



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 10:30 AM UTC

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

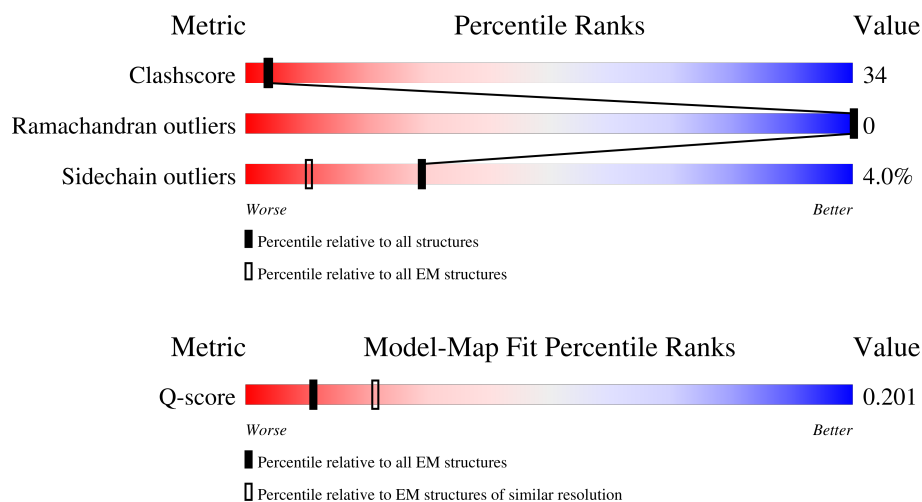
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
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 ≥ 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	
1	Ag	16	
1	Am	16	
1	As	16	

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

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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	

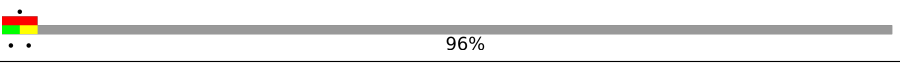
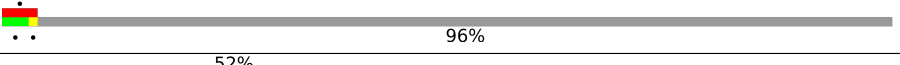
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Mol	Chain	Length	Quality of chain
6	Dl	361	
6	Dr	361	
6	Dx	361	
6	Ed	361	
7	Ee	1048	
7	Ef	1048	
7	Eg	1048	
7	Eh	1048	
7	Ei	1048	
7	Ej	1048	
7	Ek	1048	
7	El	1048	
7	Em	1048	
7	En	1048	
7	Eo	1048	
7	Ep	1048	
7	Eq	1048	
7	Er	1048	
7	Es	1048	
7	Et	1048	
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	 96%
7	Fk	1048	 96%
8	Ew	466	 52% 43% 44% 11%
8	Ex	466	 50% 43% 45% 11%
8	Ey	466	 48% 40% 48% 11%
8	Ez	466	 50% 44% 43% 11%
8	Fa	466	 49% 42% 45% 11%
9	Fb	1048	 74% 40% 40% 18%
9	Fc	1048	 77% 40% 39% 18%
9	Fd	1048	 75% 39% 41% 18%
9	Fe	1048	 75% 42% 37% 18%
9	Ff	1048	 75% 40% 40% 18%

2 Entry composition

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.

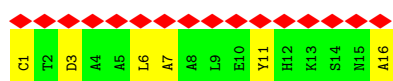
Mol	Chain	Residues	Atoms					AltConf	Trace
9	Fb	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fc	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fd	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Fe	857	Total	C	N	O	S	0	0
			6560	4256	1051	1202	51		
9	Ff	857	Total	C	N	O	S	0	0
			6560	4256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



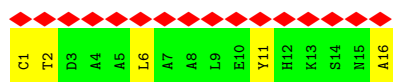
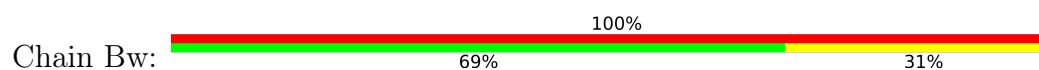
- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



- Molecule 1: unknown peptide E



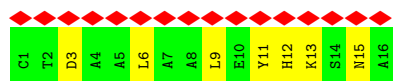
- Molecule 1: unknown peptide E



- 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



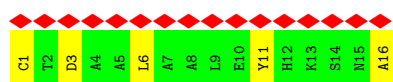
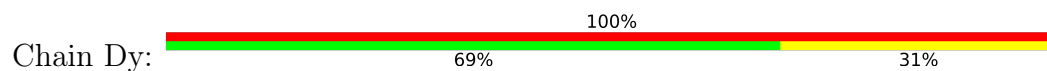
- Molecule 1: unknown peptide E



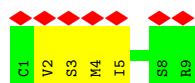
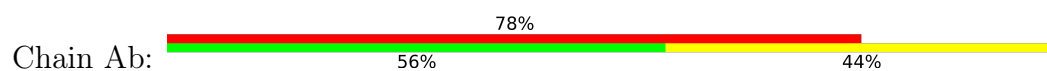
- Molecule 1: unknown peptide E



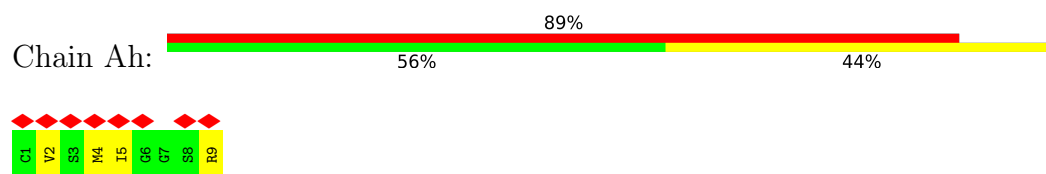
- Molecule 1: unknown peptide E



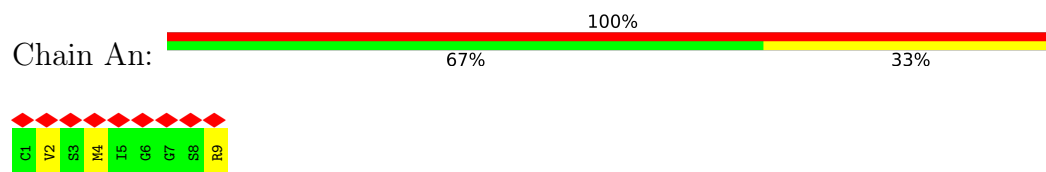
- Molecule 2: unknown peptide F



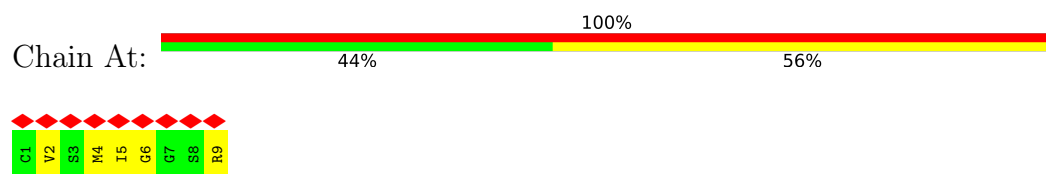
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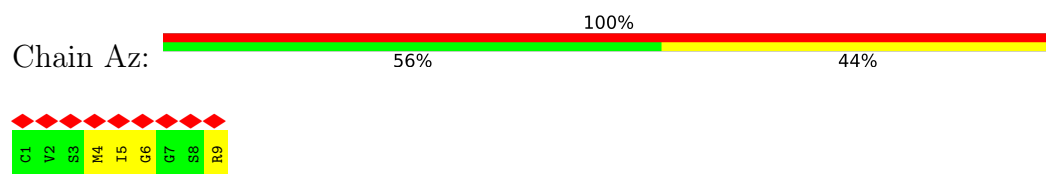
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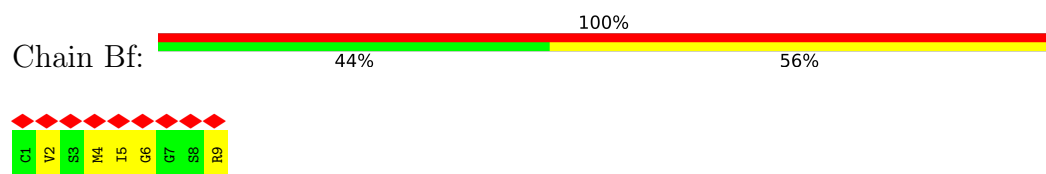
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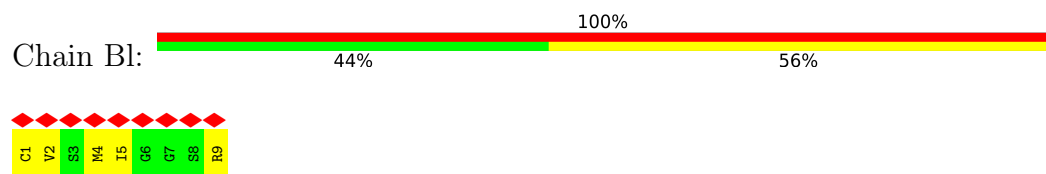
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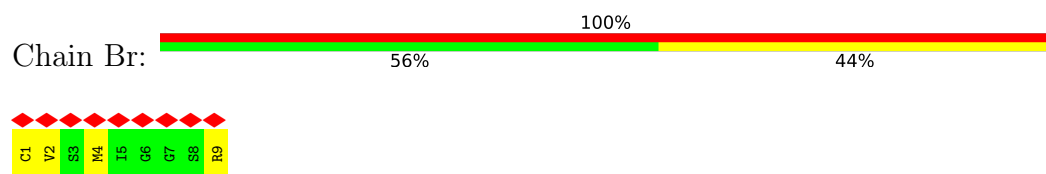
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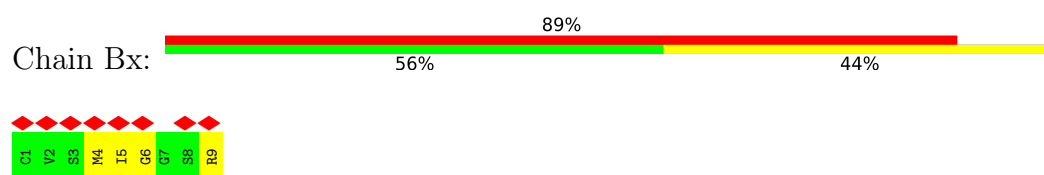
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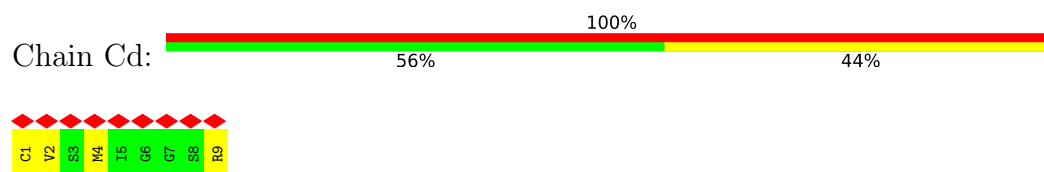
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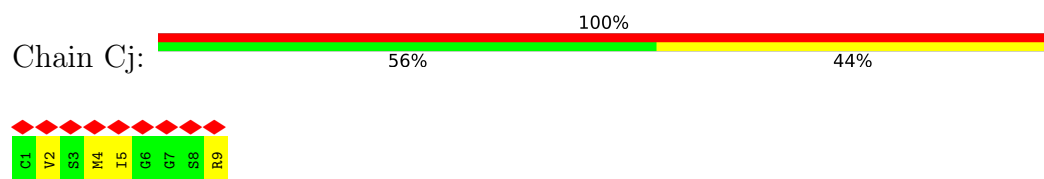
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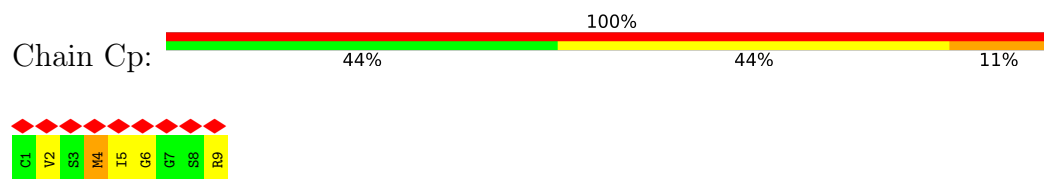
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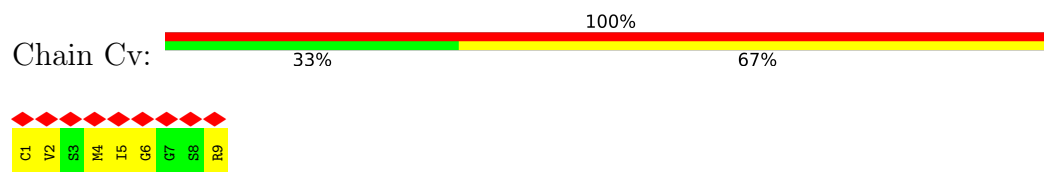
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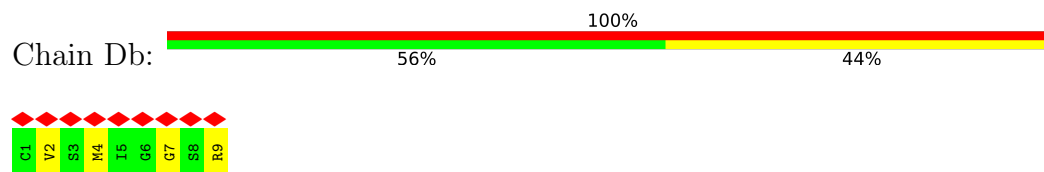
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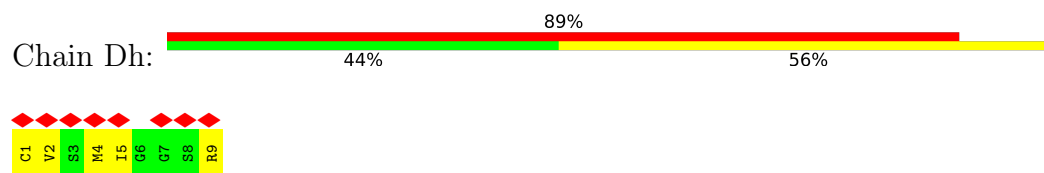
- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



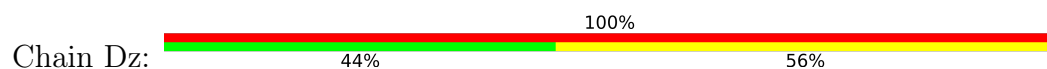
- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 2: unknown peptide F



- Molecule 3: unknown peptide G



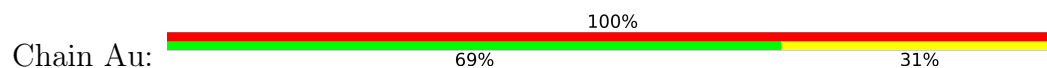
- Molecule 3: unknown peptide G



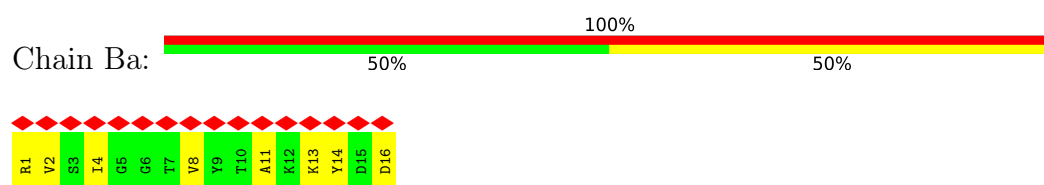
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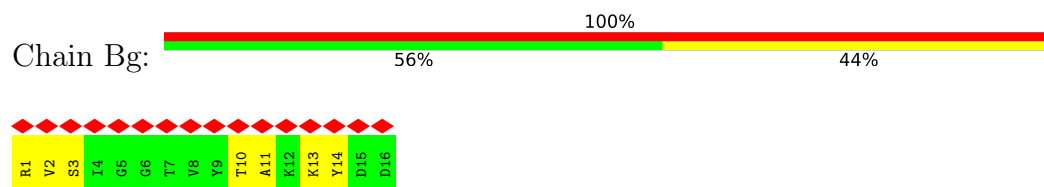
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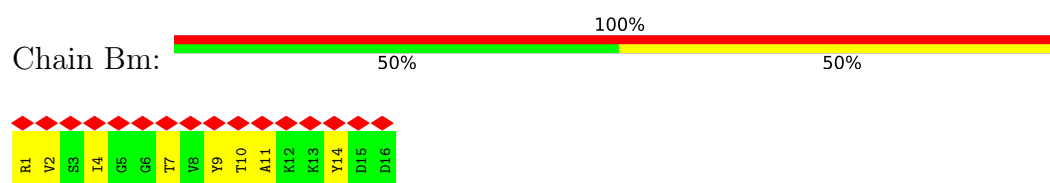
- Molecule 3: unknown peptide G



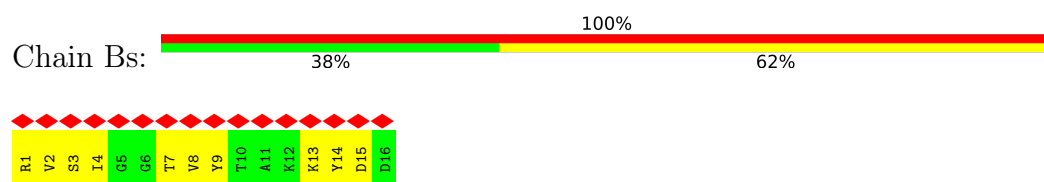
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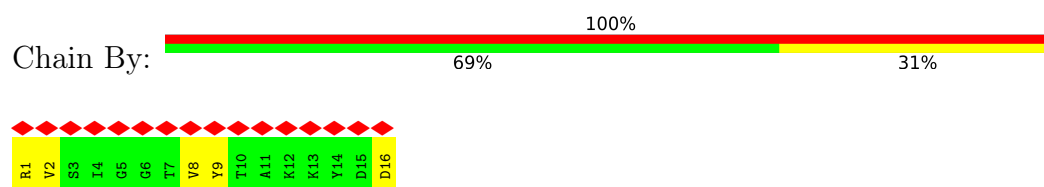
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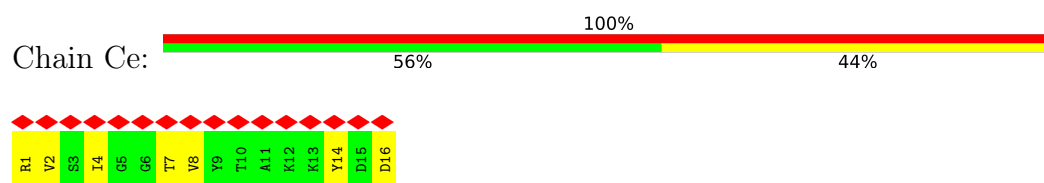
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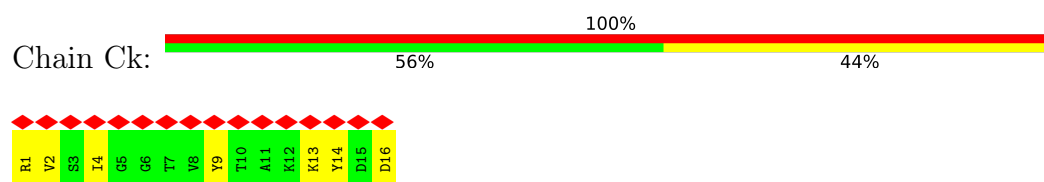
- Molecule 3: unknown peptide G



- 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



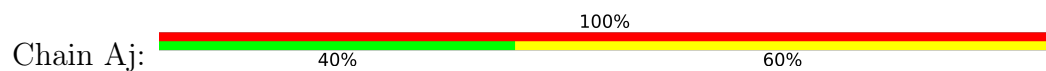
● Molecule 3: unknown peptide G



- 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



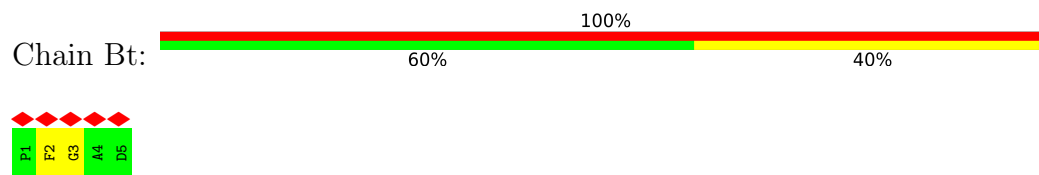
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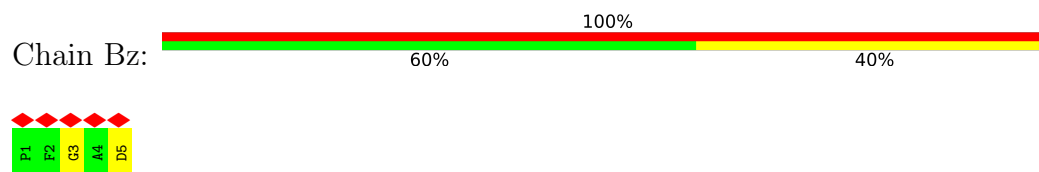
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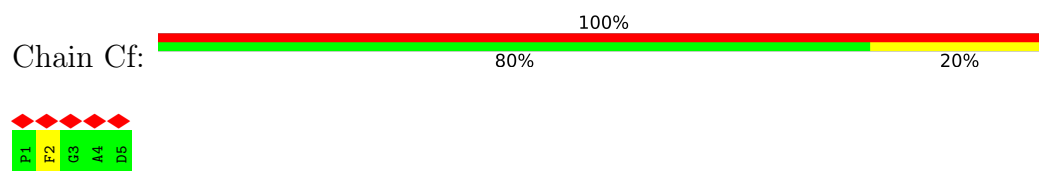
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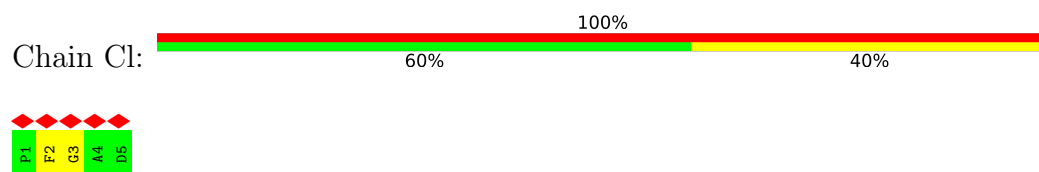
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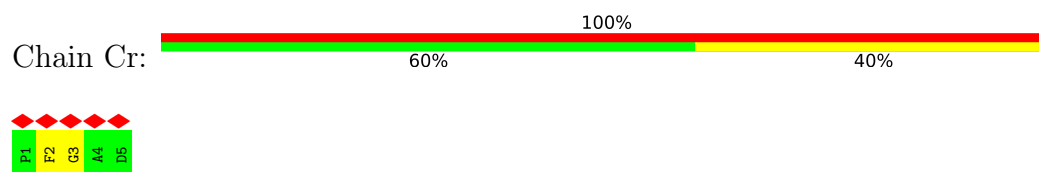
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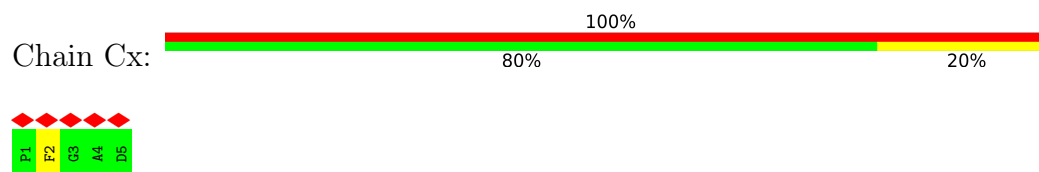
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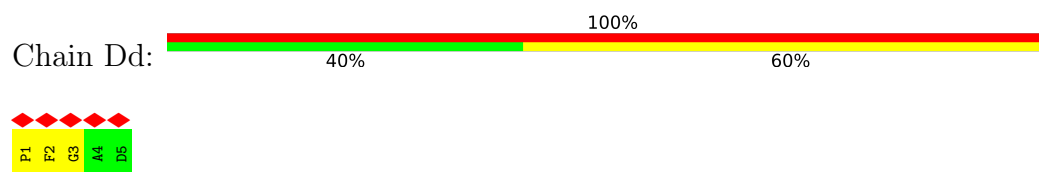
- Molecule 4: unknown peptide H



- Molecule 4: unknown peptide H

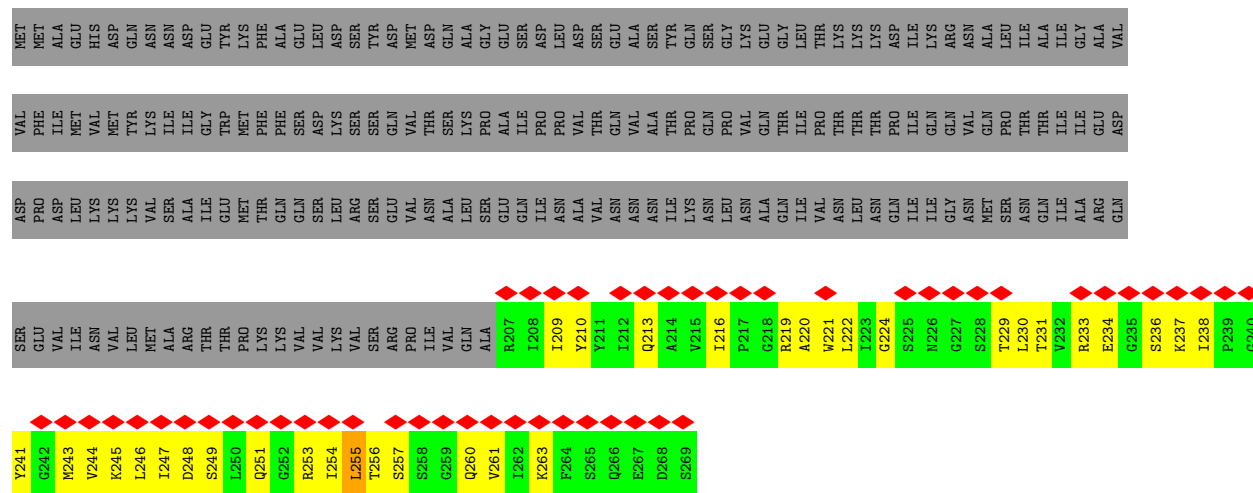


- Molecule 4: unknown peptide H

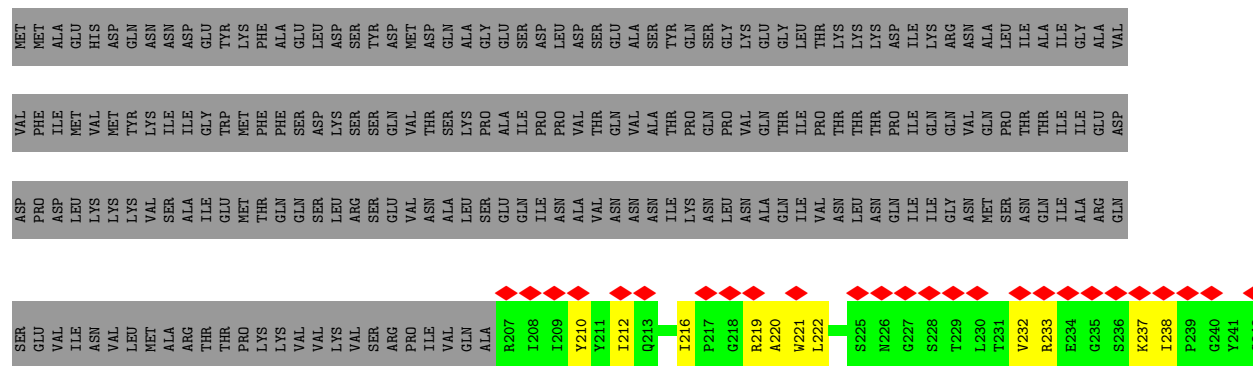


- Molecule 4: unknown peptide H

- Molecule 5: IcmG (DotF)

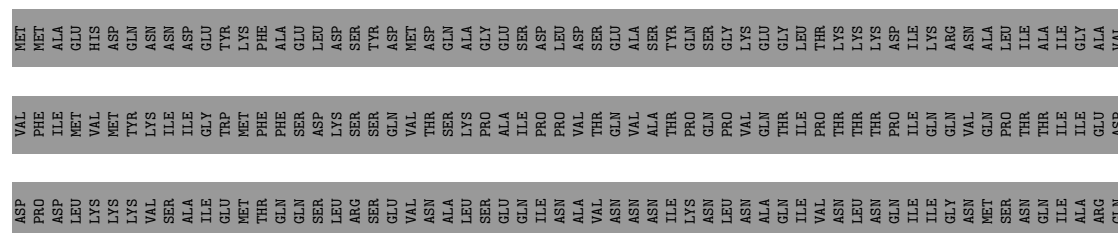


- Molecule 5: IcmG (DotF)

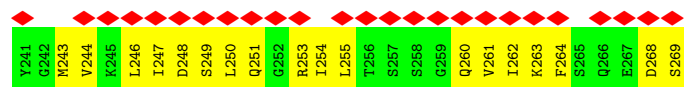
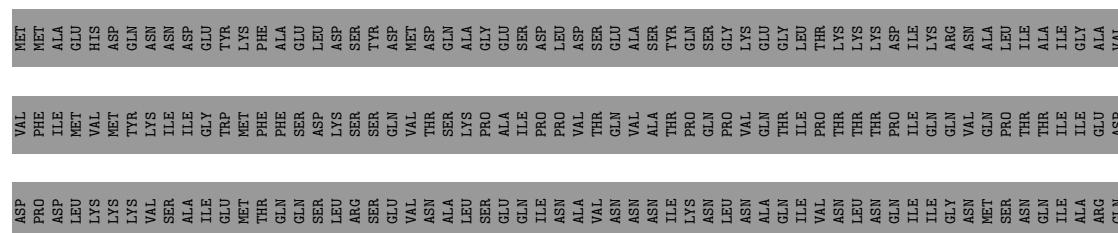




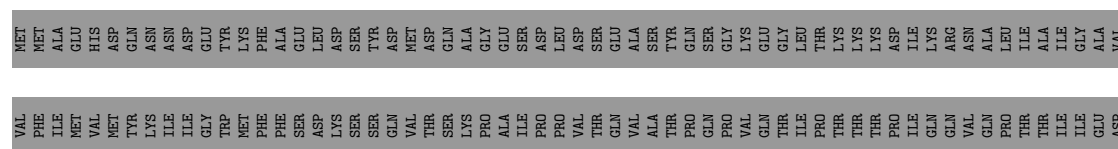
• Molecule 5: IcmG (DotF)

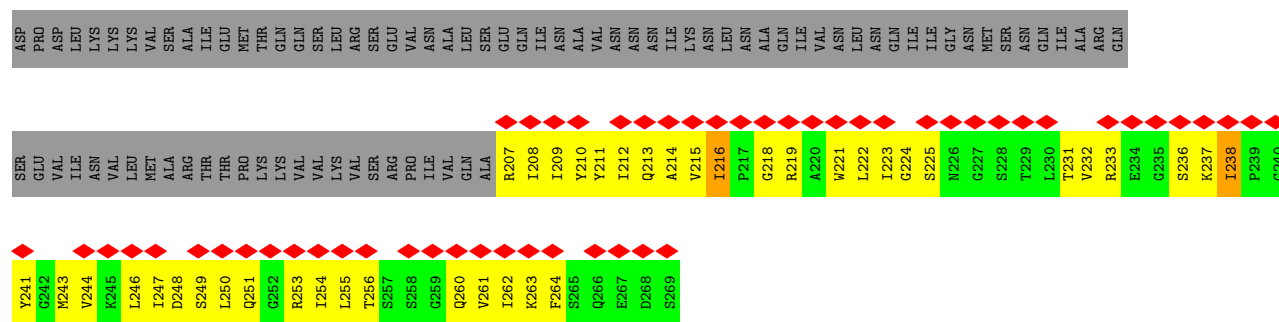


• Molecule 5: IcmG (DotF)

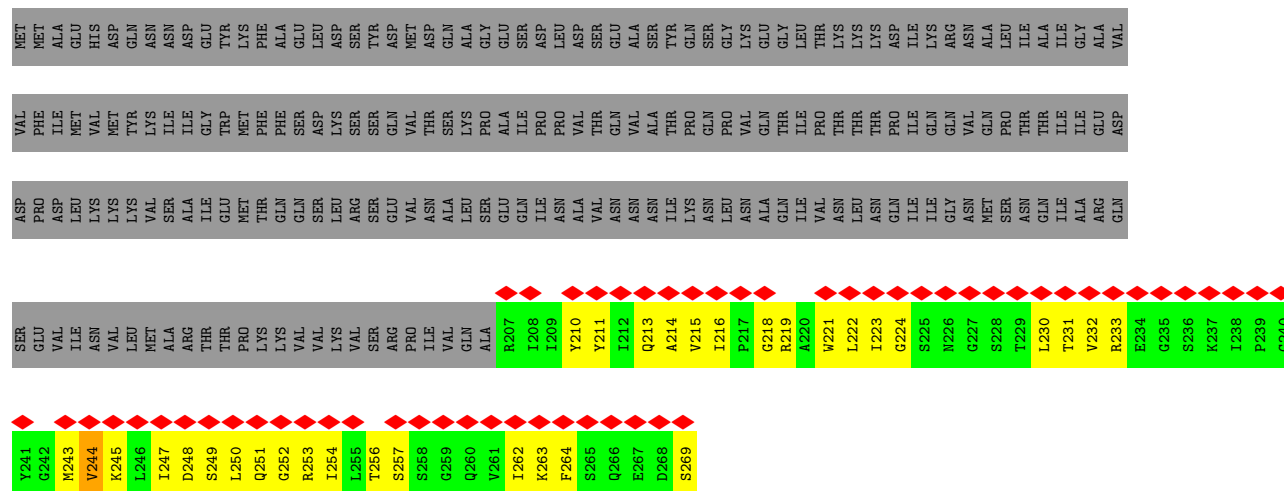


• Molecule 5: IcmG (DotF)

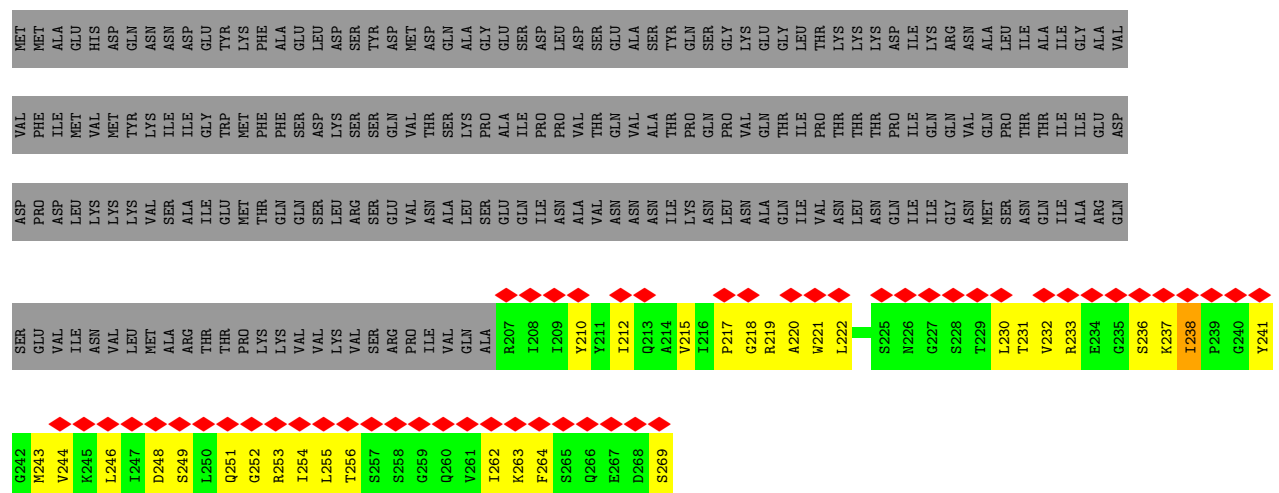




- Molecule 5: IcmG (DotF)



- Molecule 5: IcmG (DotF)

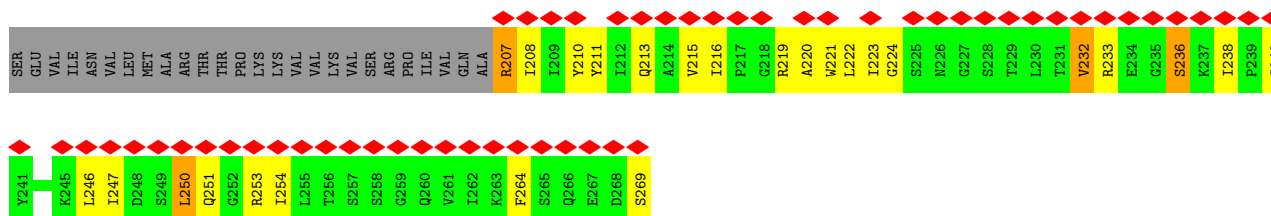


- Molecule 5: IcmG (DotF)





- Molecule 5: IcmG (DotF)

[illegible]

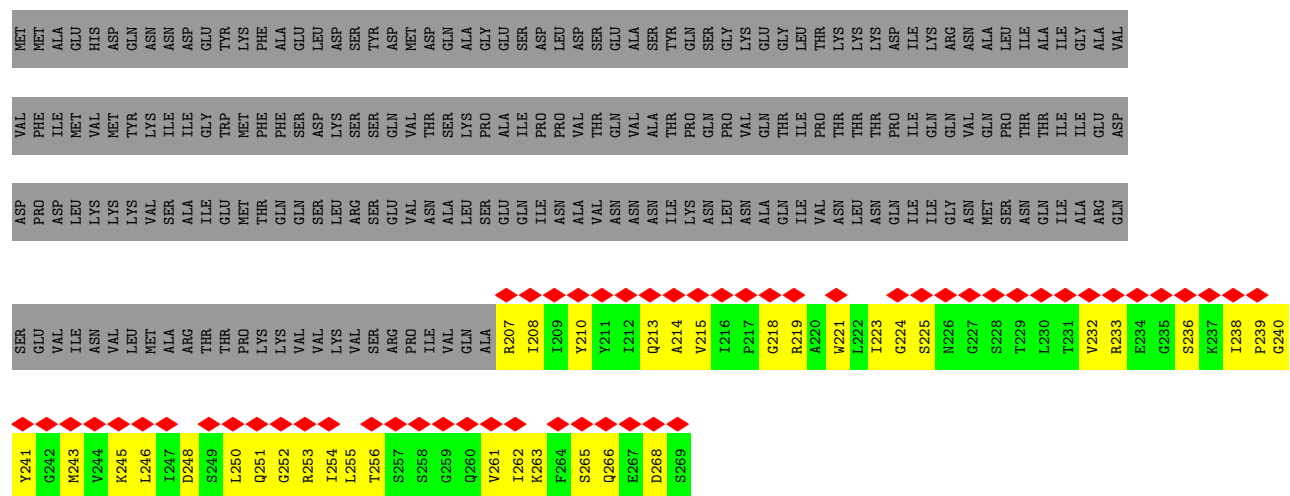
- Molecule 5: IcmG (DotF)



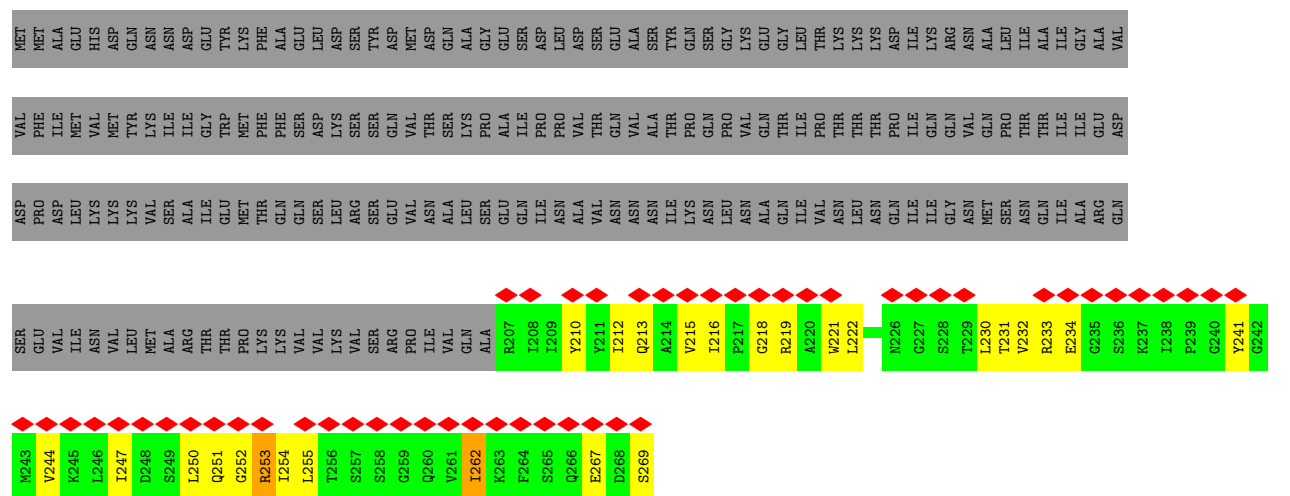
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- Molecule 5: IcmG (DotF)



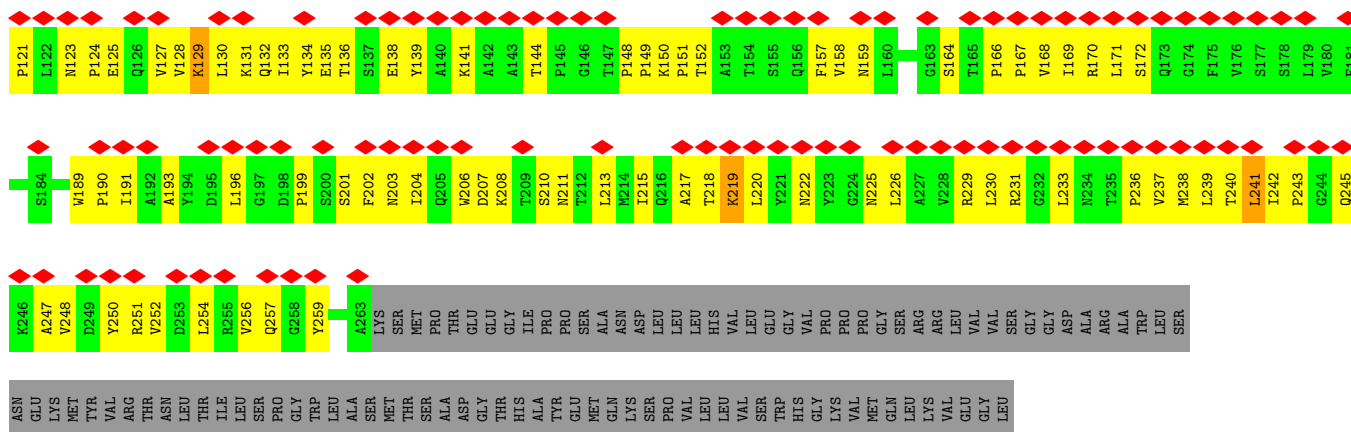
- Molecule 5: IcmG (DotF)



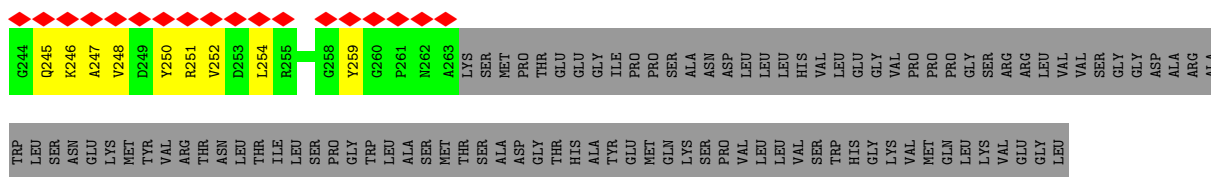
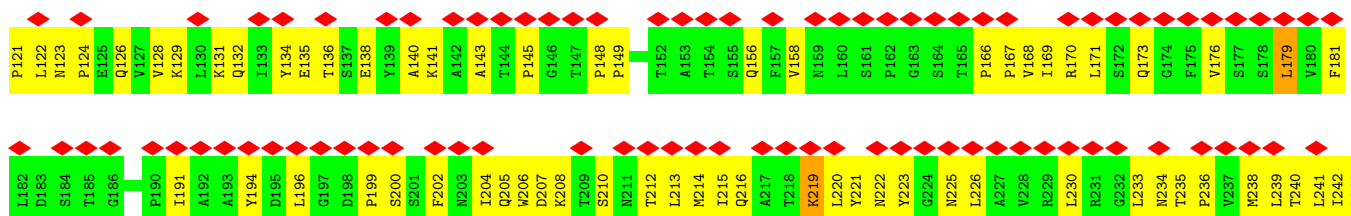
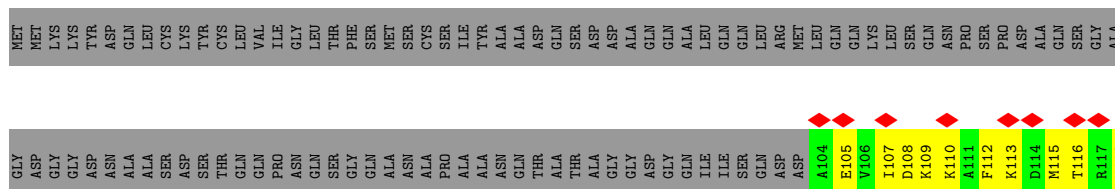
- Molecule 5: IcmG (DotF)



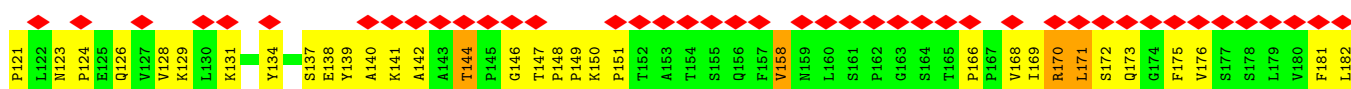
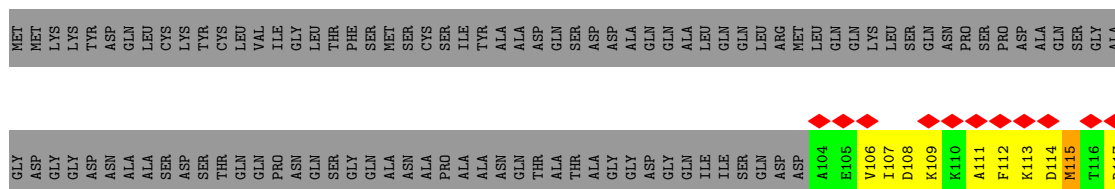
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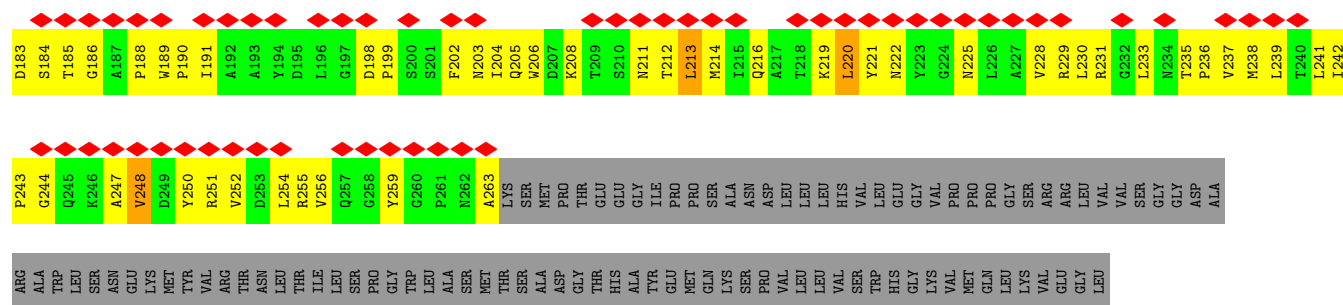


• Molecule 6: IcmK (DotH)

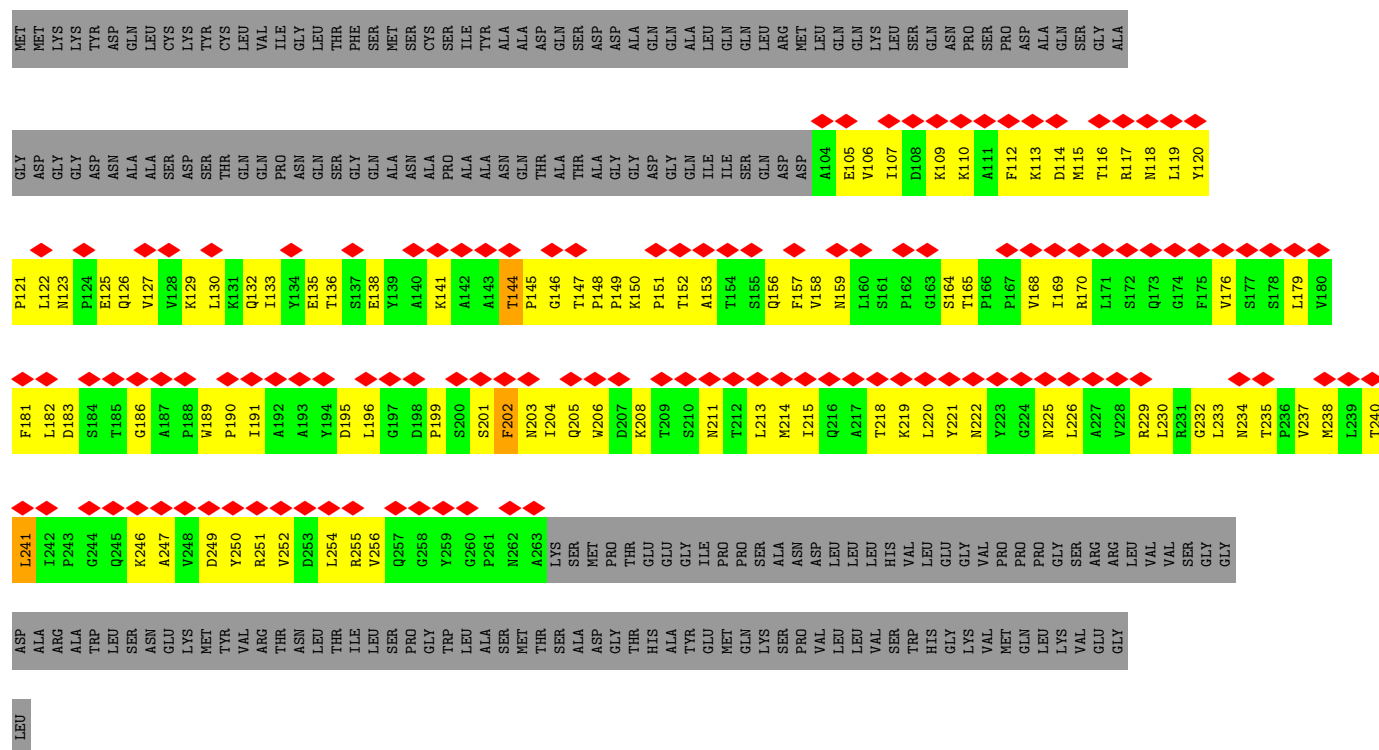


• Molecule 6: IcmK (DotH)

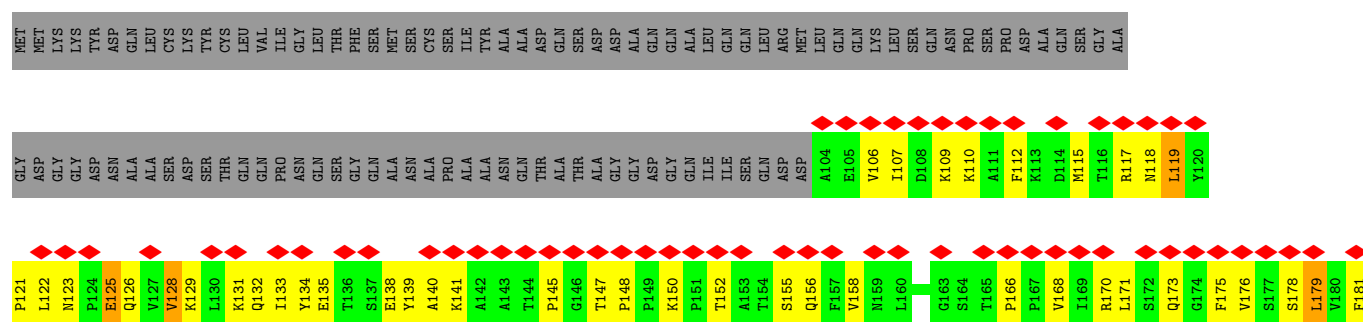




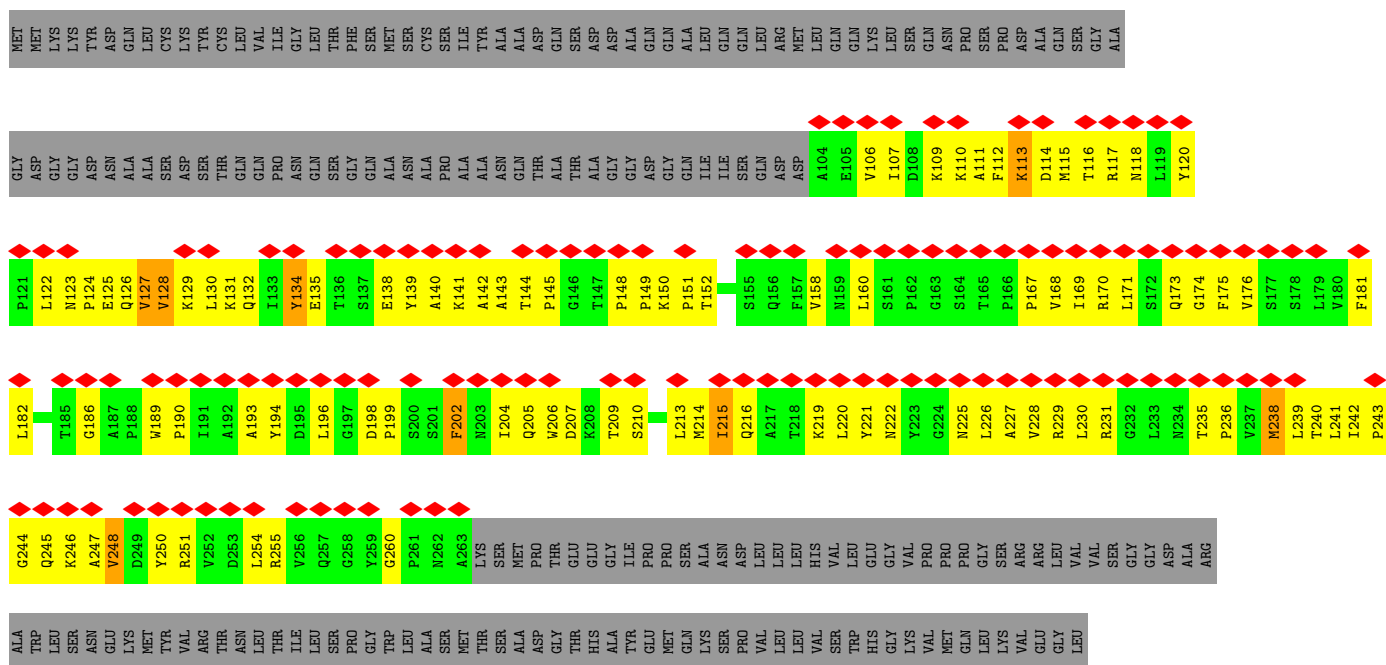
• Molecule 6: IcmK (DotH)



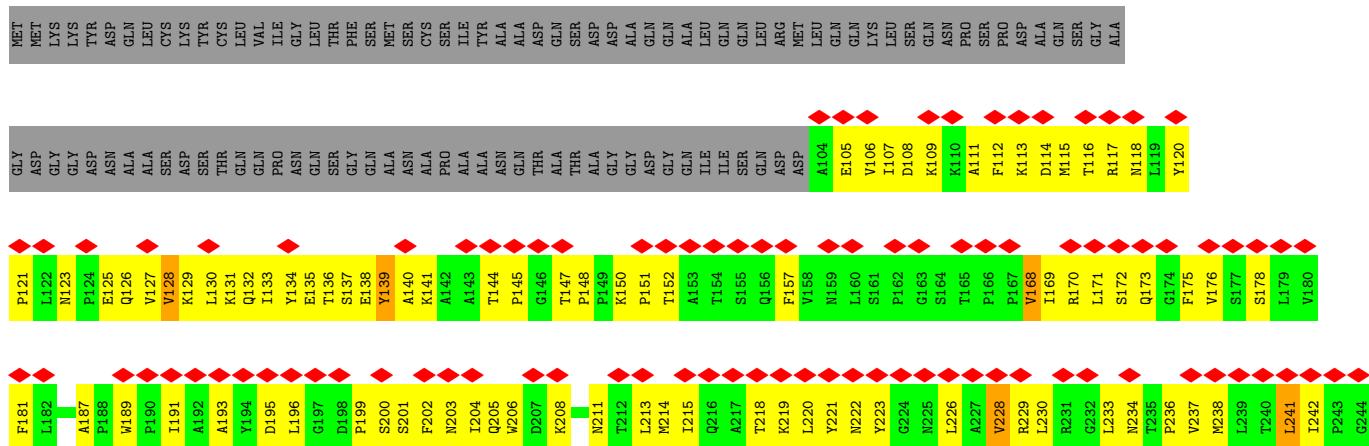
• Molecule 6: IcmK (DotH)



- Molecule 6: IcmK (DotH)



- Molecule 6: IcmK (DotH)



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LEU LEU
SER SER
ASN ASN
GLU GLU
LYS LYS
TRP TRP
MET MET
VAL VAL
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ASN ASN
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THR THR
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LEU LEU
SER SER
PRO PRO
GLY GLY
TRP TRP
LEU LEU
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SER SER
MET MET
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THR THR
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GLY GLY
LEU LEU

• Molecule 6: IcmK (DotH)

Chain Cn: 20% 32% 22% 56%

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LEU LEU
SER SER
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GLU GLU
LYS LYS
TRP TRP
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LEU LEU
THR THR
ILE ILE
LEU LEU
THR THR
PHE PHE
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LEU LEU
SER SER

• Molecule 6: IcmK (DotH)

Chain Ct: 21% 31% 23% 56%

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

GLY ASP
GLY GLY
ASP ASP
ASN ASN
ALA ALA
ALA ALA
SER SER
ASP ASP
THR THR
THR THR
GLN GLN
PRO PRO
ASN ASN
GLN GLN
SER SER
GLY GLY
THR THR
GLY GLY
GLN GLN
ALA ALA
SER SER
THR THR
ALA ALA
ASP ASP
GLY GLY
ASP ASP
GLY GLY
ILE ILE
ILE ILE
ASP ASP
MET MET
LEU LEU
GLN GLN
VAL VAL
E104
E105
V106
I107
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K110
A111
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K113
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Y120

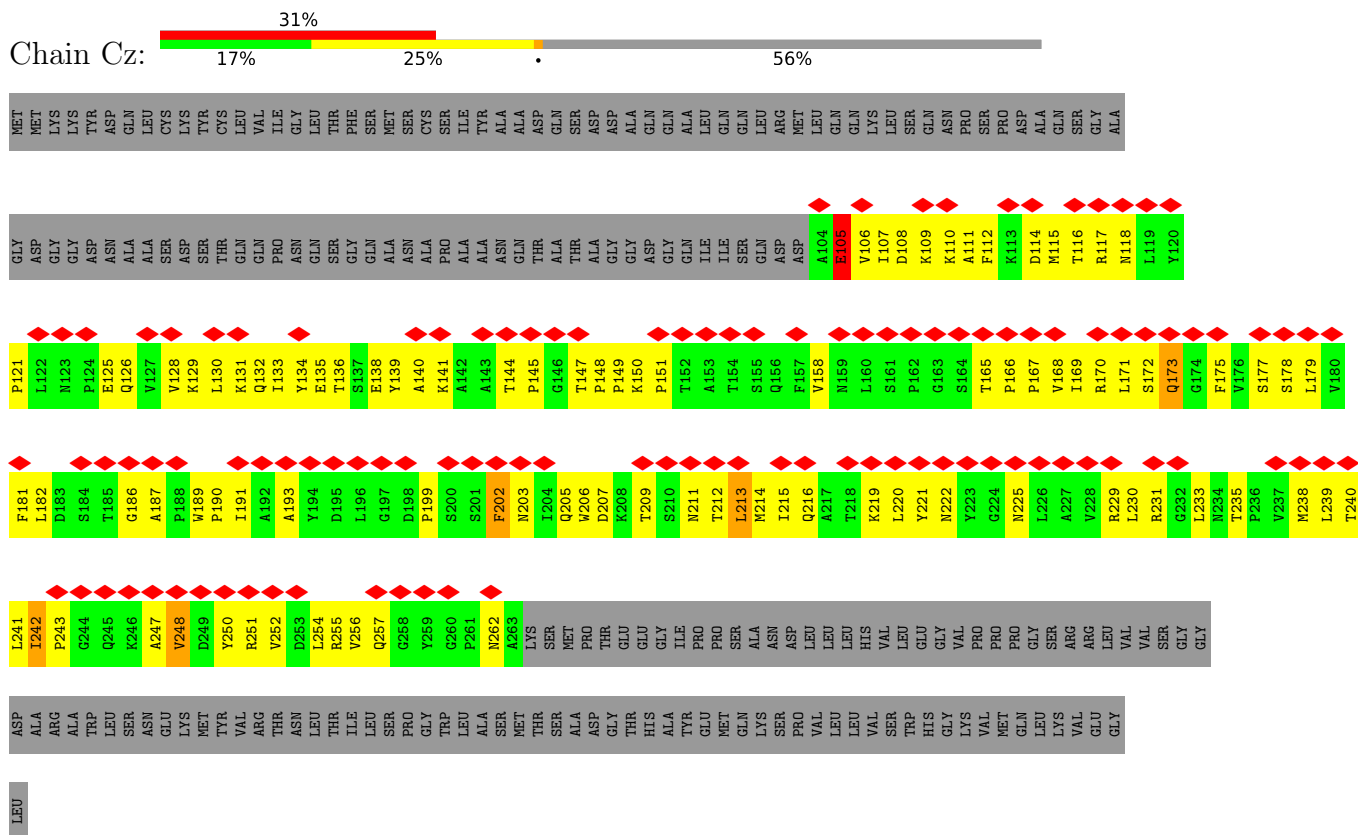
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Y134
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E138
Y139
S201
F202
K203
A142
A143
T144
P145
G146
T147
P148
P149
K150
P151
T152
A153
S155
T154
S155
Q156
L220
F157
V158
N159
S161
P162
G163
S164
T165
P166
P167
V168
I169
R170
L171
S172
Q173
G174
F175
V176
S177
L179
V180
F181

L182
D183
S184
T185
W189
P190
I191
A192
A193
Y194
D195
L196
G197
D198
P199
S200
F202
N203
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Q205
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M214
I215
Q216
A217
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K219
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Y221
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Y223
G224
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L226
A227
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L241
I242
P243

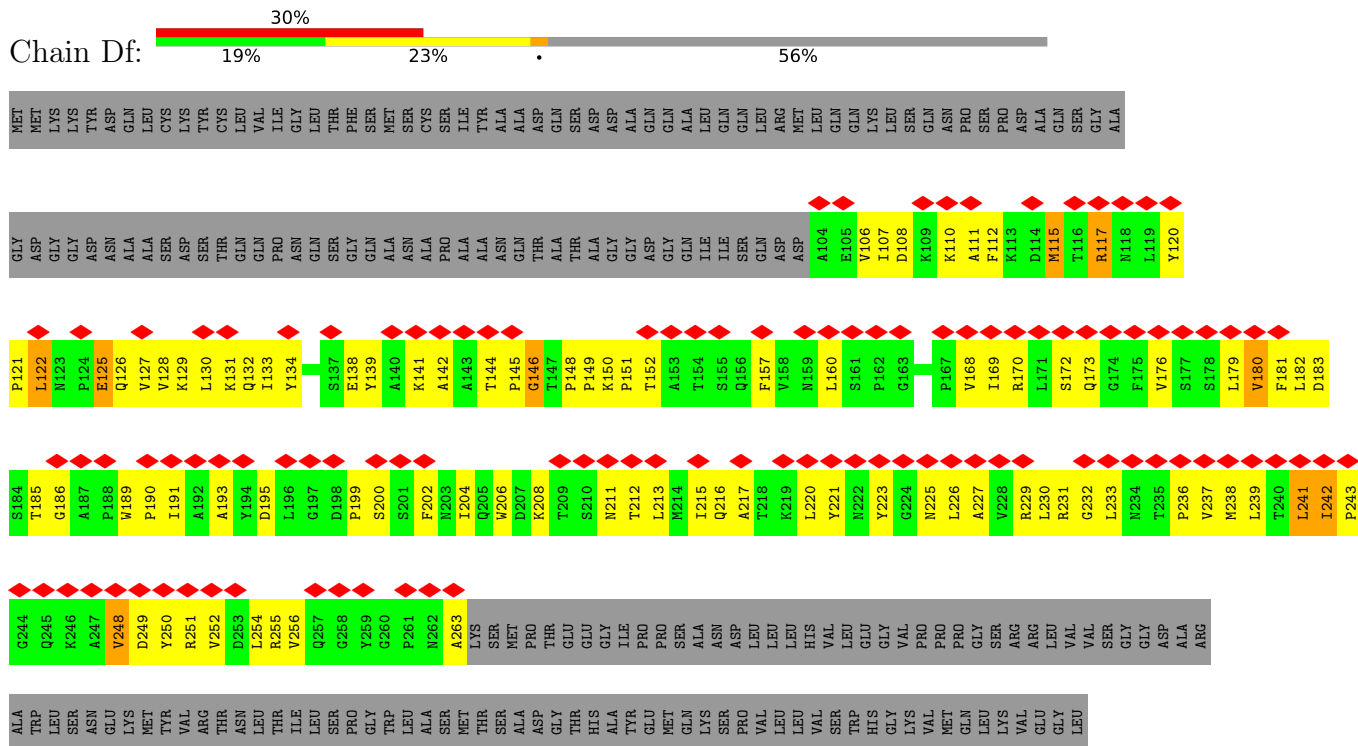
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D253
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R255
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Y259
N262
A263
LYS SER
MET MET
PRO PRO
THR THR
GLU GLU
GLY GLY
HIS HIS
ALA ALA
TYR TYR
MET MET
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VAL VAL
LEU LEU
HIS HIS
VAL VAL
SER SER
TRP TRP
HIS HIS
GLY GLY
LYS LYS
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VAL VAL
PRO PRO
PRO PRO
GLY GLY
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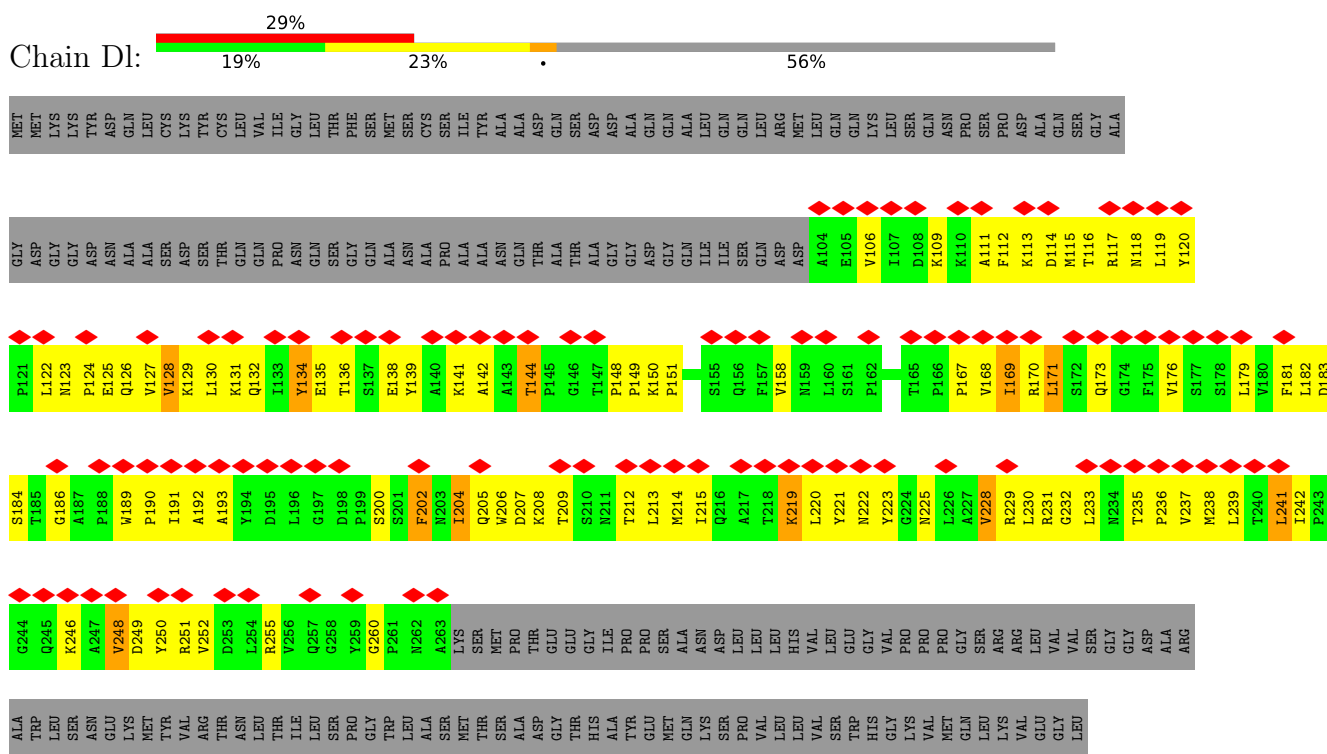
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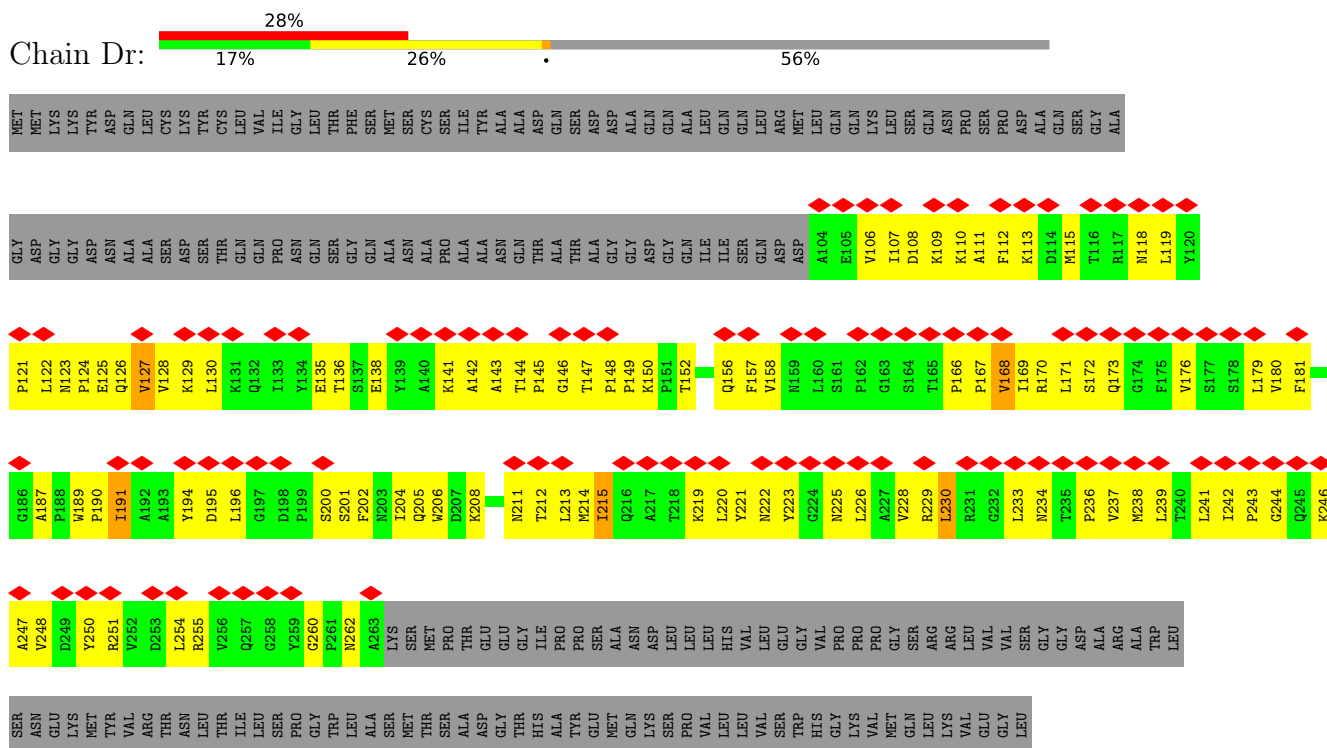
- Molecule 6: IcmK (DotH)



- Molecule 6: IcmK (DotH)



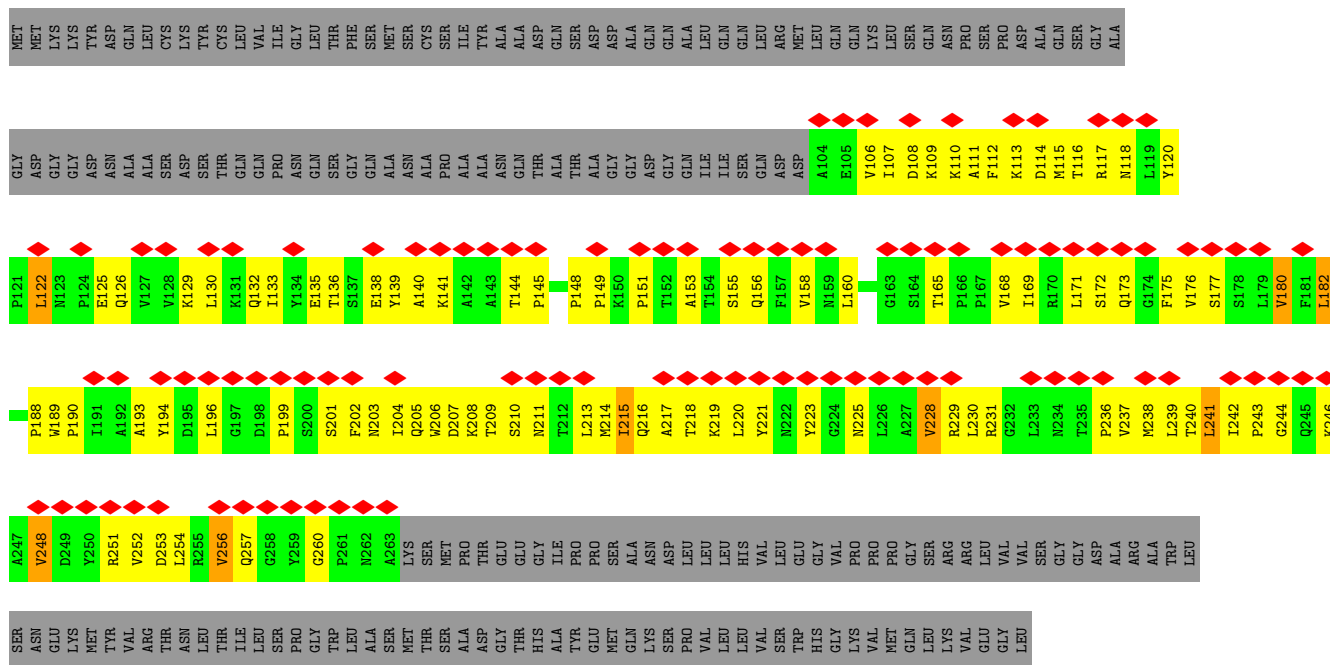
- Molecule 6: IcmK (DotH)



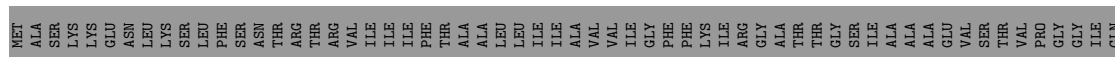
- Molecule 6: IcmK (DotH)



- Molecule 6: IcmK (DotH)



- Molecule 7: IcmE (DotG)



- Molecule 7: IcmE (DotG)



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

Chain Ei:  95%

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

Chain El: 97%

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

Chain Eq:  95%

[illegible]

- Molecule 7: IcmE (DotG)



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



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

[illegible]



- Molecule 7: IcmE (DotG)

[illegible]

- Molecule 7: IcmE (DotG)

Chain Fh:  96%





- Molecule 7: IcmE (DotG)

Chain Fj: 96%

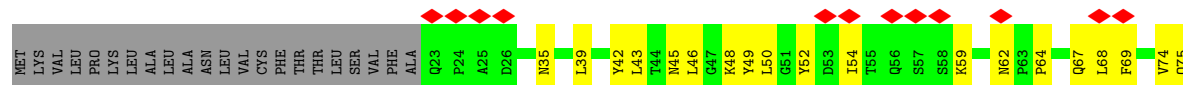


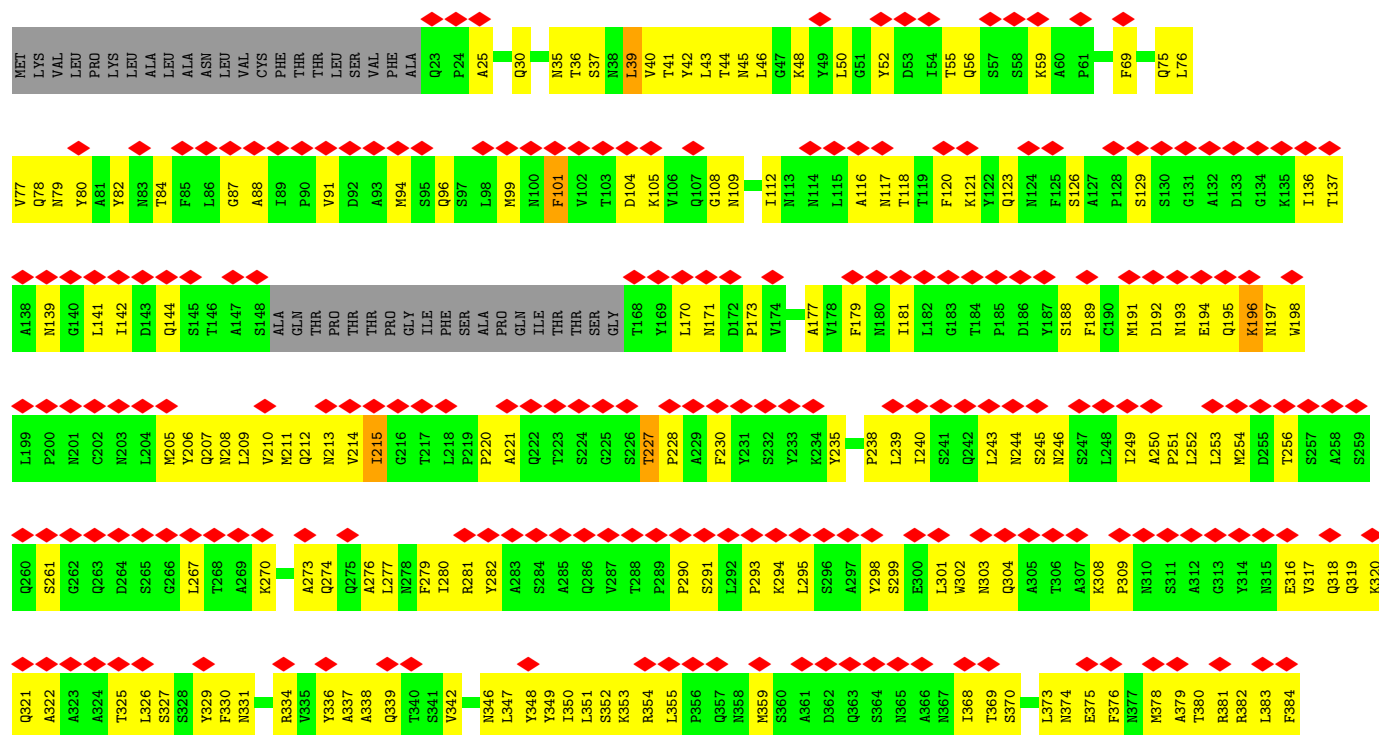
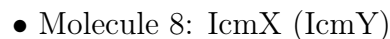
- Molecule 7: IcmE (DotG)

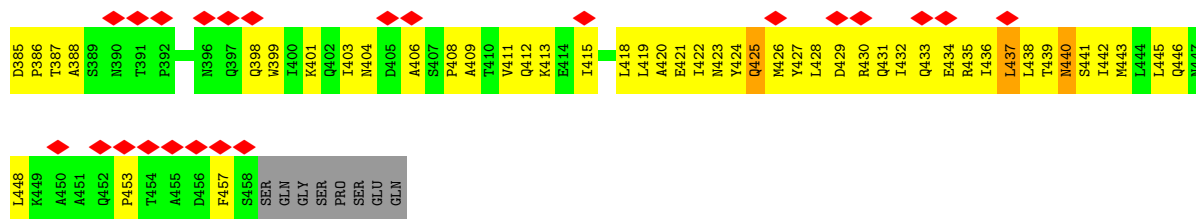
Chain Fk: 96%



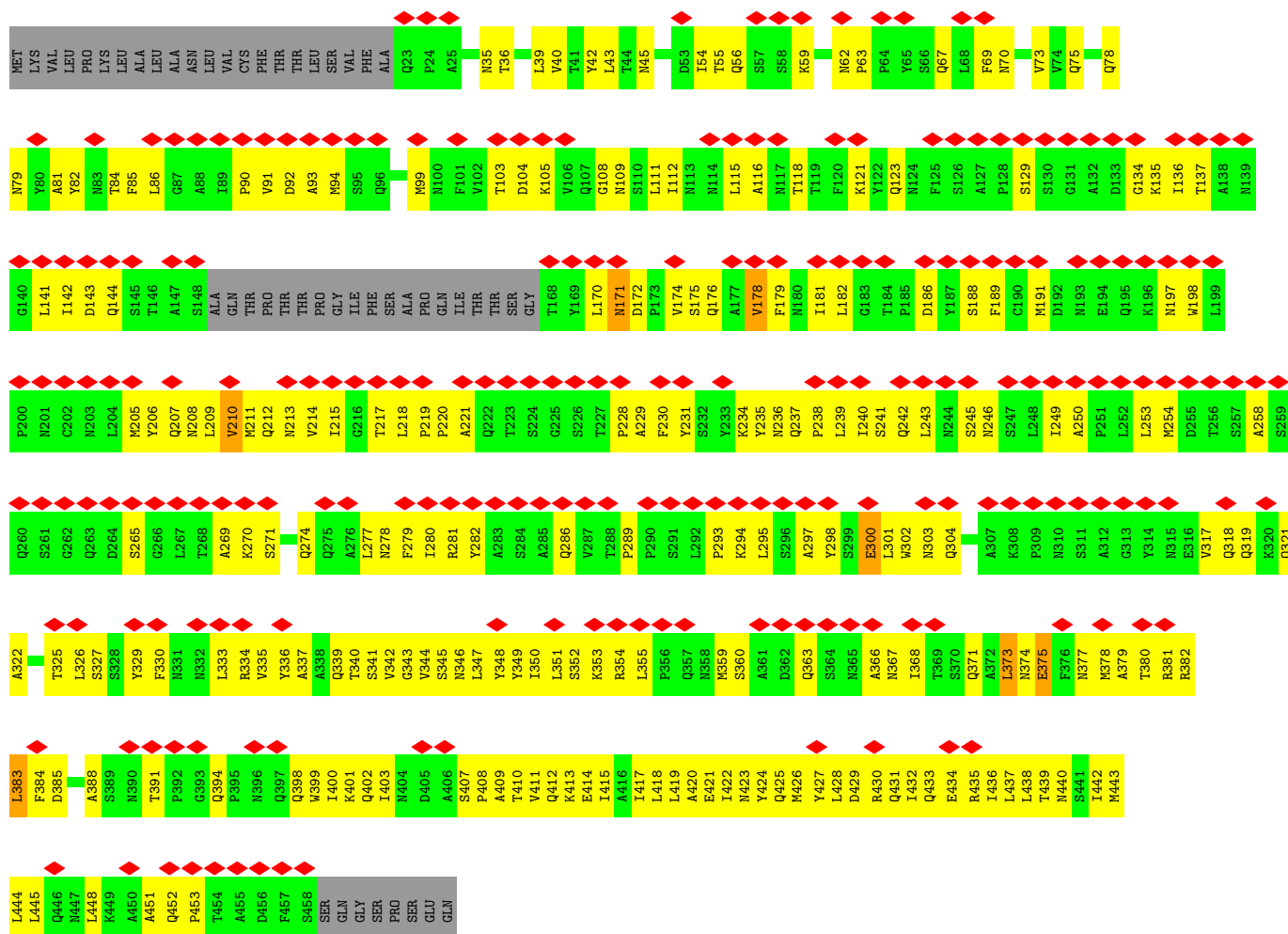
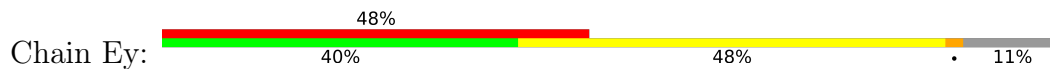
- Molecule 8: IcmX (IcmY)



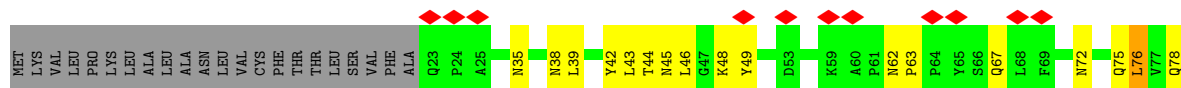
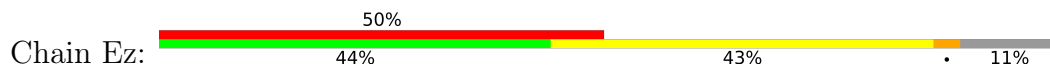


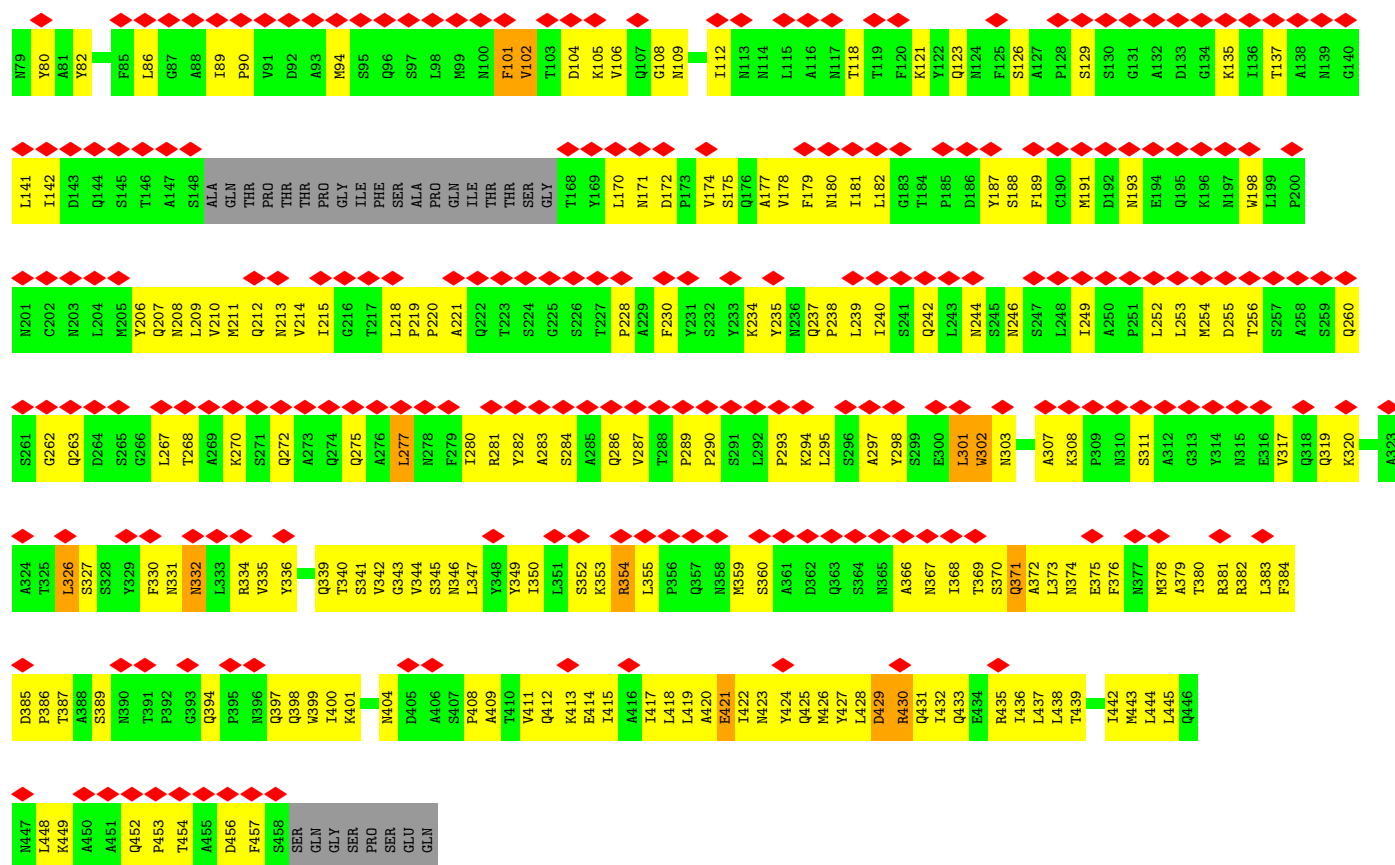


• Molecule 8: IcmX (IcmY)

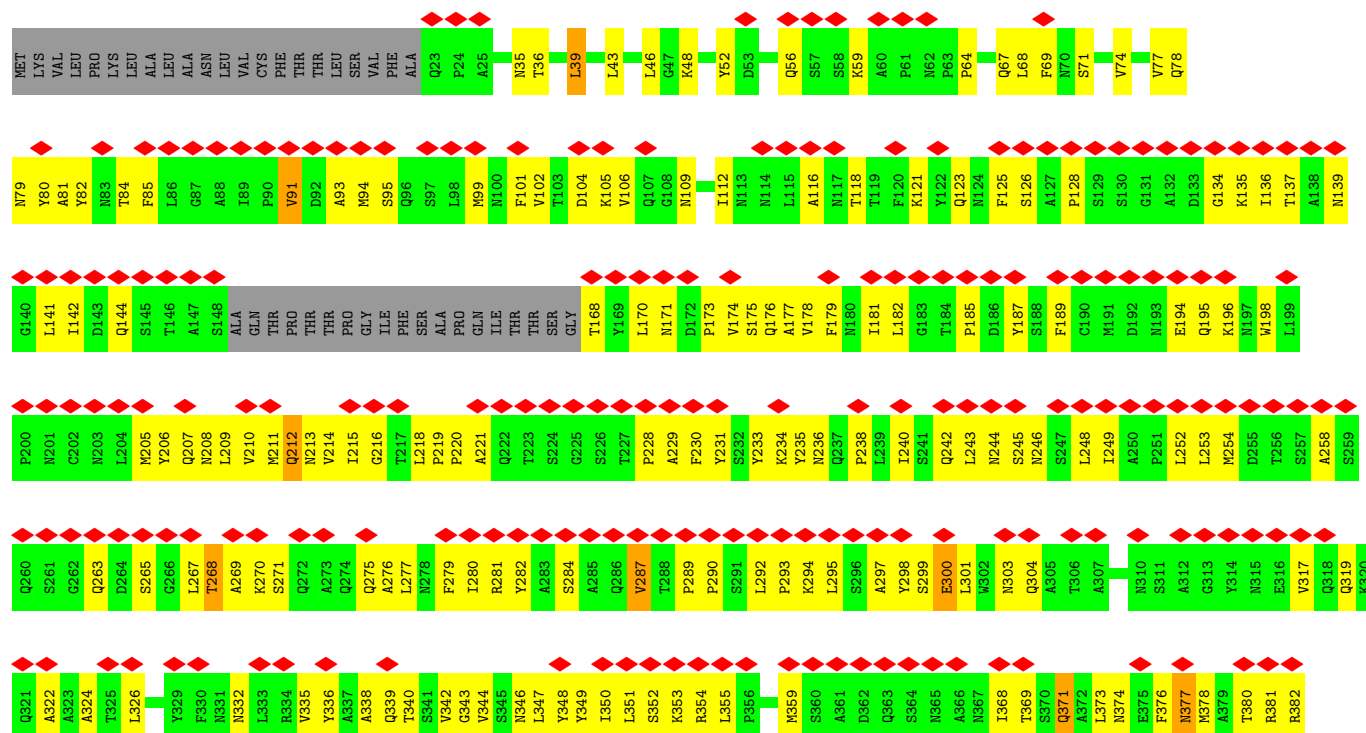


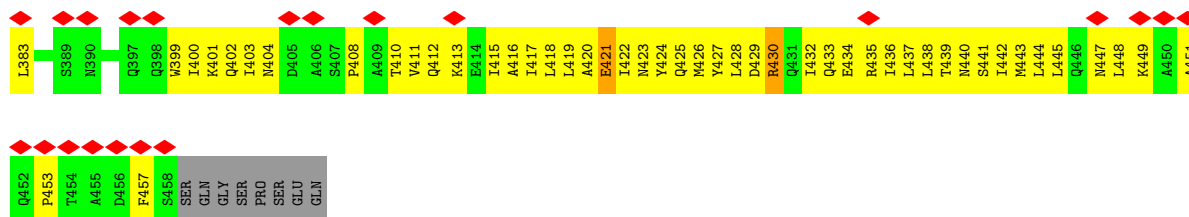
• Molecule 8: IcmX (IcmY)



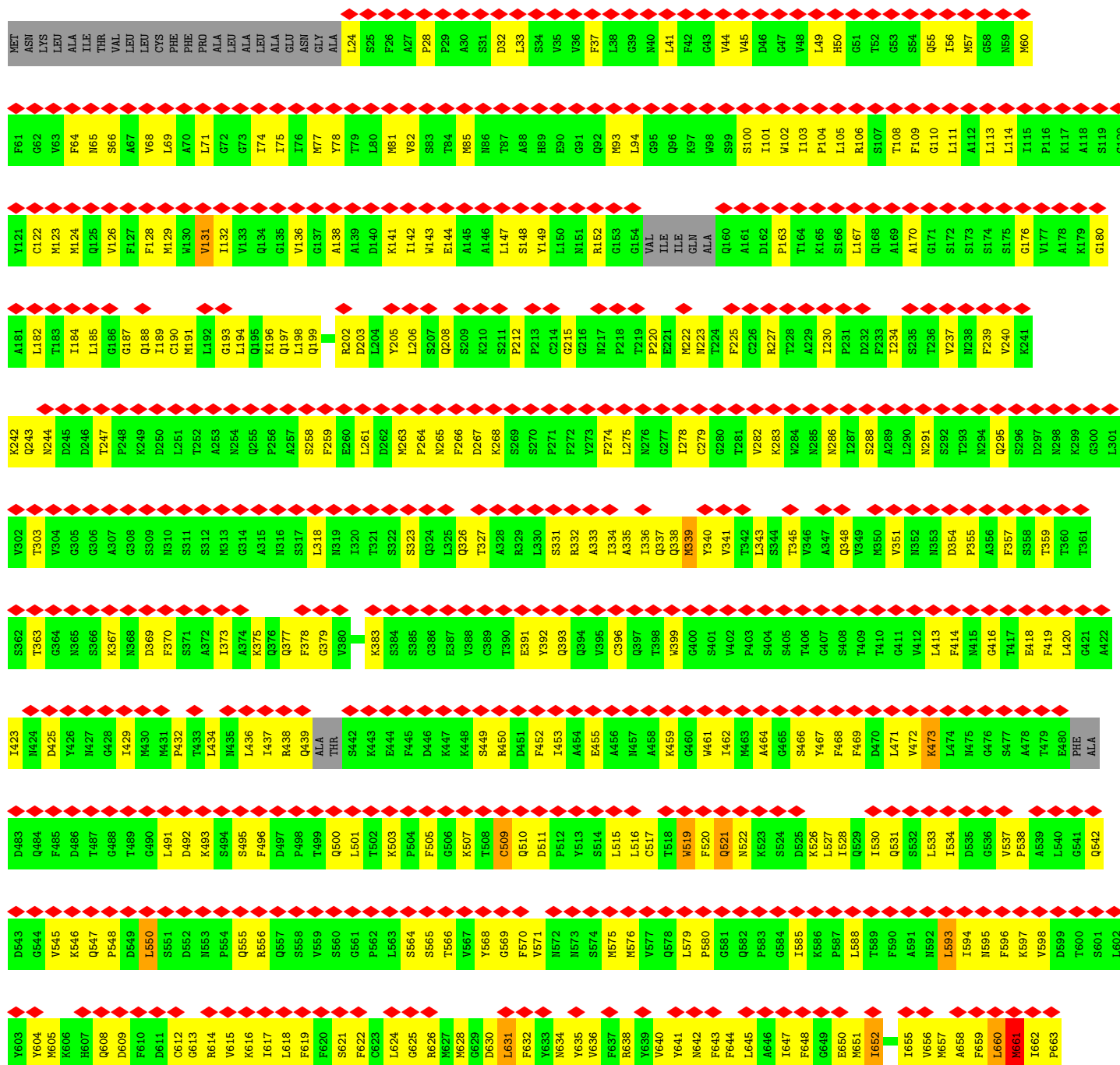
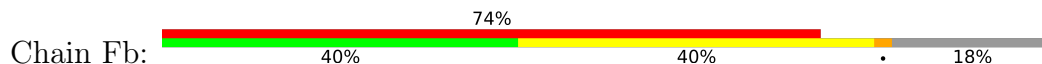


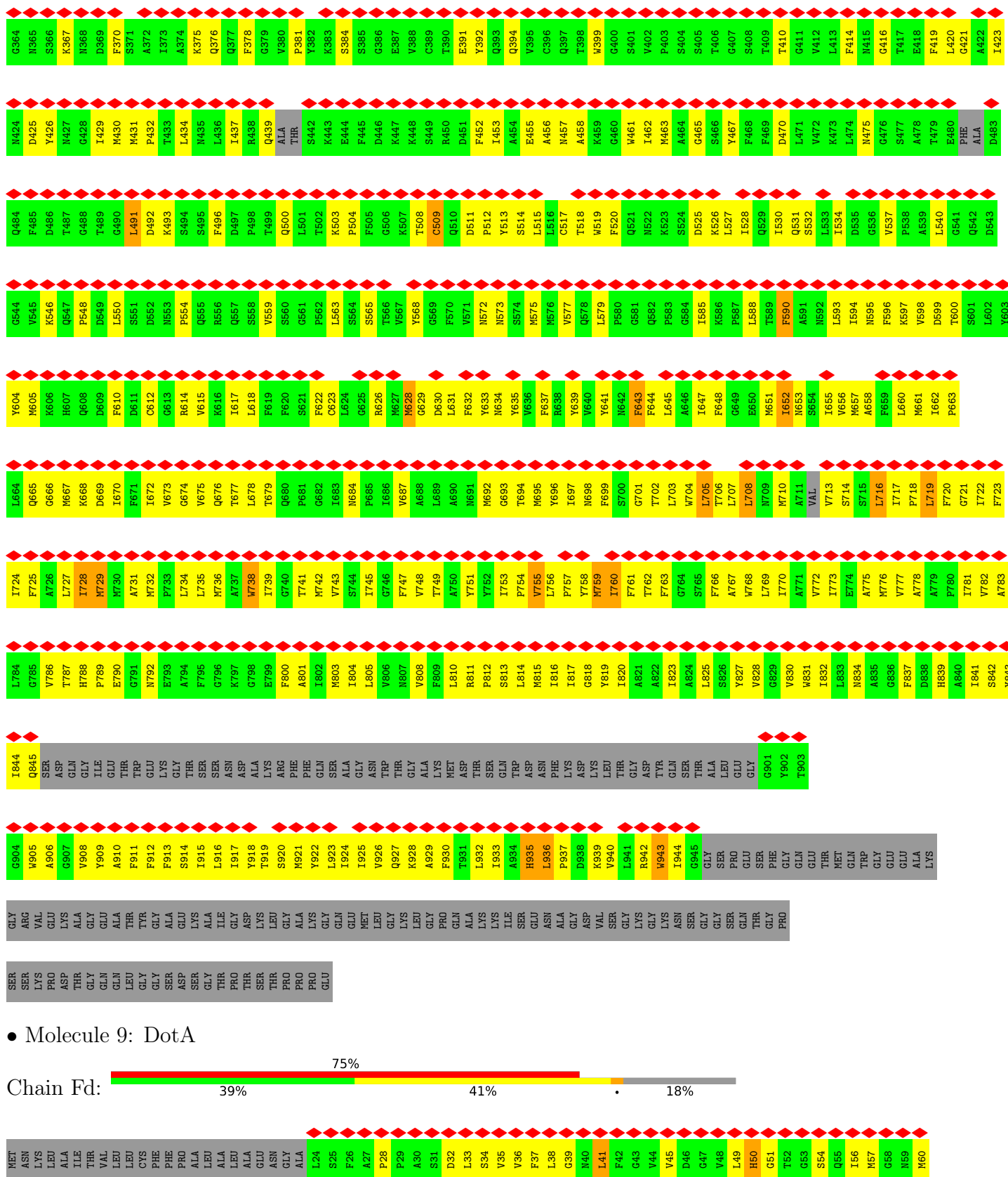
• Molecule 8: IcmX (IcmY)





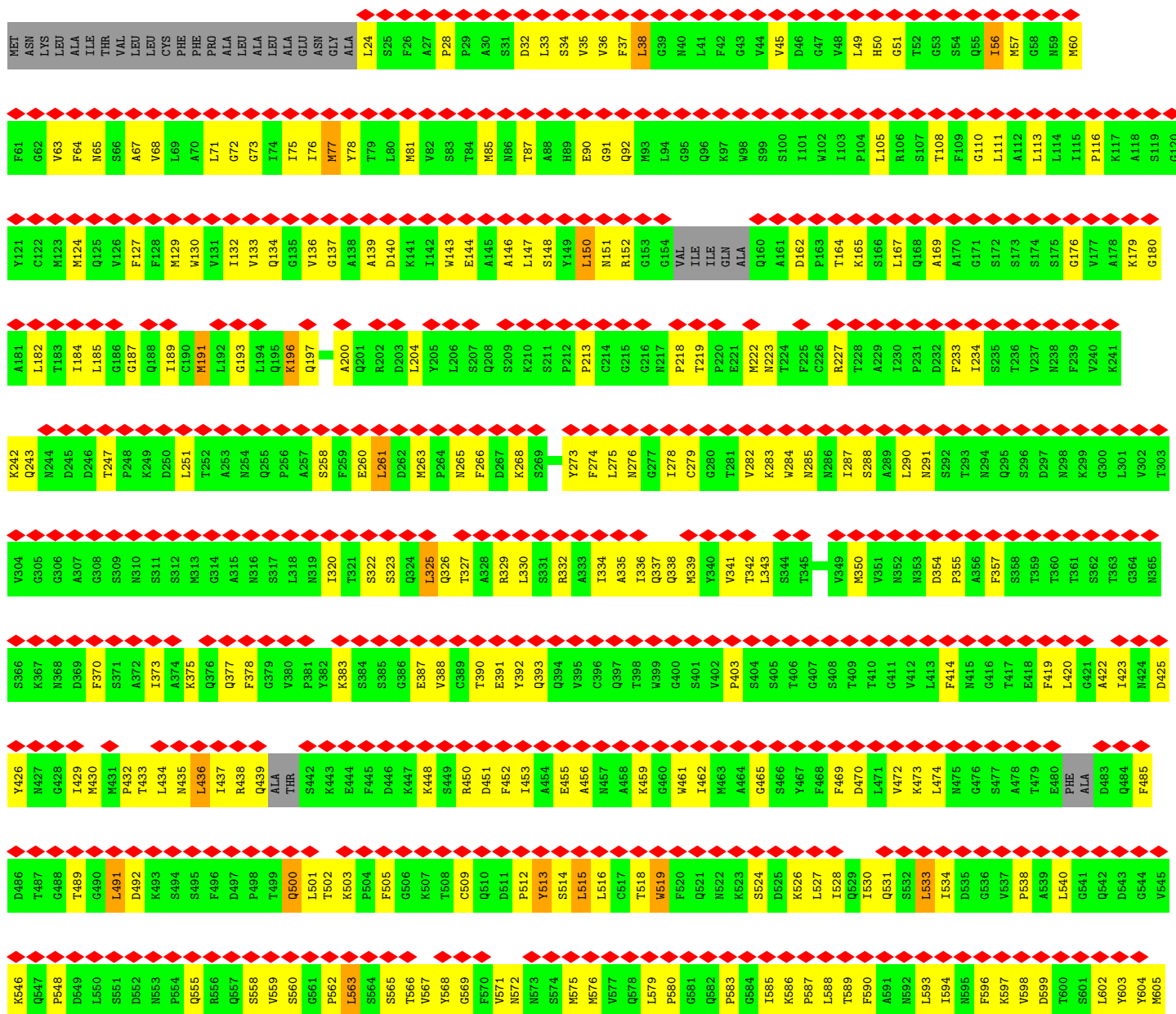
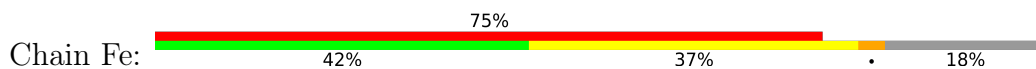
• Molecule 9: DotA





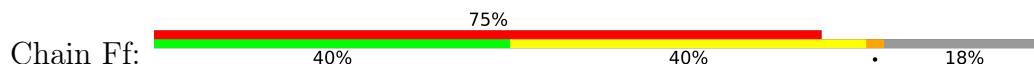
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L727	I728	M729	K730	A731	M732	P733	L734	L735	M736	A737	W738	I739	G740	T741	M742	V743	S744	I745	G746	F747	W748	T749	A750	Y751	Y752	I753	P754	Y755	L756	P757	Y758	M759	I760	F761	T762	G763	G764	S765	F766	A767	L768	W769	L770	I771	A771	W772	I773	E774	A775	M776	V777	A778	F779	P780	I781	V782	A783	L784	G785	V786			
M667	K668	D669	F670	D671	L672	M673	G674	V675	D676	T677	L678	T679	D680	P681	I682	L683	M684	P685	I686	V687	A688	L689	M690	N691	M692	G693	S813	T694	M695	Y696	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	M651	I652	N653	S654	L655	V656	M657	A658	F659	L660	R661	I662	F663	L664	G665	G666				
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	N642	F643	Q581	N582	Q582	P583	S584	G584	S585	K586	L586	P587	W709	M710	A711	VAL	W713	S714	S715	L716	I717	F718	L719	F720	G721	I722	F723	I724	F725	A726
H607	Q608	D609	F610	D611	C612	M613	R614	V615	K616	L617	L618	F619	F620	S621	F622	C623	L624	G625	R626	N627	M628	D629	D630	L631	F632	Y633	N634	G635	V636	F637	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	M651	I652	N653	S654	L655	V656	M657	A658	F659	L660	R661	I662	F663	L664	G665	G666				
M667	K668	D669	F670	D671	L672	M673	G674	V675	D676	T677	L678	T679	D680	P681	I682	L683	M684	P685	I686	V687	A688	L689	M690	N691	M692	G693	S813	T694	M695	Y696	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	M651	I652	N653	S654	L655	V656	M657	A658	F659	L660	R661	I662	F663	L664	G665	G666				
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	P754	Y755	L756	P757	Y758	M759	I760	F761	T762	G763	G764	S765	F766	A767	L768	W769	L770	I771	A771	W772	I773	E774	A775	M776	V777	A778	F779	P780	I781	V782	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	L812	S813	L814	M815	L816	I817	G818	Y819	I760	F761	A821	A822	L823	A824	L825	S826	Y827	W828	G829	W830	W831	L832	L833	N834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L784	G785	V786	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	K195	K196	Q199	R202	D203	L204	Y205	L206	S207	S211	P212	P213	C214	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	F271	P272	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	G299	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	D423	N424	D425	Y426				
N427	G428	I429	M430	M431	P432	T433	L434	M435	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	L474	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	Y519	F520	Q521	N522	K523	S524	D525	K526	L527	Y528	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	N642	F643	Q581	N582	Q582	P583	S584	G584	S585	K586	L586	P587	W709	M710	A711	VAL	W713	S714	S715	L716	I717	F718	L719	F720	G721	I722	F723	I724	F725	A726
H607	Q608	D609	F610	D611	C612	M613	R614	V615	K616	L617	L618	F619	F620	S621	F622	C623	L624	G625	R626	N627	M628	D629	D630	L631	F632	Y633	N634	G635	V636	F637	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	M651	I652	N653	S654	L655	V656	M657	A658	F659	L660	R661	I662	F663	L664	G665	G666				
M667	K668	D669	F670	D671	L672	M673	G674	V675	D676	T677	L678	T679	D680	P681	I682	L683	M684	P685	I686	V687	A688	L689	M690	N691	M692	G693	S813	T694	M695	Y696	R638	Y639	V640	Y641	N642	F643	F644	L645	A646	I647	F648	G649	E650	M651	I652	N653	S654	L655	V656	M657	A658	F659	L660	R661	I662	F663	L664	G665	G666				
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	P754	Y755	L756	P757	Y758	M759	I760	F761	T762	G763	G764	S765	F766	A767	L768	W769	L770	I771	A771	W772	I773	E774	A775	M776	V777	A778	F779	P780	I781	V782	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	L812	S813	L814	M815	L816	I817	G818	Y819	I760	F761	A821	A822	L823	A824	L825	S826	Y827	W828	G829	W830	W831	L832	L833	N834	A835	G836	F837	D838	H839	A840	I841	S842	Y843	L784	G785	V786	SER		

- Molecule 9: DotA



LYS	VAL	ASP	GLY	GLN	LEU	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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• Molecule 9: DotA



K241	K242	Q243	N244	D245	D246	T247	P248	K249	D250	L251	T252	A253	N254	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	L281	V282	K283	W284	N285	N286	I287	S288	A289	L290	N291	S292	T293	N294	Q295	S296	D297	N298	K299	G300																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

SER	GLY	G904	L784	L664	L602	Q542	ALA	A422	T361	L301
SER	ARG	W905	G785	Q665	Y603	D543	D483	I423	S362	V302
PRO	VAL	A906	V786	G666	Y604	G544	Q484	N424	T363	T303
THR	LYS	G907	T787	M667	M605	V545	F485	Y426	G364	V304
THR	ALA	W908	H788	M668	K606	Q547	D486	G428	N365	G305
GLY	GLY	Y909	P789	D669	H607	Q548	T487	G429	S366	G306
GLU	ALA	A910	E790	I670	Q608	P548	G488	M430	A367	A307
THR	THR	F911	G791	F671	F610	D549	T489	M431	N368	G308
GLY	GLY	F912	N792	I672	F611	L550	G490	M432	D369	S309
GLY	LYS	F913	E793	G673	D611	S551	L491	P432	F370	N310
ALA	GLY	S914	A794	G674	C612	D552	D492	A372	S371	S311
GLY	THR	L915	F795	V675	G613	N553	K493	I373	S312	S312
ALA	SER	L916	L796	Q676	R614	P554	S494	A374	M313	M313
GLY	ILE	L917	K797	T677	V615	Q555	S495	G314	G314	G314
ASP	ASP	Y918	G798	L678	K616	R556	F496	A315	A315	A315
THR	ALA	T919	E799	T679	I617	Q557	D497	N316	N316	N316
LYS	LYS	S920	G740	Q680	L618	S558	P498	S317	S317	S317
LEU	ARG	M921	T741	P681	F619	V559	T499	G379	G379	G379
GLY	PHE	N922	M742	G682	F620	S560	Q500	V380	V380	N319
ALA	GLN	L923	M743	I683	S821	G561	L501	I320	I320	I320
GLN	ALA	I924	S744	N684	F622	P562	T502	T321	T321	T321
MET	GLY	T925	L745	P685	C623	L563	K503	S322	S322	S322
LEU	ASN	W926	I746	I686	L624	S564	P504	S384	S384	S384
GLY	TRP	Q927	G746	V687	G625	T566	F505	S385	S385	S385
LYS	THR	K928	F747	G688	R626	S567	G506	G386	G386	G386
LEU	GLY	N929	V748	A689	M627	Y567	K507	E387	E387	L326
GLY	ALA	F930	T749	A690	M628	Y568	T508	V388	V388	L326
PRO	MET	L810	A750	N691	L631	G569	C509	C389	C389	T327
ALA	ASP	R811	Y751	G692	F632	F570	Q510	T390	T390	A328
GLN	THR	P812	Y752	G693	Y633	N571	D511	E391	E391	R329
LYS	SER	L932	L753	T694	M634	N573	P512	Y392	Y392	R329
LYS	GLN	T933	T695	G696	Y635	N574	Y513	Q393	Q393	S331
ILE	TRP	A934	L814	Y696	Y636	S574	S514	Q394	Q394	R332
SER	ASP	H935	M815	I697	V636	M575	L515	V395	V395	A333
GLU	ASN	L936	T816	N698	F637	M576	L516	C396	C396	I334
ALA	PHE	P937	L817	G699	R638	V577	C517	Q397	Q397	A335
GLY	LYS	F938	G818	F699	Y640	Q578	T518	T398	T398	I336
ASP	ASP	K939	C818	G701	V641	L579	W519	W399	W399	Q338
VAL	LEU	W940	Y819	T702	N642	P580	F520	G400	G400	Q338
SER	THR	L941	T820	L703	F643	Q581	Q521	M339	M339	V340
GLY	GLY	R942	A821	W704	F644	Q582	N522	S401	S401	Y340
LYS	TYR	W943	A822	T705	F645	P583	K523	V402	V402	V341
LYS	GLN	I944	T823	L706	L646	G584	S524	P403	P403	V341
ASN	SER	Q945	A824	T707	I647	G585	D525	A404	A404	T342
GLY	THR	GLY	S826	L708	F648	I585	K526	S405	S405	L343
GLY	LEU	SER	Y827	N709	M651	K586	L527	G406	G406	S344
PRO	GLU	PRO	W828	W710	I652	P587	L528	T406	T406	T345
GLN	GLY	SER	C829	VAL	G653	L588	Q529	G407	G407	V346
THR	GLY	PHE	W831	V713	S654	T589	I530	S408	S408	Q348
GLY	GLY	GLY	T832	S714	I655	F590	Q531	T409	T409	V349
THR	THR	THR	L833	S715	V656	M591	L471	M350	M350	M350
GLN	GLN	GLN	L834	L716	A658	N592	V472	T410	T410	V351
TRP	TRP	TRP	M835	I717	F659	L593	K473	L413	L413	N353
GLY	GLY	GLY	A836	P718	M660	I594	L474	F414	F414	D354
GLU	GLU	GLU	G836	L719	L661	N595	N475	M415	M415	P355
ALA	ALA	ALA	F837	L720	M662	K597	G476	G416	G416	A356
LYS	LYS	LYS	D838	F721	I662	V598	S477	T417	T417	F357
			H839	I722	P663	D599	A478	E418	E418	S358
			A840	F723		T600	T479	F419	F419	T359
			S842			S601	E480	L420	L420	T360
			Y843				PHE	G421	G421	

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 ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >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%)	9	28
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%)	9	28
1	Ci	11/11 (100%)	9 (82%)	2 (18%)	2	10
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%)	9	28
1	Dm	11/11 (100%)	10 (91%)	1 (9%)	9	28
1	Ds	11/11 (100%)	10 (91%)	1 (9%)	9	28
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%)	3	14
2	Cp	7/7 (100%)	6 (86%)	1 (14%)	3	14
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%)	12	32
3	Ai	13/13 (100%)	12 (92%)	1 (8%)	12	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Ao	13/13 (100%)	12 (92%)	1 (8%)	12	32
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%)	12	32
3	Ce	13/13 (100%)	12 (92%)	1 (8%)	12	32
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%)	12	32
3	Di	13/13 (100%)	12 (92%)	1 (8%)	12	32
3	Do	13/13 (100%)	11 (85%)	2 (15%)	2	13
3	Du	13/13 (100%)	13 (100%)	0	100	100
3	Ea	13/13 (100%)	12 (92%)	1 (8%)	12	32
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%)	50	66
5	Ak	53/237 (22%)	52 (98%)	1 (2%)	50	66
5	Aq	53/237 (22%)	50 (94%)	3 (6%)	18	40
5	Aw	53/237 (22%)	51 (96%)	2 (4%)	29	50
5	Bc	53/237 (22%)	50 (94%)	3 (6%)	18	40
5	Bi	53/237 (22%)	52 (98%)	1 (2%)	50	66
5	Bo	53/237 (22%)	49 (92%)	4 (8%)	12	33
5	Bu	53/237 (22%)	51 (96%)	2 (4%)	29	50
5	Ca	53/237 (22%)	52 (98%)	1 (2%)	50	66
5	Cg	53/237 (22%)	49 (92%)	4 (8%)	12	33
5	Cm	53/237 (22%)	47 (89%)	6 (11%)	5	20
5	Cs	53/237 (22%)	53 (100%)	0	100	100
5	Cy	53/237 (22%)	51 (96%)	2 (4%)	29	50
5	De	53/237 (22%)	51 (96%)	2 (4%)	29	50
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%)	18	40
5	Ec	53/237 (22%)	53 (100%)	0	100	100
6	Af	137/300 (46%)	127 (93%)	10 (7%)	13	34
6	Al	137/300 (46%)	131 (96%)	6 (4%)	25	47
6	Ar	137/300 (46%)	135 (98%)	2 (2%)	57	70
6	Ax	137/300 (46%)	128 (93%)	9 (7%)	15	37
6	Bd	137/300 (46%)	132 (96%)	5 (4%)	31	52
6	Bj	137/300 (46%)	132 (96%)	5 (4%)	31	52
6	Bp	137/300 (46%)	128 (93%)	9 (7%)	15	37
6	Bv	137/300 (46%)	130 (95%)	7 (5%)	21	43
6	Cb	137/300 (46%)	128 (93%)	9 (7%)	15	37
6	Ch	137/300 (46%)	130 (95%)	7 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	Cn	137/300 (46%)	127 (93%)	10 (7%)	13	34
6	Ct	137/300 (46%)	135 (98%)	2 (2%)	57	70
6	Cz	137/300 (46%)	130 (95%)	7 (5%)	21	43
6	Df	137/300 (46%)	128 (93%)	9 (7%)	15	37
6	Dl	137/300 (46%)	125 (91%)	12 (9%)	9	29
6	Dr	137/300 (46%)	128 (93%)	9 (7%)	15	37
6	Dx	137/300 (46%)	131 (96%)	6 (4%)	25	47
6	Ed	137/300 (46%)	127 (93%)	10 (7%)	13	34
7	Ee	31/765 (4%)	29 (94%)	2 (6%)	15	37
7	Ef	51/765 (7%)	48 (94%)	3 (6%)	18	40
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%)	5	19
7	Ej	50/765 (6%)	48 (96%)	2 (4%)	28	49
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%)	8	25
7	En	31/765 (4%)	29 (94%)	2 (6%)	15	37
7	Eo	31/765 (4%)	30 (97%)	1 (3%)	34	55
7	Ep	31/765 (4%)	31 (100%)	0	100	100
7	Eq	50/765 (6%)	48 (96%)	2 (4%)	28	49
7	Er	31/765 (4%)	31 (100%)	0	100	100
7	Es	50/765 (6%)	44 (88%)	6 (12%)	5	18
7	Et	44/765 (6%)	42 (96%)	2 (4%)	24	46
7	Eu	51/765 (7%)	50 (98%)	1 (2%)	48	65
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%)	19	41
7	Fk	36/765 (5%)	34 (94%)	2 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	Ew	360/401 (90%)	350 (97%)	10 (3%)	38	59
8	Ex	360/401 (90%)	349 (97%)	11 (3%)	35	56
8	Ey	360/401 (90%)	352 (98%)	8 (2%)	45	64
8	Ez	360/401 (90%)	348 (97%)	12 (3%)	33	55
8	Fa	360/401 (90%)	353 (98%)	7 (2%)	50	66
9	Fb	715/858 (83%)	691 (97%)	24 (3%)	32	54
9	Fc	715/858 (83%)	682 (95%)	33 (5%)	24	46
9	Fd	715/858 (83%)	693 (97%)	22 (3%)	35	56
9	Fe	715/858 (83%)	676 (94%)	39 (6%)	19	42
9	Ff	715/858 (83%)	688 (96%)	27 (4%)	29	50
All	All	10292/34168 (30%)	9877 (96%)	415 (4%)	29	49

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.

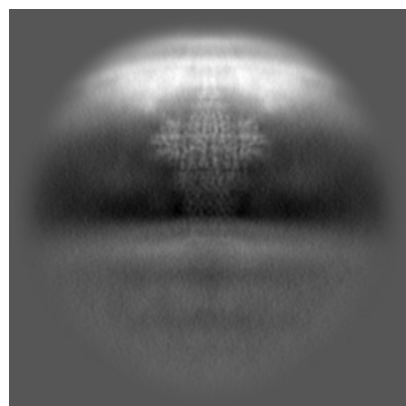
6 Map visualisation [i](#)

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.

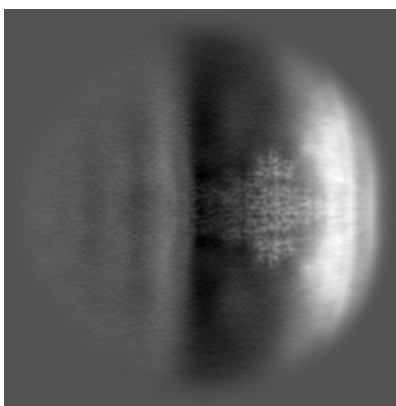
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

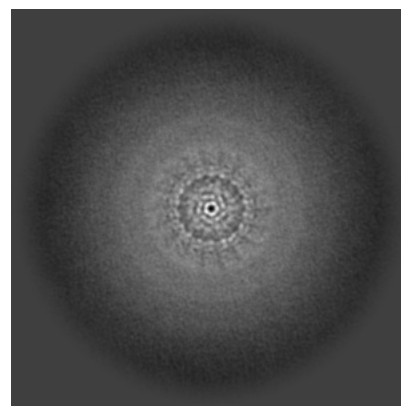
6.1.1 Primary map



X

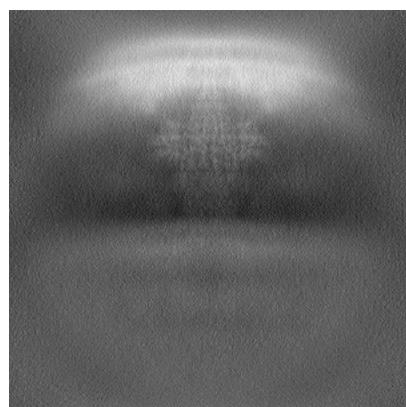


Y

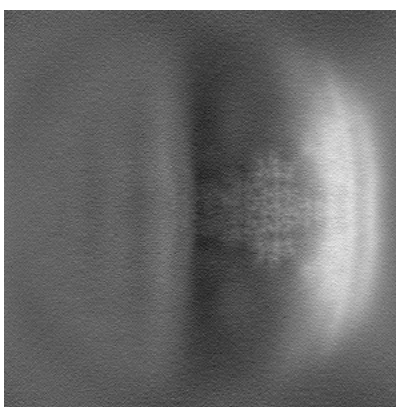


Z

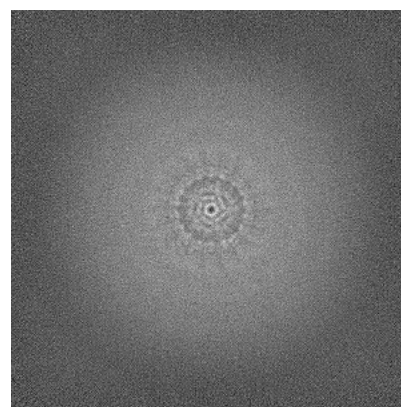
6.1.2 Raw map



X



Y

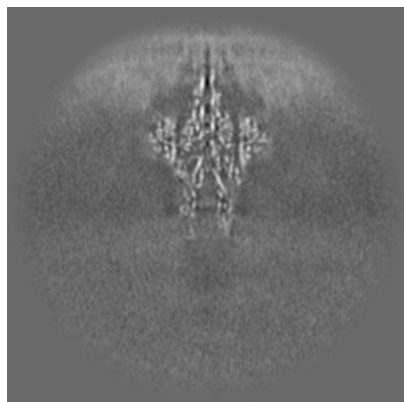


Z

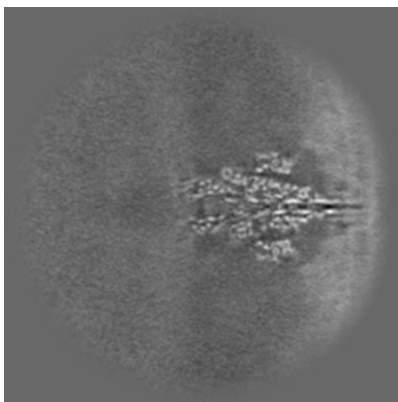
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

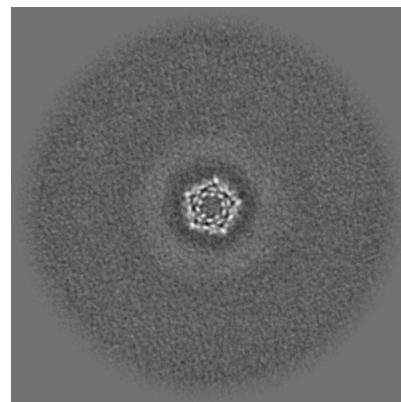
6.2.1 Primary map



X Index: 256

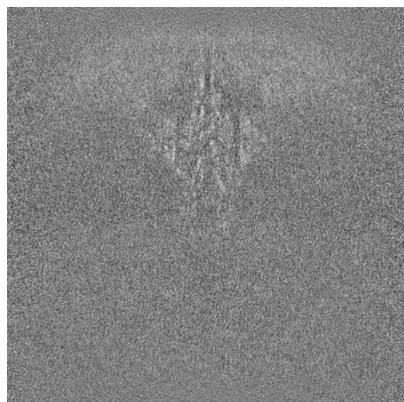


Y Index: 256

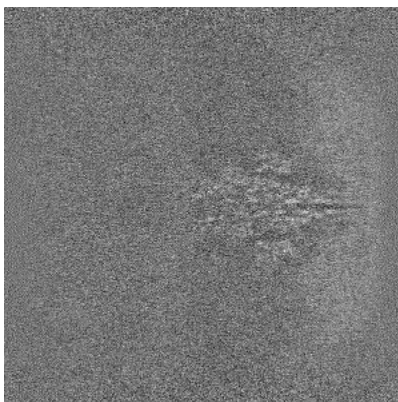


Z Index: 256

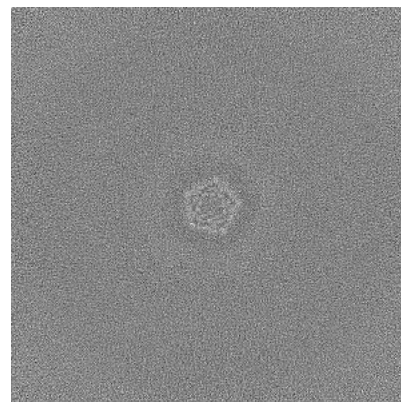
6.2.2 Raw map



X Index: 256



Y Index: 256

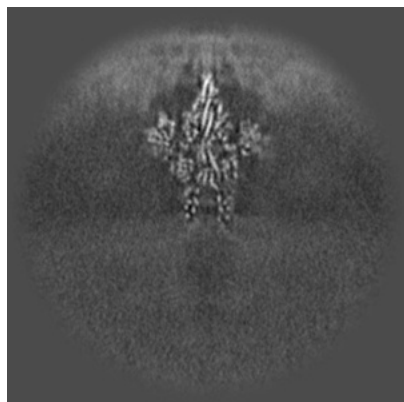


Z Index: 256

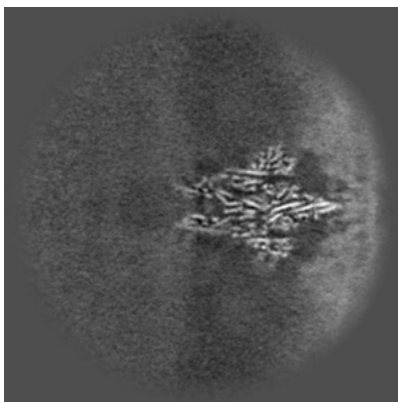
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

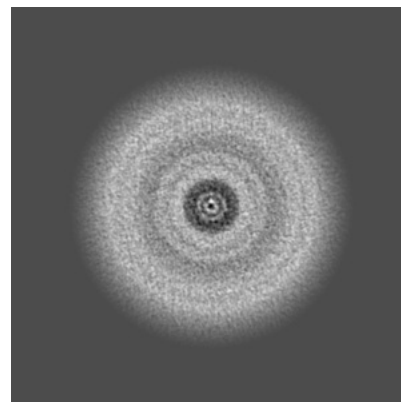
6.3.1 Primary map



X Index: 250

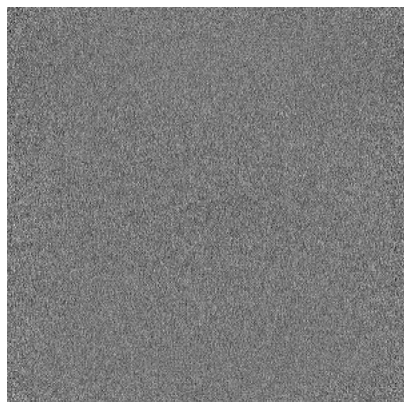


Y Index: 263

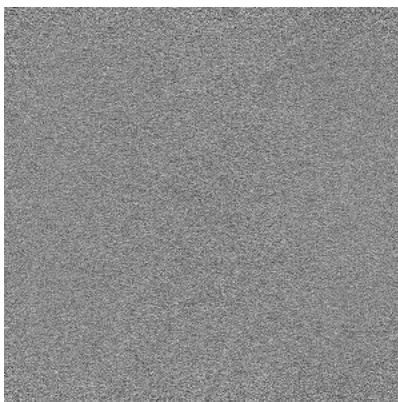


Z Index: 430

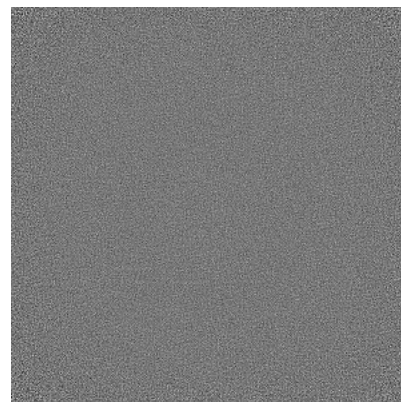
6.3.2 Raw map



X Index: 0



Y Index: 0

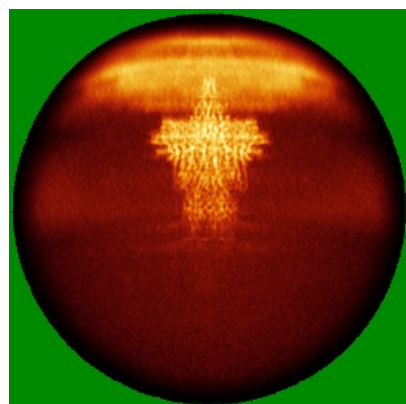


Z Index: 511

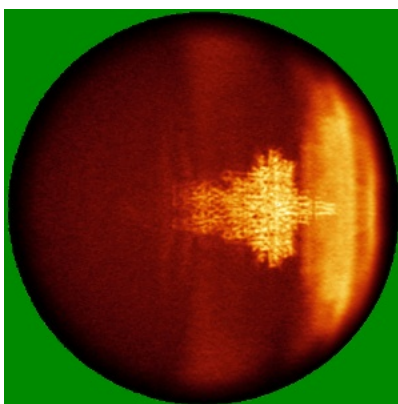
The images above show the largest variance slices of the map in three orthogonal directions.

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

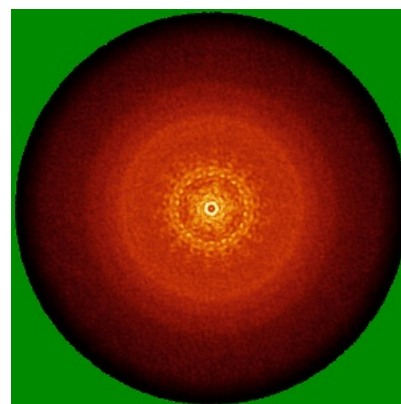
6.4.1 Primary map



X

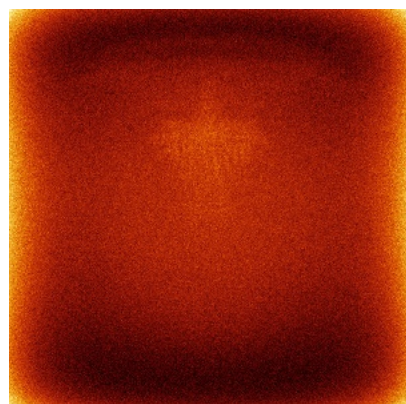


Y

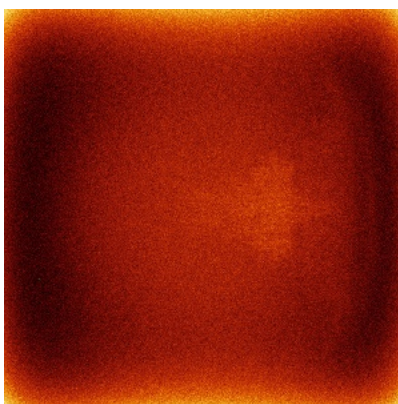


Z

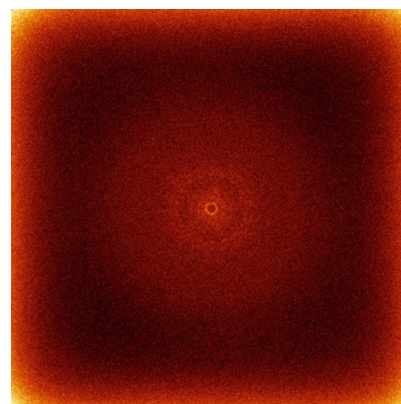
6.4.2 Raw map



X



Y

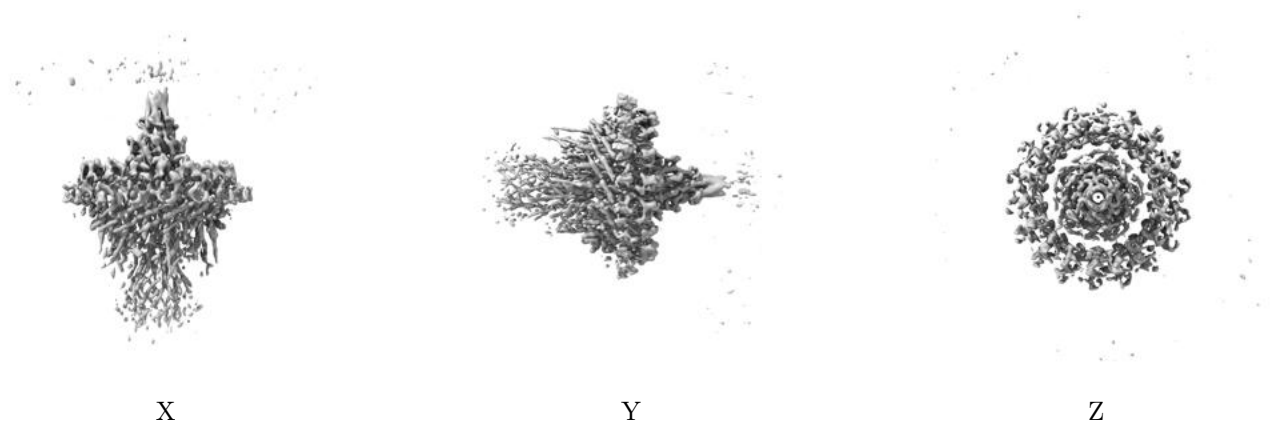


Z

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.

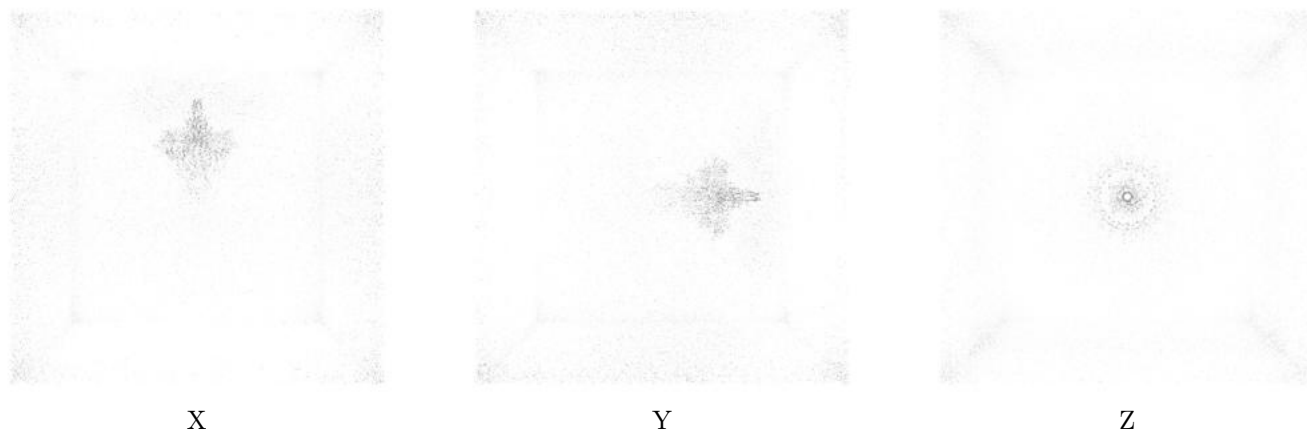
6.5 Orthogonal surface views [i](#)

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.

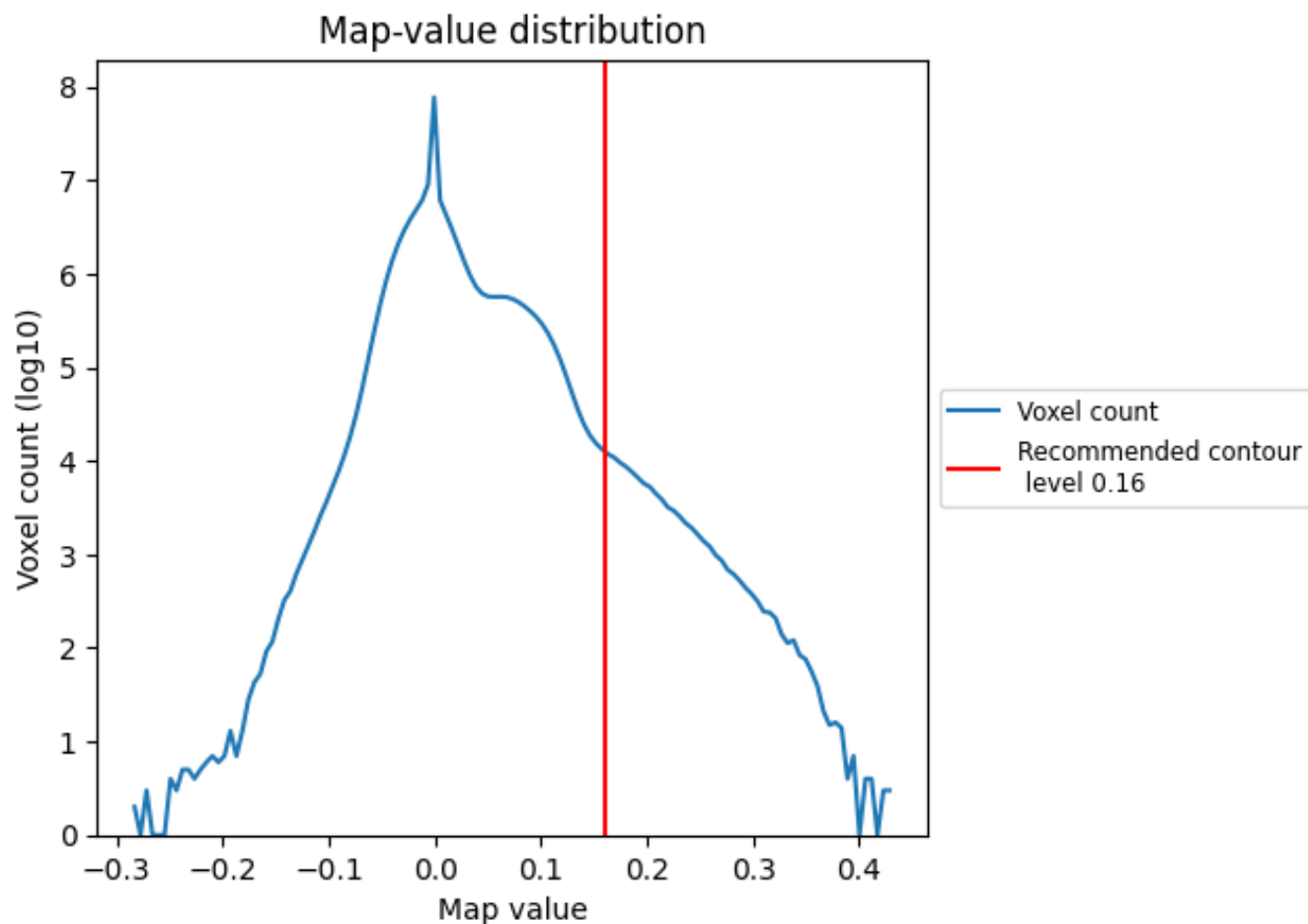
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

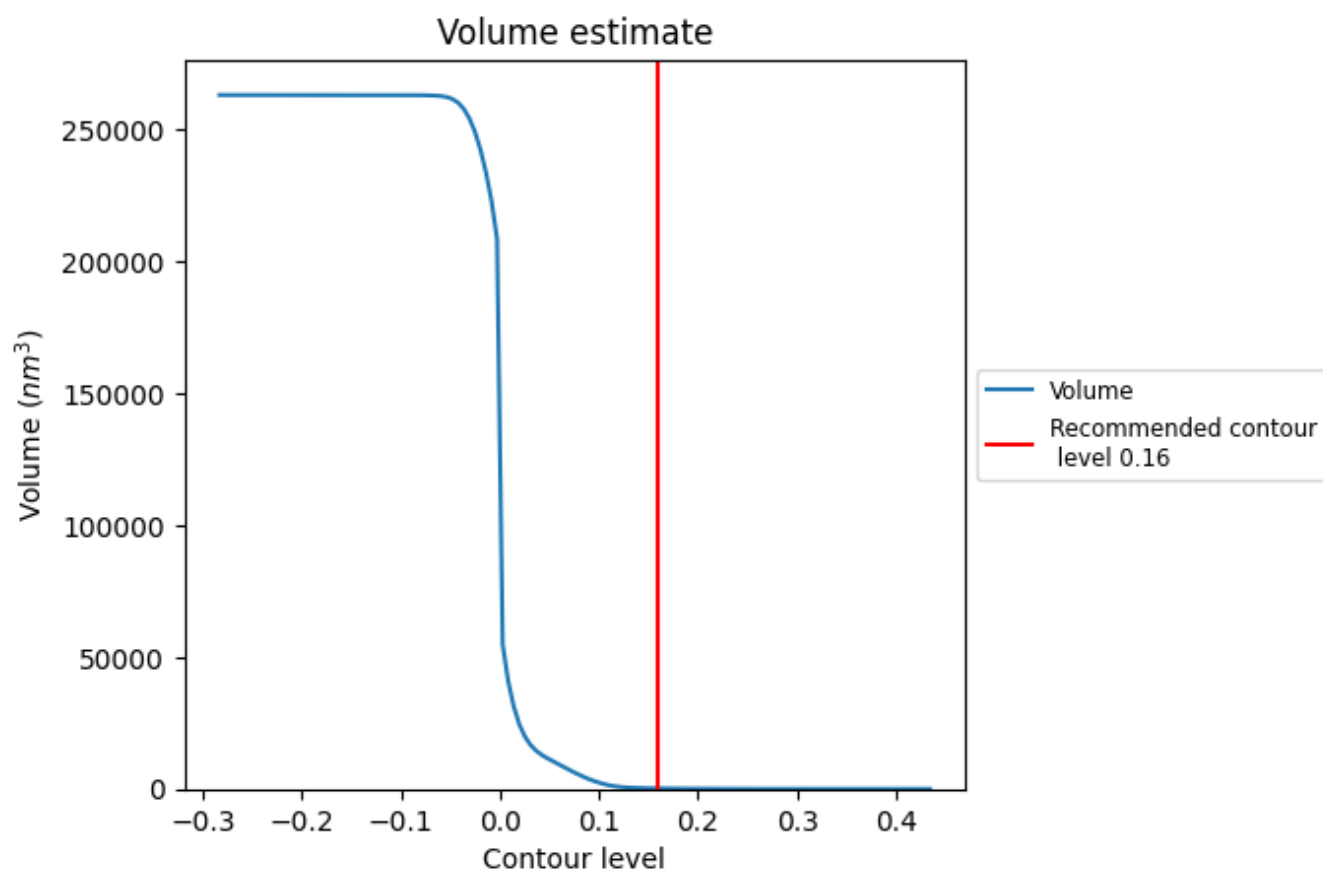
This section contains the results of statistical analysis of the map.

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.

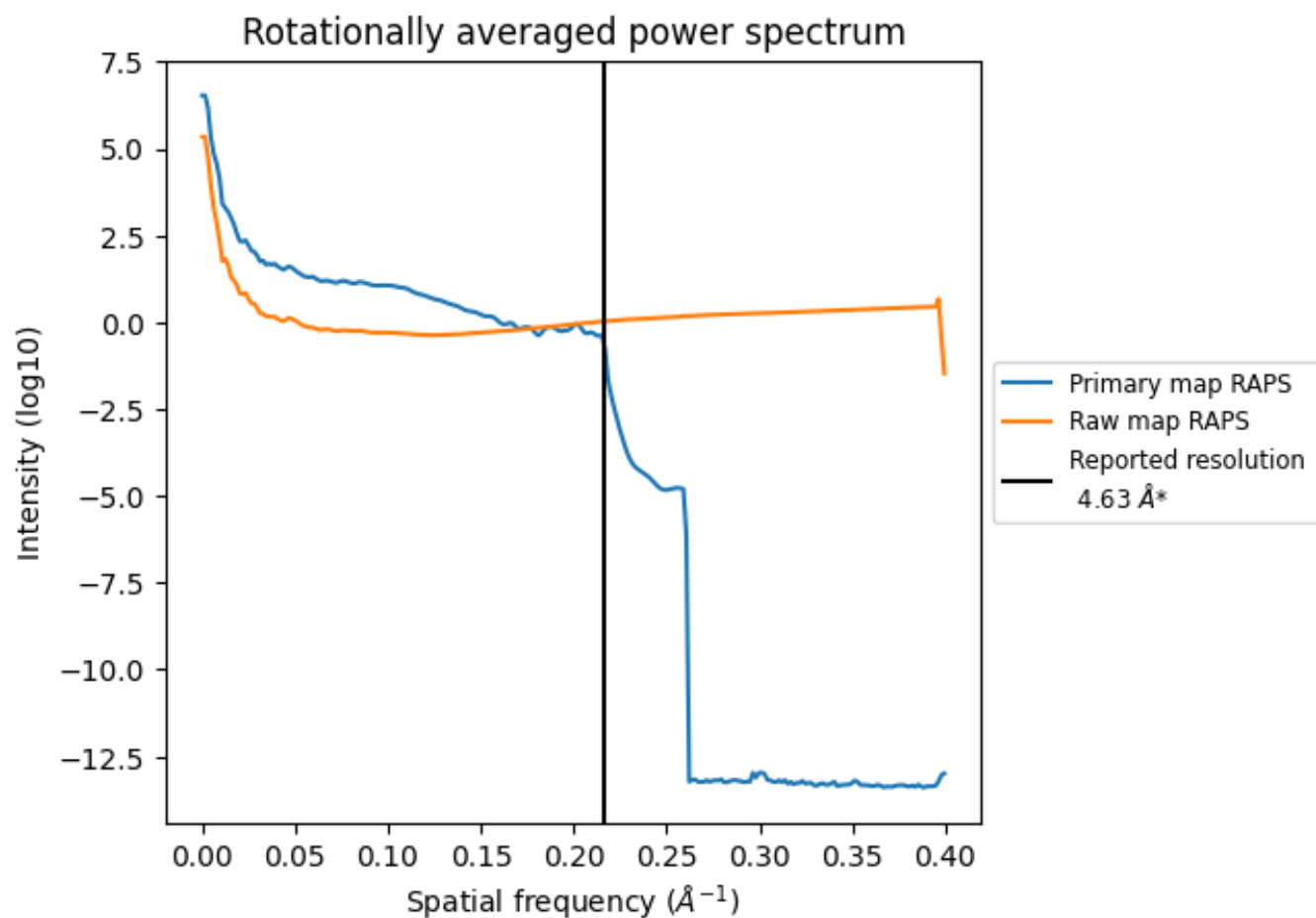
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 207 nm^3 ; 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 ⓘ

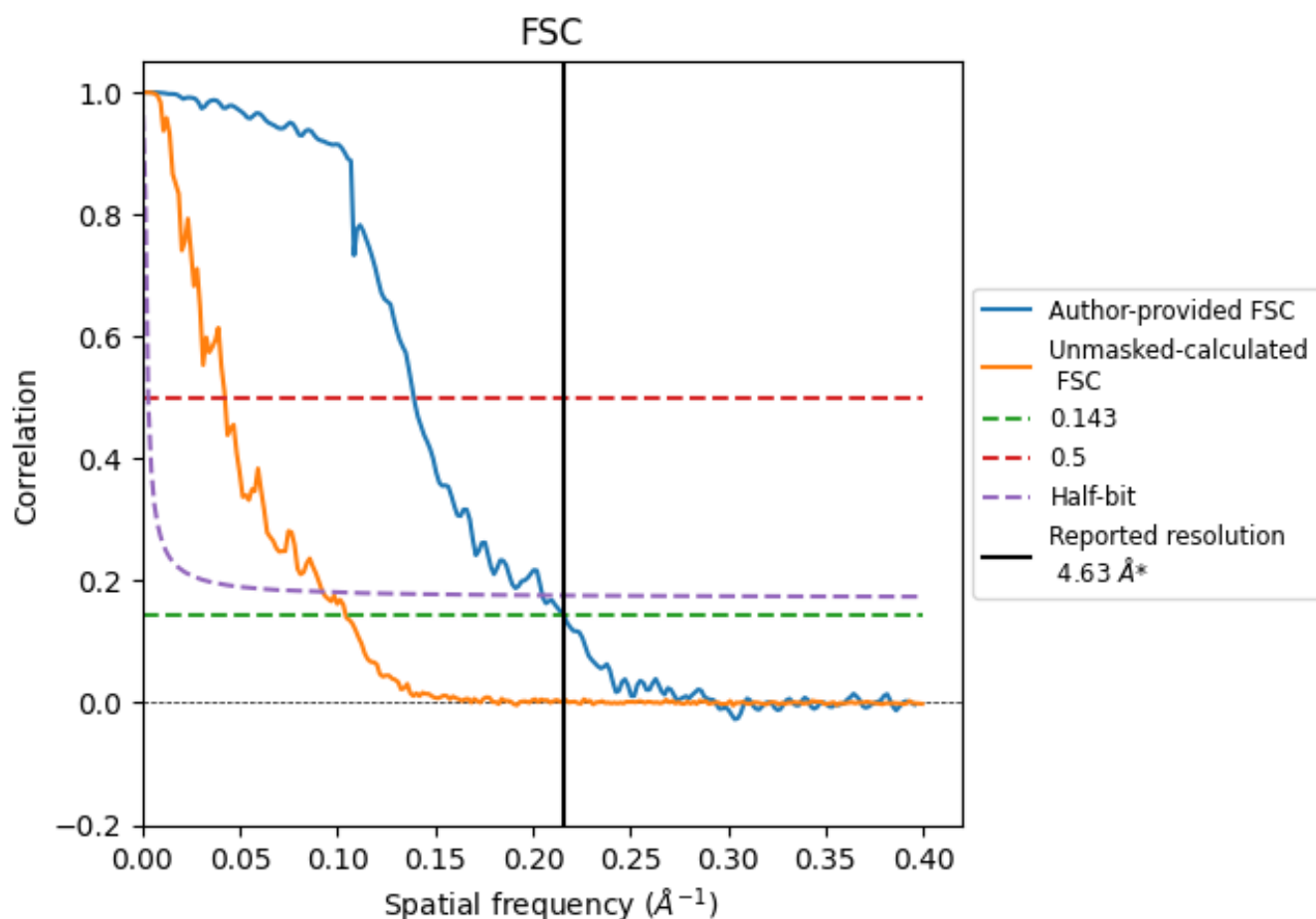


*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.216 Å⁻¹

8.2 Resolution estimates [i](#)

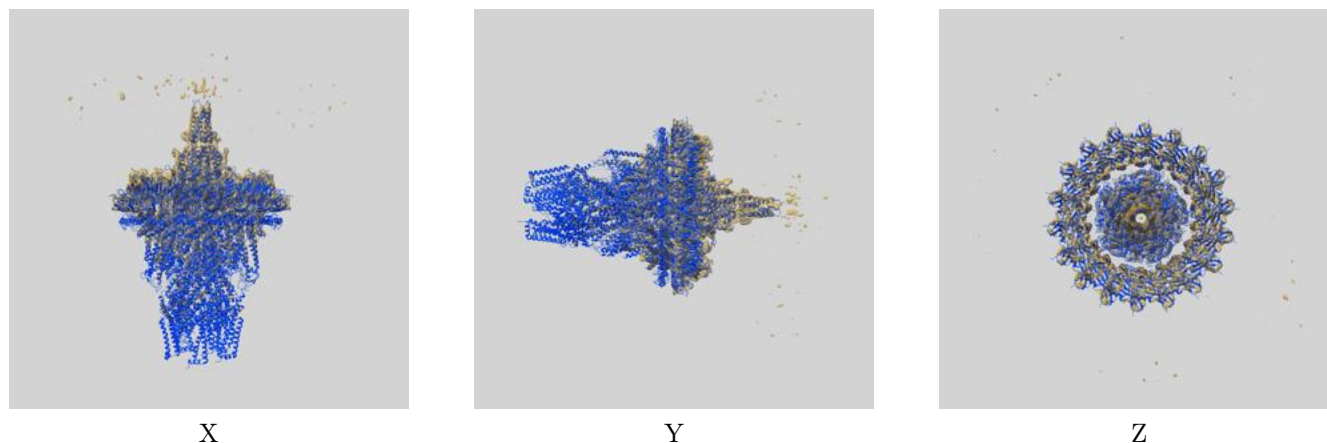
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.63	-	-
Author-provided FSC curve	4.63	7.19	4.88
Unmasked-calculated*	9.59	23.64	10.82

*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](#)

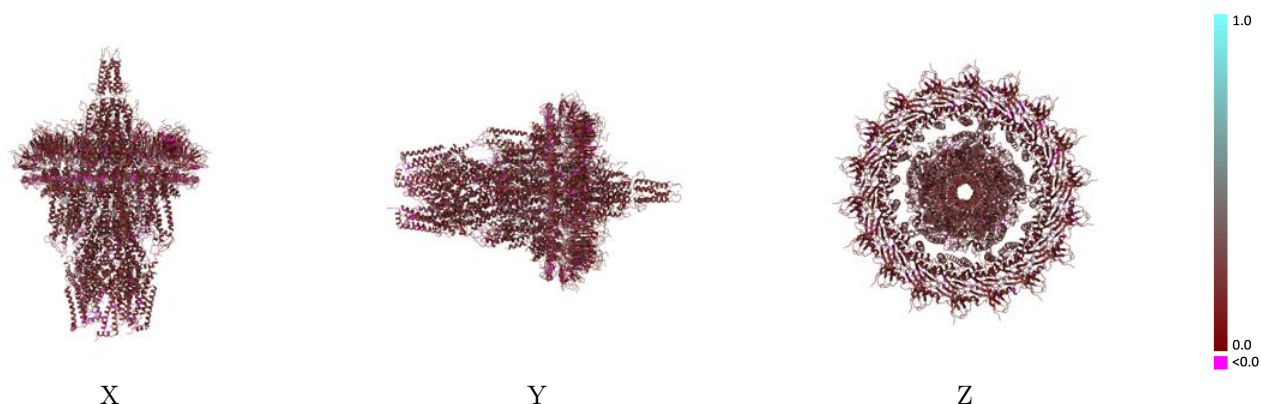
This section contains information regarding the fit between EMDB map EMD-49398 and PDB model 9NH0. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



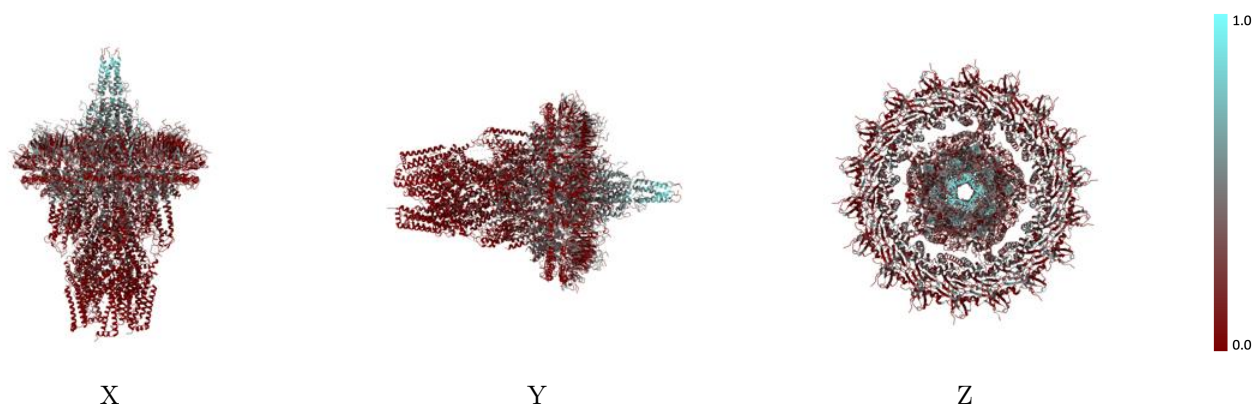
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



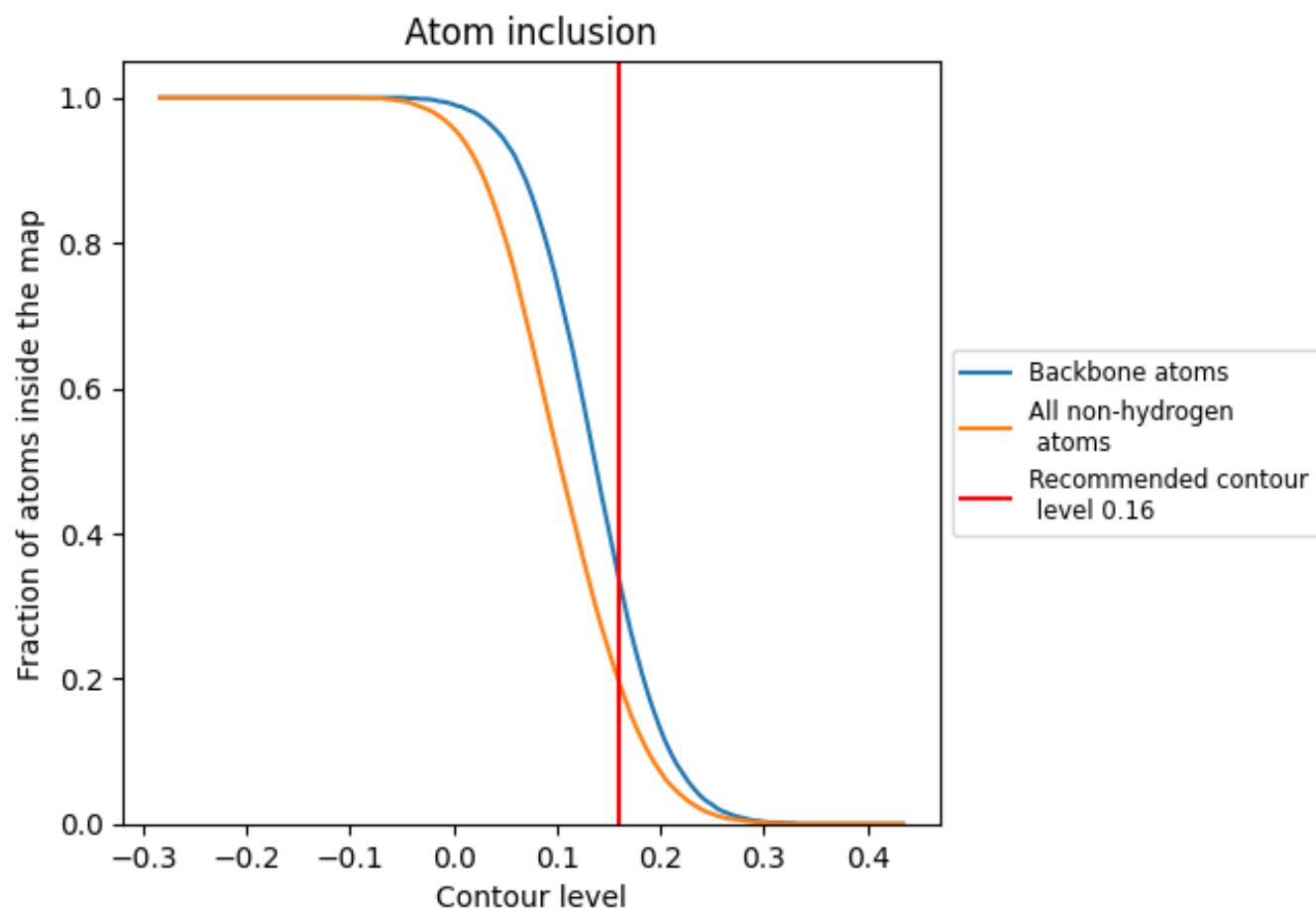
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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