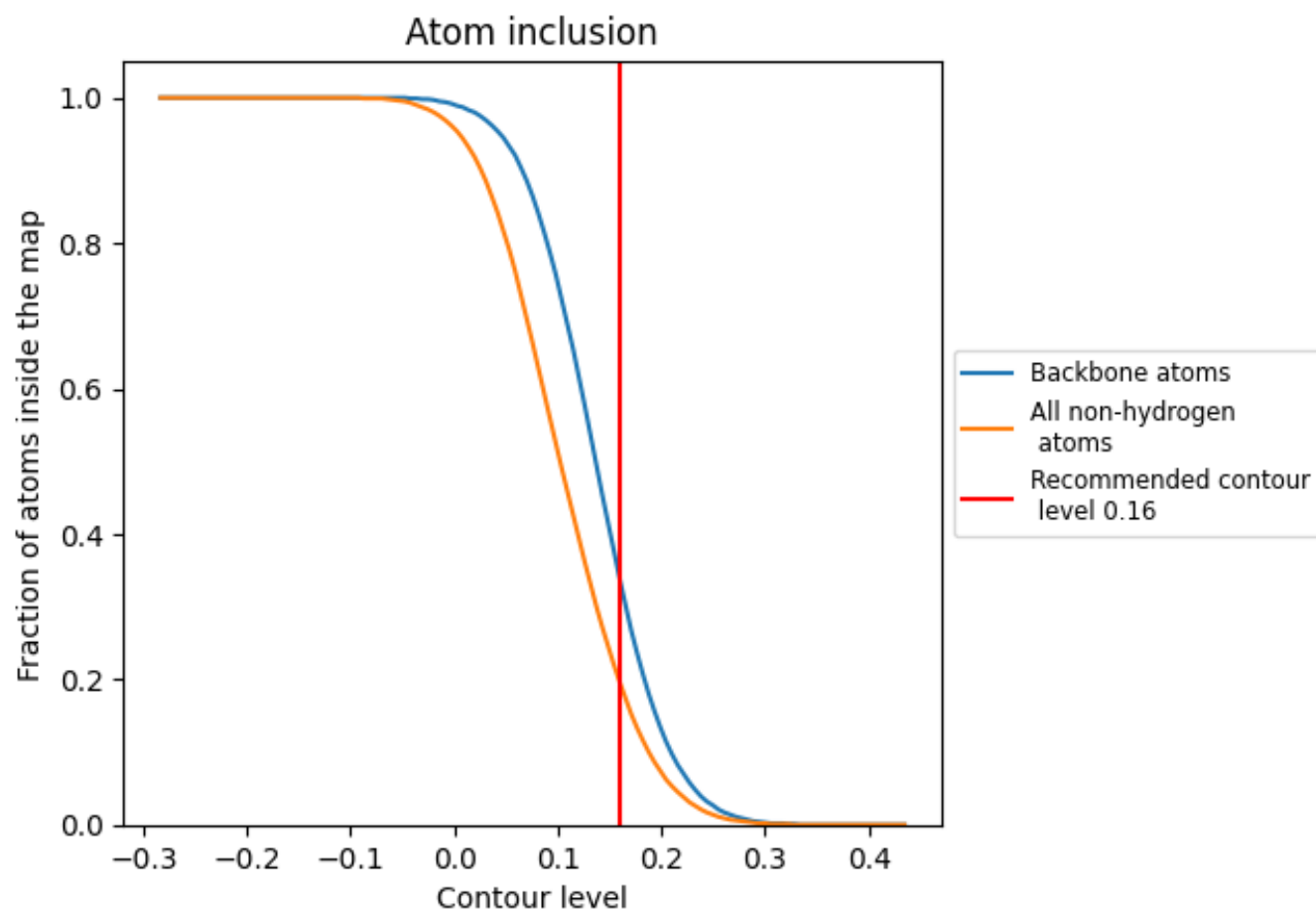
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.16).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 20% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1950	 0.2010
Aa	 0.0000	 0.1650
Ab	 0.1020	 0.2220
Ac	 0.0000	 0.0490
Ad	 0.0000	 0.0010
Ae	 0.1820	 0.2010
Af	 0.2550	 0.2080
Ag	 0.0000	 0.1660
Ah	 0.0850	 0.2400
Ai	 0.0000	 0.1260
Aj	 0.0000	 0.0980
Ak	 0.1630	 0.1880
Al	 0.2810	 0.1980
Am	 0.0170	 0.1750
An	 0.0510	 0.1430
Ao	 0.0000	 0.0930
Ap	 0.0000	 0.1540
Aq	 0.1720	 0.1620
Ar	 0.2430	 0.1920
As	 0.0000	 0.1420
At	 0.0340	 0.1620
Au	 0.0000	 0.1150
Av	 0.0000	 0.0400
Aw	 0.1610	 0.1890
Ax	 0.2470	 0.1940
Ay	 0.0000	 0.2180
Az	 0.0000	 0.1730
Ba	 0.0000	 0.1710
Bb	 0.0000	 0.0750
Bc	 0.1000	 0.1690
Bd	 0.2420	 0.2050
Be	 0.0000	 0.1880
Bf	 0.0510	 0.2300
Bg	 0.0000	 0.0930
Bh	 0.0000	 0.0110























































































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Chain	Atom inclusion	Q-score
Bi	0.1360	0.1830
Bj	0.2520	0.2000
Bk	0.0000	0.1890
Bl	0.0000	0.1900
Bm	0.0000	0.0510
Bn	0.0000	-0.0730
Bo	0.1480	0.1810
Bp	0.2170	0.2080
Bq	0.0000	0.1350
Br	0.0170	0.2190
Bs	0.0000	0.1200
Bt	0.0000	-0.0550
Bu	0.1060	0.1760
Bv	0.2710	0.2130
Bw	0.0000	0.1840
Bx	0.1190	0.1440
By	0.0000	0.1100
Bz	0.0000	0.0110
Ca	0.1500	0.1780
Cb	0.2840	0.2030
Cc	0.0000	0.1760
Cd	0.0340	0.2270
Ce	0.0000	0.1640
Cf	0.0000	0.0570
Cg	0.1290	0.1830
Ch	0.2440	0.2080
Ci	0.0000	0.1620
Cj	0.0000	0.2090
Ck	0.0000	0.1040
Cl	0.0000	0.0000
Cm	0.1440	0.1950
Cn	0.2430	0.2060
Co	0.0000	0.2150
Cp	0.0000	0.1820
Cq	0.0000	0.1010
Cr	0.0000	0.0150
Cs	0.1840	0.1950
Ct	0.2650	0.2070
Cu	0.0000	0.1530
Cv	0.0000	0.0810
Cw	0.0000	0.1330
Cx	0.0000	0.2220

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Chain	Atom inclusion	Q-score
Cy	 0.1590	 0.2020
Cz	 0.2540	 0.1970
Da	 0.0170	 0.1990
Db	 0.0340	 0.1430
Dc	 0.0000	 0.1050
Dd	 0.0000	 0.0980
De	 0.1440	 0.1760
Df	 0.2800	 0.2120
Dg	 0.0000	 0.1630
Dh	 0.0510	 0.1860
Di	 0.0000	 0.1560
Dj	 0.0000	 -0.0640
Dk	 0.1400	 0.2010
Dl	 0.3170	 0.2130
Dm	 0.0000	 0.1880
Dn	 0.0510	 0.2040
Do	 0.0000	 0.1220
Dp	 0.0000	 0.0190
Dq	 0.1780	 0.2090
Dr	 0.3140	 0.2180
Ds	 0.0000	 0.1690
Dt	 0.0340	 0.2350
Du	 0.0000	 0.0600
Dv	 0.0000	 0.0040
Dw	 0.1570	 0.1980
Dx	 0.2860	 0.2140
Dy	 0.0090	 0.1720
Dz	 0.0510	 0.2220
Ea	 0.0000	 0.0810
Eb	 0.0000	 0.0330
Ec	 0.1630	 0.1890
Ed	 0.3060	 0.2140
Ee	 0.3820	 0.2380
Ef	 0.2420	 0.2250
Eg	 0.3160	 0.2360
Eh	 0.2420	 0.2220
Ei	 0.2620	 0.1950
Ej	 0.2610	 0.2150
Ek	 0.3530	 0.2600
El	 0.4410	 0.2450
Em	 0.2930	 0.2330
En	 0.4410	 0.2370

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Chain	Atom inclusion	Q-score
Eo	 0.3460	 0.2380
Ep	 0.3570	 0.2350
Eq	 0.3080	 0.2110
Er	 0.3310	 0.2280
Es	 0.2450	 0.2300
Et	 0.3110	 0.2280
Eu	 0.2330	 0.2250
Ev	 0.4520	 0.2440
Ew	 0.3370	 0.2190
Ex	 0.3450	 0.2180
Ey	 0.3480	 0.2260
Ez	 0.3470	 0.2230
Fa	 0.3440	 0.2270
Fb	 0.1150	 0.1980
Fc	 0.0960	 0.1970
Fd	 0.1050	 0.1970
Fe	 0.1070	 0.1970
Ff	 0.1080	 0.1980
Fg	 0.0000	 0.1920
Fh	 0.0030	 0.1620
Fi	 0.0000	 0.1850
Fj	 0.0000	 0.1730
Fk	 0.0000	 0.1810