wwPDB EM Validation Summary Report (i)

Mar 6, 2026 – 03:08 PM UTC

PDB ID	:	9NGV / pdb_00009ngv
EMDB ID	:	EMD-49394
Title	:	In situ cryo-EM structure of periplasmic ring (PR) of the Legionella Dot/Icm T4SS machine.
Authors	:	Yue, J.; Jun, L.
Deposited on	:	2025-02-22
Resolution	:	3.04 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 (i) 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 (i)) were used in the production of this report:

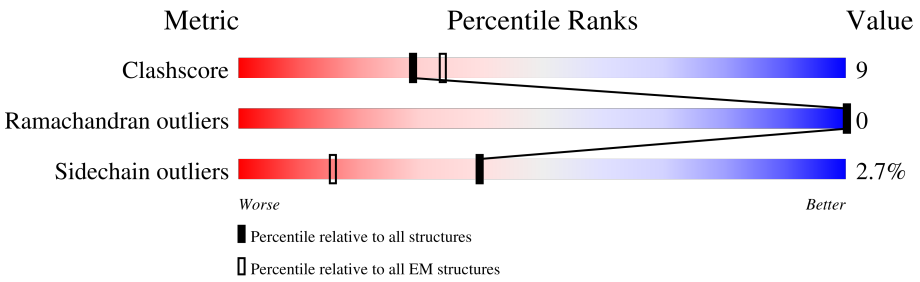
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

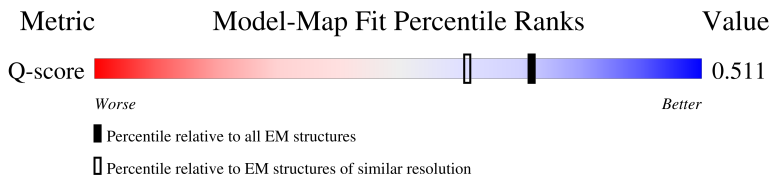
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.04 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	13952 (2.54 - 3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	Aa	16	12% 69% 31%
1	Ah	16	19% 81% 19%
1	Ao	16	19% 62% 38%
1	Av	16	6% 81% 19%

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Mol	Chain	Length	Quality of chain
1	Bc	16	12% 75% 25%
1	Bj	16	6% 75% 25%
1	Bq	16	6% 81% 19%
1	Bx	16	19% 88% 12%
1	Ce	16	6% 75% 25%
1	Cl	16	12% 69% 31%
1	Cs	16	12% 75% 25%
1	Cz	16	12% 69% 31%
1	Dg	16	19% 75% 25%
1	Dn	16	12% 75% 25%
1	Du	16	6% 81% 19%
1	Eb	16	6% 75% 25%
1	Ei	16	19% 88% 12%
1	Ep	16	12% 69% 31%
2	Ab	9	33% 67% 33%
2	Ai	9	22% 67% 33%
2	Ap	9	22% 67% 22% 11%
2	Aw	9	11% 67% 33%
2	Bd	9	22% 78% 22%
2	Bk	9	11% 78% 22%
2	Br	9	11% 67% 33%
2	By	9	11% 67% 33%
2	Cf	9	11% 78% 22%
2	Cm	9	22% 56% 33% 11%
2	Ct	9	33% 44% 56%

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Mol	Chain	Length	Quality of chain
2	Da	9	22% 67% 22% 11%
2	Dh	9	22% 56% 33% 11%
2	Do	9	22% 56% 44%
2	Dv	9	11% 56% 44%
2	Ec	9	11% 67% 33%
2	Ej	9	11% 44% 33% 22%
2	Eq	9	22% 67% 33%
3	Ac	16	50% 50% 44% 6%
3	Aj	16	50% 62% 31% 6%
3	Aq	16	38% 50% 38% 12%
3	Ax	16	44% 62% 38%
3	Be	16	38% 75% 25%
3	Bl	16	44% 50% 50%
3	Bs	16	50% 75% 25%
3	Bz	16	44% 62% 31% 6%
3	Cg	16	38% 56% 31% 12%
3	Cn	16	50% 50% 44% 6%
3	Cu	16	50% 44% 50% 6%
3	Db	16	31% 44% 44% 12%
3	Di	16	44% 56% 44%
3	Dp	16	38% 56% 31% 12%
3	Dw	16	44% 62% 31% 6%
3	Ed	16	50% 69% 31%
3	Ek	16	44% 56% 38% 6%
3	Er	16	38% 50% 38% 12%

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Mol	Chain	Length	Quality of chain
4	Ad	5	60% / 60% / 40%
4	Ak	5	60% / 80% / 20%
4	Ar	5	60% / 60% / 40%
4	Ay	5	60% / 80% / 20%
4	Bf	5	60% / 80% / 20%
4	Bm	5	60% / 80% / 20%
4	Bt	5	60% / 80% / 20%
4	Ca	5	60% / 80% / 20%
4	Ch	5	40% / 80% / 20%
4	Co	5	40% / 60% / 40%
4	Cv	5	60% / 80% / 20%
4	Dc	5	60% / 60% / 40%
4	Dj	5	60% / 60% / 40%
4	Dq	5	60% / 80% / 20%
4	Dx	5	40% / 80% / 20%
4	Ee	5	60% / 80% / 20%
4	El	5	60% / 60% / 40%
4	Es	5	40% / 80% / 20%
5	Ae	269	19% / 5% / 77%
5	Al	269	19% / 5% / 77%
5	As	269	19% / 5% / 77%
5	Az	269	18% / 6% / 77%
5	Bg	269	19% / • / 77%
5	Bn	269	19% / • / 77%
5	Bu	269	18% / 6% / 77%

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Mol	Chain	Length	Quality of chain
5	Cb	269	18% 6% 77%
5	Ci	269	19% • 77%
5	Cp	269	18% 5% 77%
5	Cw	269	18% 5% 77%
5	Dd	269	19% 5% 77%
5	Dk	269	18% 5% 77%
5	Dr	269	19% 5% 77%
5	Dy	269	18% 5% 77%
5	Ef	269	18% 5% 77%
5	Em	269	18% 5% 77%
5	Et	269	19% • 77%
6	Af	1048	• • 97%
6	Am	1048	• • 97%
6	At	1048	• 97%
6	Ba	1048	• 97%
6	Bh	1048	• 97%
6	Bo	1048	• 97%
6	Bv	1048	• • 97%
6	Cc	1048	• 97%
6	Cj	1048	• 97%
6	Cq	1048	• 97%
6	Cx	1048	• • 97%
6	De	1048	• 97%
6	Dl	1048	• 97%
6	Ds	1048	• 97%

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Mol	Chain	Length	Quality of chain
6	Dz	1048	97%
6	Eg	1048	97%
6	En	1048	97%
6	Eu	1048	97%
7	Ag	361	33% 10% 56%
7	An	361	35% 9% 56%
7	Au	361	34% 10% 56%
7	Bb	361	36% 9% 56%
7	Bi	361	35% 9% 56%
7	Bp	361	32% 12% 56%
7	Bw	361	37% 7% 56%
7	Cd	361	34% 10% 56%
7	Ck	361	37% 7% 56%
7	Cr	361	34% 9% 56%
7	Cy	361	35% 9% 56%
7	Df	361	34% 9% 56%
7	Dm	361	35% 9% 56%
7	Dt	361	34% 9% 56%
7	Ea	361	31% 13% 56%
7	Eh	361	35% 9% 56%
7	Eo	361	34% 10% 56%
7	Ev	361	36% 8% 56%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 42066 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 A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Aa	16	117	71	20	25	1	0	0
1	Ah	16	117	71	20	25	1	0	0
1	Ao	16	117	71	20	25	1	0	0
1	Av	16	117	71	20	25	1	0	0
1	Bc	16	117	71	20	25	1	0	0
1	Bj	16	117	71	20	25	1	0	0
1	Bq	16	117	71	20	25	1	0	0
1	Bx	16	117	71	20	25	1	0	0
1	Ce	16	117	71	20	25	1	0	0
1	Cl	16	117	71	20	25	1	0	0
1	Cs	16	117	71	20	25	1	0	0
1	Cz	16	117	71	20	25	1	0	0
1	Dg	16	117	71	20	25	1	0	0
1	Dn	16	117	71	20	25	1	0	0
1	Du	16	117	71	20	25	1	0	0
1	Eb	16	117	71	20	25	1	0	0
1	Ei	16	117	71	20	25	1	0	0

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

- Molecule 2 is a protein called unknown peptide B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Ab	9	61	35	12	12	2	0	0
2	Ai	9	61	35	12	12	2	0	0
2	Ap	9	61	35	12	12	2	0	0
2	Aw	9	61	35	12	12	2	0	0
2	Bd	9	61	35	12	12	2	0	0
2	Bk	9	61	35	12	12	2	0	0
2	Br	9	61	35	12	12	2	0	0
2	By	9	61	35	12	12	2	0	0
2	Cf	9	61	35	12	12	2	0	0
2	Cm	9	61	35	12	12	2	0	0
2	Ct	9	61	35	12	12	2	0	0
2	Da	9	61	35	12	12	2	0	0
2	Dh	9	61	35	12	12	2	0	0
2	Do	9	61	35	12	12	2	0	0
2	Dv	9	61	35	12	12	2	0	0
2	Ec	9	61	35	12	12	2	0	0
2	Ej	9	61	35	12	12	2	0	0
2	Eq	9	61	35	12	12	2	0	0

- Molecule 3 is a protein called unknown peptide C.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Ac	16	125	78	21	26	0	0
3	Aj	16	125	78	21	26	0	0
3	Aq	16	125	78	21	26	0	0
3	Ax	16	125	78	21	26	0	0
3	Be	16	125	78	21	26	0	0
3	Bl	16	125	78	21	26	0	0
3	Bs	16	125	78	21	26	0	0
3	Bz	16	125	78	21	26	0	0
3	Cg	16	125	78	21	26	0	0
3	Cn	16	125	78	21	26	0	0
3	Cu	16	125	78	21	26	0	0
3	Db	16	125	78	21	26	0	0
3	Di	16	125	78	21	26	0	0
3	Dp	16	125	78	21	26	0	0
3	Dw	16	125	78	21	26	0	0
3	Ed	16	125	78	21	26	0	0
3	Ek	16	125	78	21	26	0	0
3	Er	16	125	78	21	26	0	0

- Molecule 4 is a protein called unknown peptide D.

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

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	Ak	5	36	23	5	8	0	0
4	Ar	5	36	23	5	8	0	0
4	Ay	5	36	23	5	8	0	0
4	Bf	5	36	23	5	8	0	0
4	Bm	5	36	23	5	8	0	0
4	Bt	5	36	23	5	8	0	0
4	Ca	5	36	23	5	8	0	0
4	Ch	5	36	23	5	8	0	0
4	Co	5	36	23	5	8	0	0
4	Cv	5	36	23	5	8	0	0
4	Dc	5	36	23	5	8	0	0
4	Dj	5	36	23	5	8	0	0
4	Dq	5	36	23	5	8	0	0
4	Dx	5	36	23	5	8	0	0
4	Ee	5	36	23	5	8	0	0
4	El	5	36	23	5	8	0	0
4	Es	5	36	23	5	8	0	0

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	As	63	484	308	84	91	1	0	0
5	Az	63	484	308	84	91	1	0	0
5	Bg	63	484	308	84	91	1	0	0
5	Bn	63	484	308	84	91	1	0	0
5	Bu	63	484	308	84	91	1	0	0
5	Cb	63	484	308	84	91	1	0	0
5	Ci	63	484	308	84	91	1	0	0
5	Cp	63	484	308	84	91	1	0	0
5	Cw	63	484	308	84	91	1	0	0
5	Dd	63	484	308	84	91	1	0	0
5	Dk	63	484	308	84	91	1	0	0
5	Dr	63	484	308	84	91	1	0	0
5	Dy	63	484	308	84	91	1	0	0
5	Ef	63	484	308	84	91	1	0	0
5	Em	63	484	308	84	91	1	0	0
5	Et	63	484	308	84	91	1	0	0

- Molecule 6 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Af	34	276	168	47	60	1	0	0
6	Am	34	276	168	47	60	1	0	0
6	At	34	276	168	47	60	1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Ba	34	276	168	47	60	1	0	0
6	Bh	34	276	168	47	60	1	0	0
6	Bo	34	276	168	47	60	1	0	0
6	Bv	34	276	168	47	60	1	0	0
6	Cc	34	276	168	47	60	1	0	0
6	Cj	34	276	168	47	60	1	0	0
6	Cq	34	276	168	47	60	1	0	0
6	Cx	34	276	168	47	60	1	0	0
6	De	34	276	168	47	60	1	0	0
6	Dl	34	276	168	47	60	1	0	0
6	Ds	34	276	168	47	60	1	0	0
6	Dz	34	276	168	47	60	1	0	0
6	Eg	34	276	168	47	60	1	0	0
6	En	34	276	168	47	60	1	0	0
6	Eu	34	276	168	47	60	1	0	0

- Molecule 7 is a protein called IcmK (DotH).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Ag	160	1238	795	207	233	3	0	0
7	An	160	1238	795	207	233	3	0	0
7	Au	160	1238	795	207	233	3	0	0
7	Bb	160	1238	795	207	233	3	0	0

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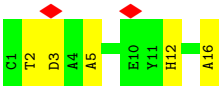
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Bi	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Bp	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Bw	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Cd	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Ck	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Cr	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Cy	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Df	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Dm	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Dt	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Ea	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Eh	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Eo	160	1238	795	207	233	3	0	0
			Total	C	N	O	S		
7	Ev	160	1238	795	207	233	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

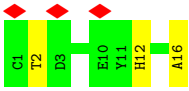
- Molecule 1: unknown peptide A

Chain Aa:



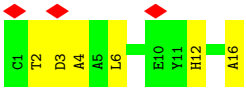
- Molecule 1: unknown peptide A

Chain Ah:



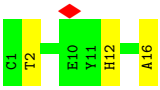
- Molecule 1: unknown peptide A

Chain Ao:



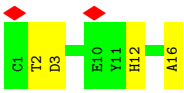
- Molecule 1: unknown peptide A

Chain Av:



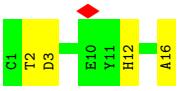
- Molecule 1: unknown peptide A

Chain Bc:



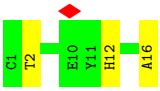
- Molecule 1: unknown peptide A

Chain Bj: 6% 75% 25%



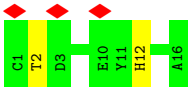
- Molecule 1: unknown peptide A

Chain Bq: 6% 81% 19%



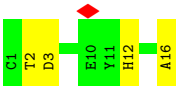
- Molecule 1: unknown peptide A

Chain Bx: 19% 88% 12%



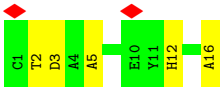
- Molecule 1: unknown peptide A

Chain Ce: 6% 75% 25%



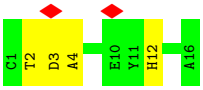
- Molecule 1: unknown peptide A

Chain Cl: 12% 69% 31%



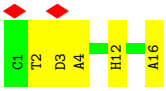
- Molecule 1: unknown peptide A

Chain Cs: 12% 75% 25%



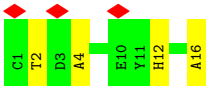
- Molecule 1: unknown peptide A

Chain Cz: 12% 69% 31%



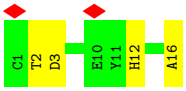
• Molecule 1: unknown peptide A

Chain Dg:



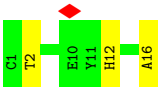
• Molecule 1: unknown peptide A

Chain Dn:



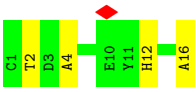
• Molecule 1: unknown peptide A

Chain Du:



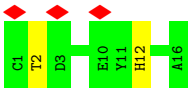
• Molecule 1: unknown peptide A

Chain Eb:



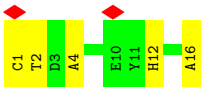
• Molecule 1: unknown peptide A

Chain Ei:



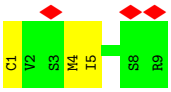
• Molecule 1: unknown peptide A

Chain Ep:



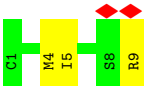
• Molecule 2: unknown peptide B

Chain Ab:



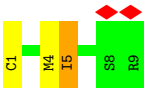
• Molecule 2: unknown peptide B

Chain Ai:



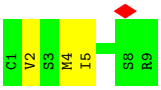
• Molecule 2: unknown peptide B

Chain Ap:



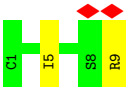
• Molecule 2: unknown peptide B

Chain Aw:



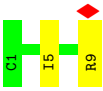
• Molecule 2: unknown peptide B

Chain Bd:



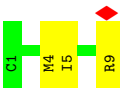
• Molecule 2: unknown peptide B

Chain Bk:



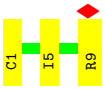
• Molecule 2: unknown peptide B

Chain Br:



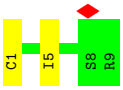
- Molecule 2: unknown peptide B

Chain By:



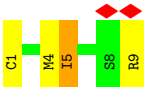
- Molecule 2: unknown peptide B

Chain Cf:



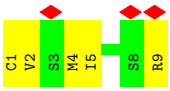
- Molecule 2: unknown peptide B

Chain Cm:



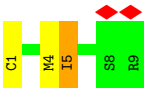
- Molecule 2: unknown peptide B

Chain Ct:



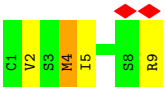
- Molecule 2: unknown peptide B

Chain Da:



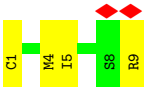
- Molecule 2: unknown peptide B

Chain Dh:



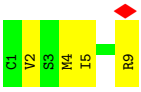
- Molecule 2: unknown peptide B

Chain Do:



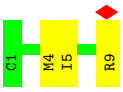
• Molecule 2: unknown peptide B

Chain Dv:



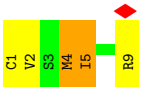
• Molecule 2: unknown peptide B

Chain Ec:



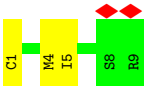
• Molecule 2: unknown peptide B

Chain Ej:



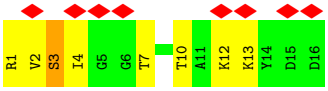
• Molecule 2: unknown peptide B

Chain Eq:



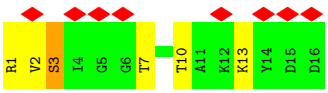
• Molecule 3: unknown peptide C

Chain Ac:



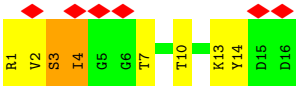
• Molecule 3: unknown peptide C

Chain Aj:



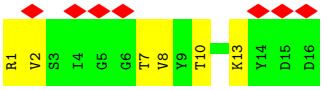
• Molecule 3: unknown peptide C

Chain Aq:



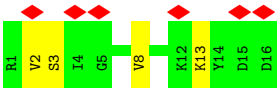
- Molecule 3: unknown peptide C

Chain Ax:



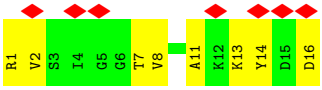
- Molecule 3: unknown peptide C

Chain Be:



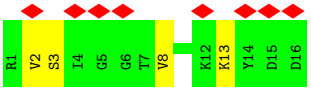
- Molecule 3: unknown peptide C

Chain Bl:



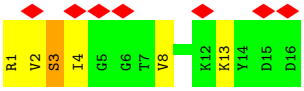
- Molecule 3: unknown peptide C

Chain Bs:



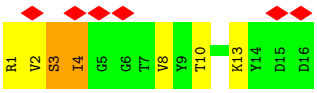
- Molecule 3: unknown peptide C

Chain Bz:



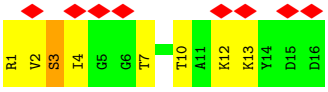
- Molecule 3: unknown peptide C

Chain Cg:



• Molecule 3: unknown peptide C

Chain Cn:



• Molecule 3: unknown peptide C

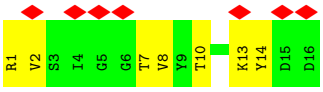
Chain Cu:

• Molecule 3: unknown peptide C

Chain Db:

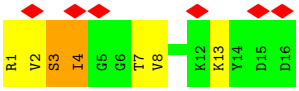
• Molecule 3: unknown peptide C

Chain Di:



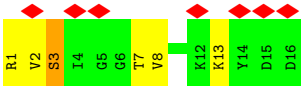
• Molecule 3: unknown peptide C

Chain Dp:



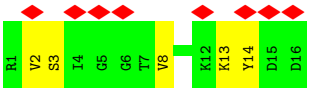
• Molecule 3: unknown peptide C

Chain Dw:



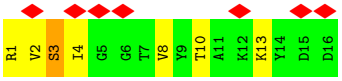
• Molecule 3: unknown peptide C

Chain Ed: 50% 69% 31%



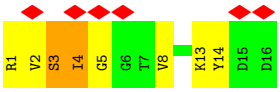
• Molecule 3: unknown peptide C

Chain Ek: 44% 56% 38% 6%



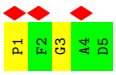
• Molecule 3: unknown peptide C

Chain Er: 38% 50% 38% 12%



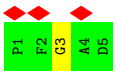
• Molecule 4: unknown peptide D

Chain Ad: 60% 60% 40%



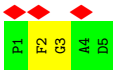
• Molecule 4: unknown peptide D

Chain Ak: 60% 80% 20%



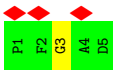
• Molecule 4: unknown peptide D

Chain Ar: 60% 60% 40%



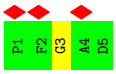
• Molecule 4: unknown peptide D

Chain Ay: 60% 80% 20%



• Molecule 4: unknown peptide D

Chain Bf:

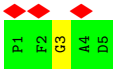


• Molecule 4: unknown peptide D

Chain Bm:

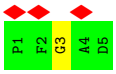
• Molecule 4: unknown peptide D

Chain Bt:



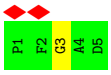
• Molecule 4: unknown peptide D

Chain Ca:



• Molecule 4: unknown peptide D

Chain Ch:



• Molecule 4: unknown peptide D

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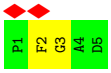
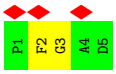


• Molecule 4: unknown peptide D

Chain Cv:

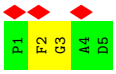
• Molecule 4: unknown peptide D

Chain Dc:



- Molecule 4: unknown peptide D

Chain Dj:



- Molecule 4: unknown peptide D

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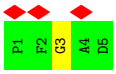
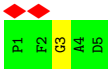


- Molecule 4: unknown peptide D

Chain Dx:



- Molecule 4: unknown peptide D

Chain Ee:

- Molecule 4: unknown peptide D

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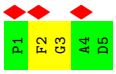
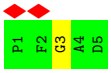


- Molecule 4: unknown peptide D

Chain Es:



- Molecule 5: IcmG (DotF)

Chain Ae: 19% 5% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 Q213 I216 R219 A220 W221 R253 I254 L255 V261 I262 K263 F264 S269

- Molecule 5: IcmG (DotF)

Chain Al: 19% 5% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 Q213 R219 I223 D248 R253 I254 L255 V261 I262 K263 F264 S269

- Molecule 5: IcmG (DotF)

Chain As: 19% 5% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

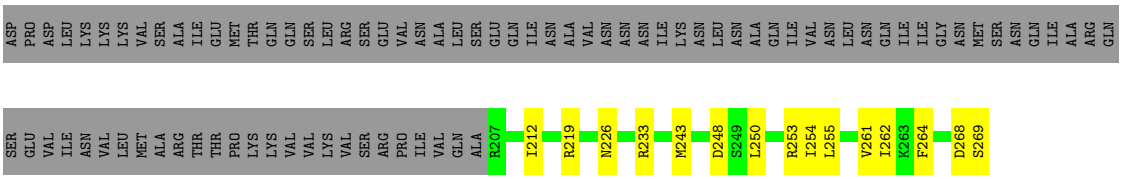
SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 R219 R233 L250 R253 I254 L255 V261 I262 K263 F264 D268 S269

- Molecule 5: IcmG (DotF)

Chain Az: 18% 6% 77%

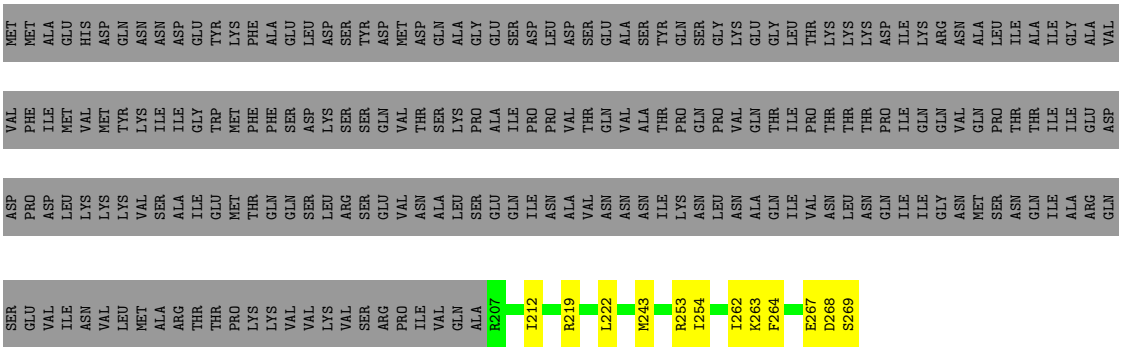
MET MET ALA GLU HIS ASP GLN ASN ASN ASP GLU TYR LYS PHE ALA GLU LEU ASP SER TYR ASP MET ASP GLN ALA GLY GLU SER ASP LEU ASP SER GLU ALA SER TYR GLN SER GLY LYS GLU GLY LEU THR LYS LYS ASP ILE LYS ARG ASN ALA LEU ILE ALA ILE GLY ALA VAL

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP



• Molecule 5: IcmG (DotF)

Chain Bg:



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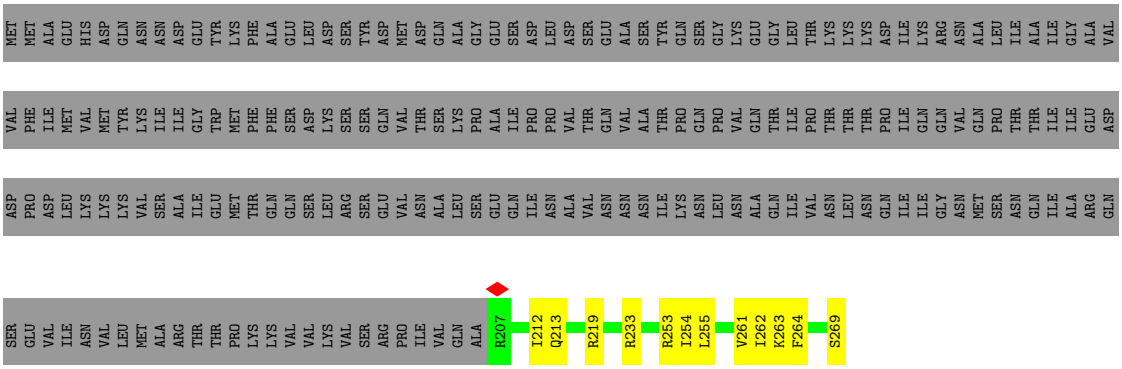

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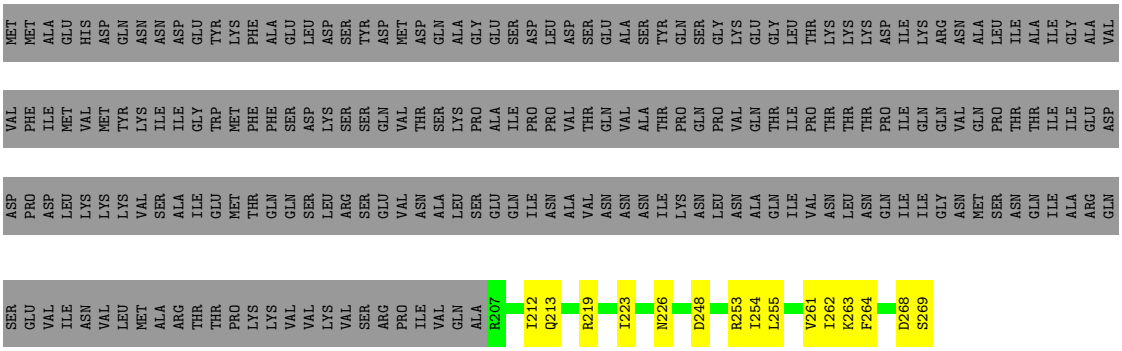


• Molecule 5: IcmG (DotF)

Chain Cb: 18% 6% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 G218 R219 R233 K237 R253 I254 L255 V261 I262 K263 F264 S265 D268 S269

- Molecule 5: IcmG (DotF)

Chain Ci: 19% • 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 Q213 R219 R233 S249 L250 Q251 G252 R253 I254 L255 I262 K263 F264 S269

- Molecule 5: IcmG (DotF)

Chain Cp: 18% 5% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP

ASP PRO ASP LEU LYS LYS LYS VAL SER ALA ILE GLU MET THR GLN GLN SER LEU ARG SER GLU VAL ASN ALA LEU SER GLU GLN ILE ASN ALA VAL ASN ASN ASN ILE LYS ASN LEU ASN ALA GLN ILE VAL ASN LEU ASN GLN ILE ILE GLY ASN MET SER ASN GLN ILE ALA ARG GLN

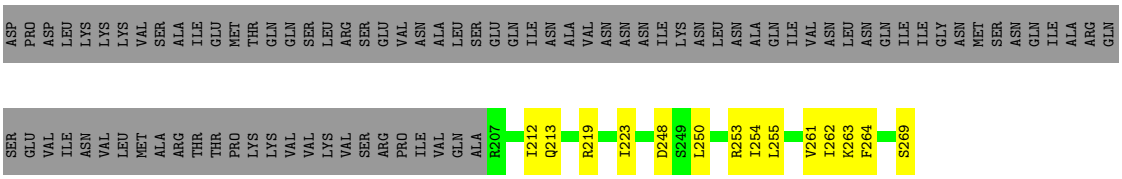
SER GLU VAL ILE ASN VAL LEU MET ALA ARG THR THR PRO LYS LYS VAL VAL LYS VAL SER ARG PRO ILE VAL GLN ALA R207 I212 Q213 I216 R219 A220 W221 Q251 G252 R253 I254 L255 V261 I262 K263 F264 S269

- Molecule 5: IcmG (DotF)

Chain Cw: 18% 5% 77%

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

VAL PHE ILE MET VAL MET TYR LYS ILE ILE GLY TRP MET PHE PHE SER ASP LYS SER SER GLN VAL THR SER LYS PRO ALA ILE PRO PRO VAL THR GLN VAL ALA THR PRO GLN PRO VAL GLN THR ILE PRO THR THR THR PRO ILE GLN GLN VAL GLN PRO THR THR ILE ILE GLU ASP



• Molecule 5: IcmG (DotF)

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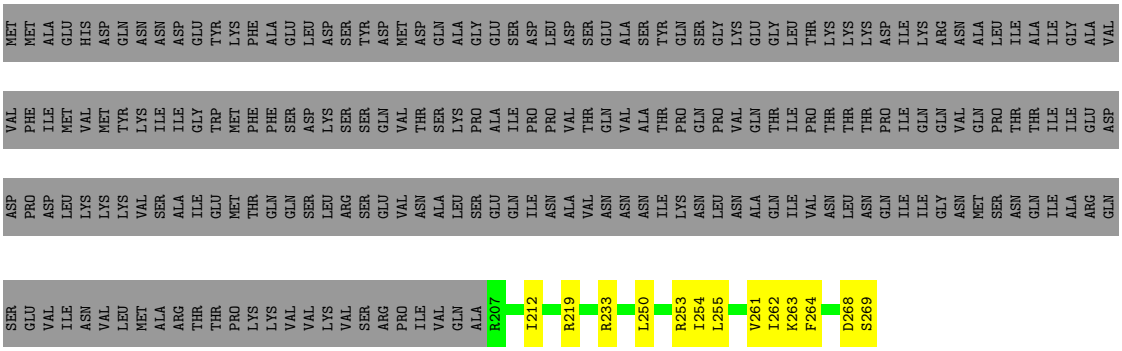

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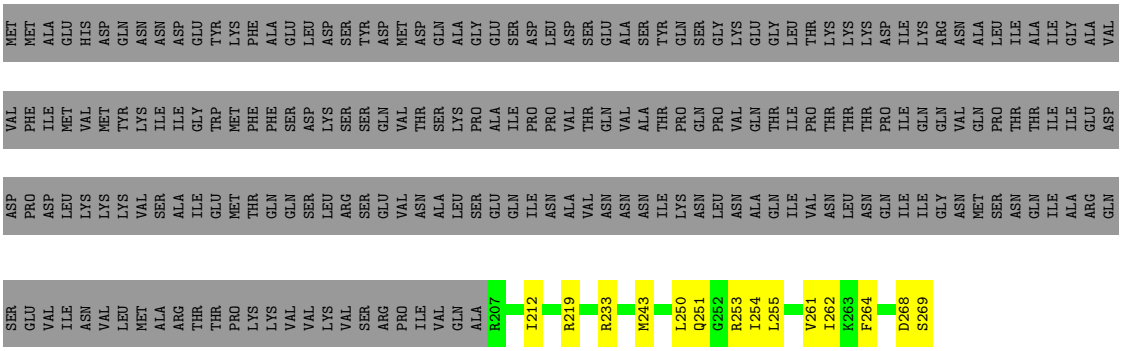

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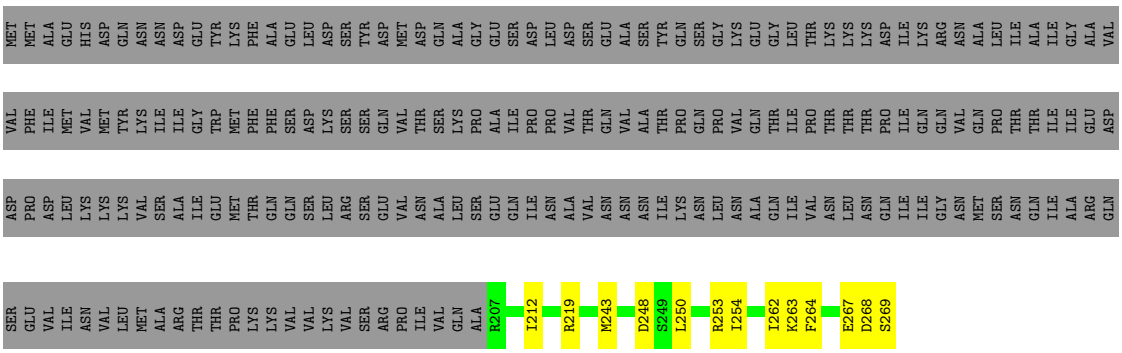
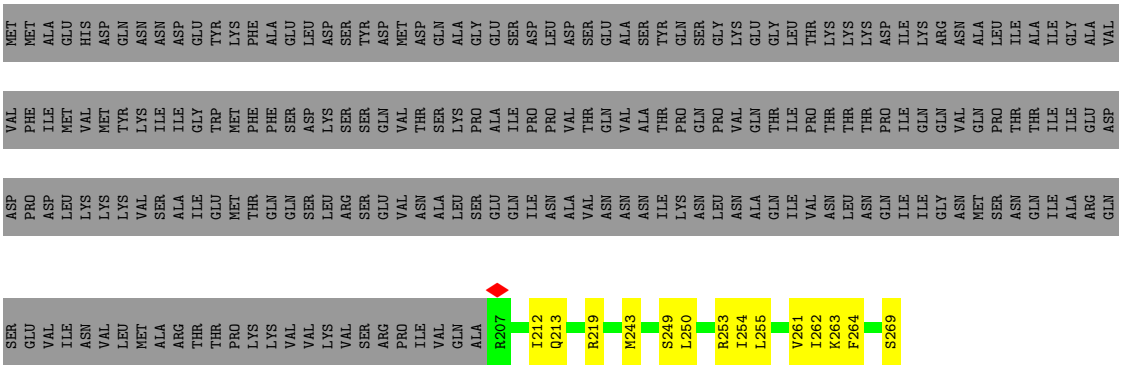


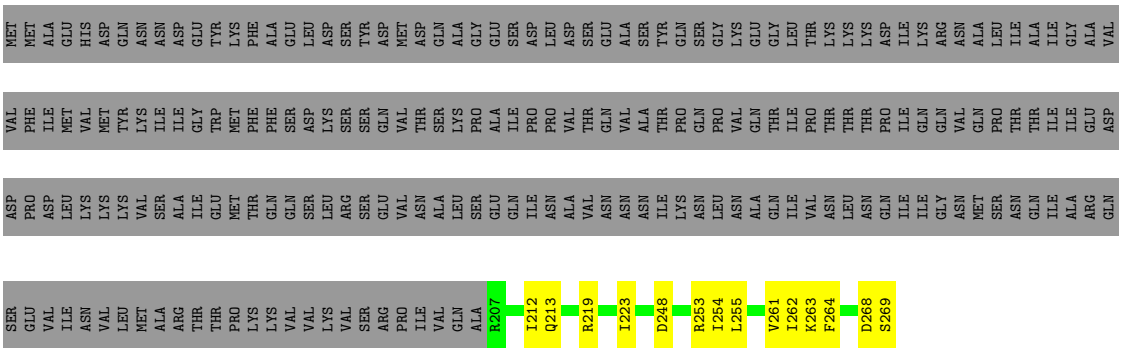
• Molecule 5: IcmG (DotF)

Chain Dy: 18% 5% 77%



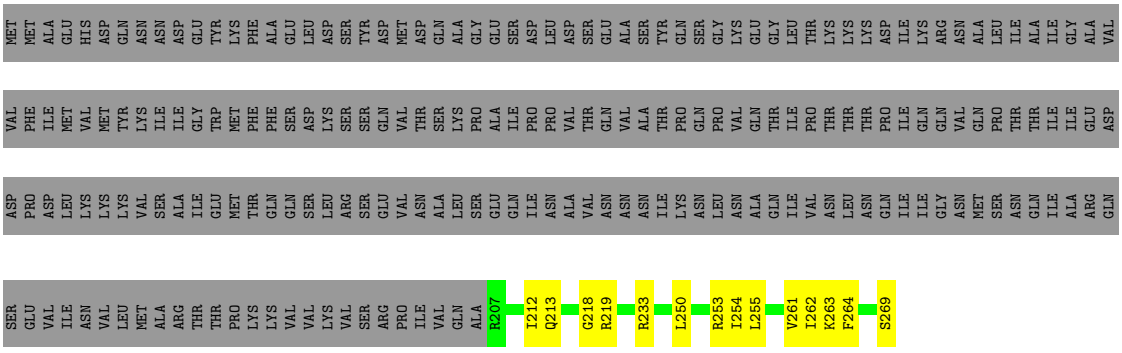
• Molecule 5: IcmG (DotF)

Chain Ef: 18% 5% 77%



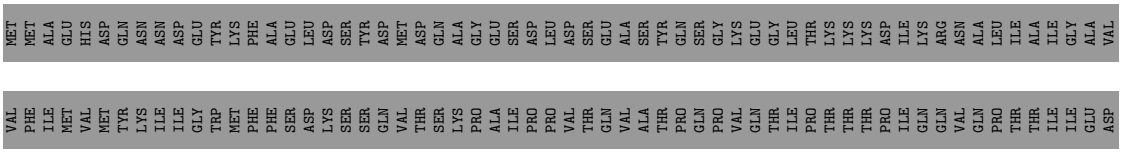
• Molecule 5: IcmG (DotF)

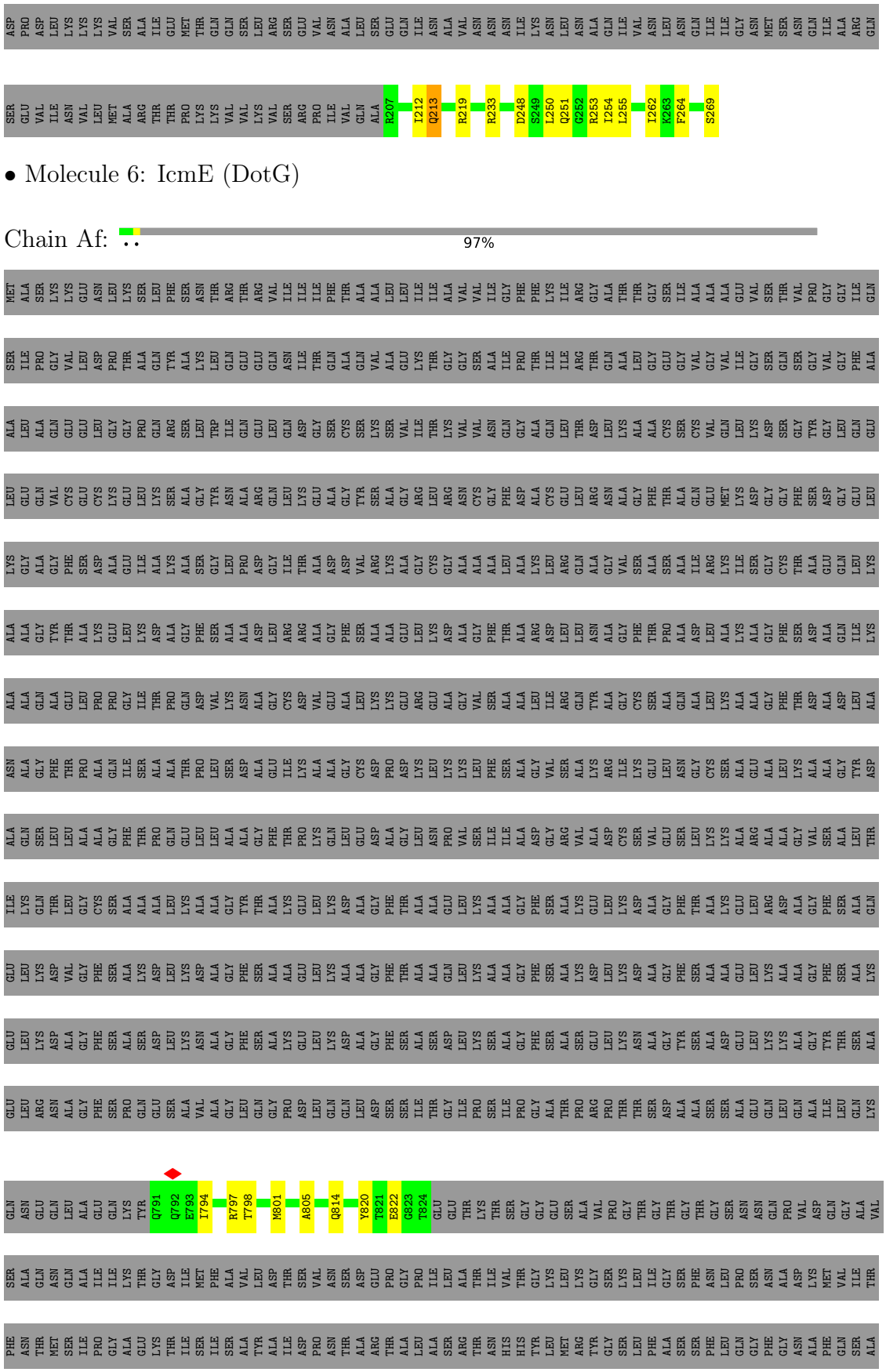
Chain Em: 18% 5% 77%



• Molecule 5: IcmG (DotF)

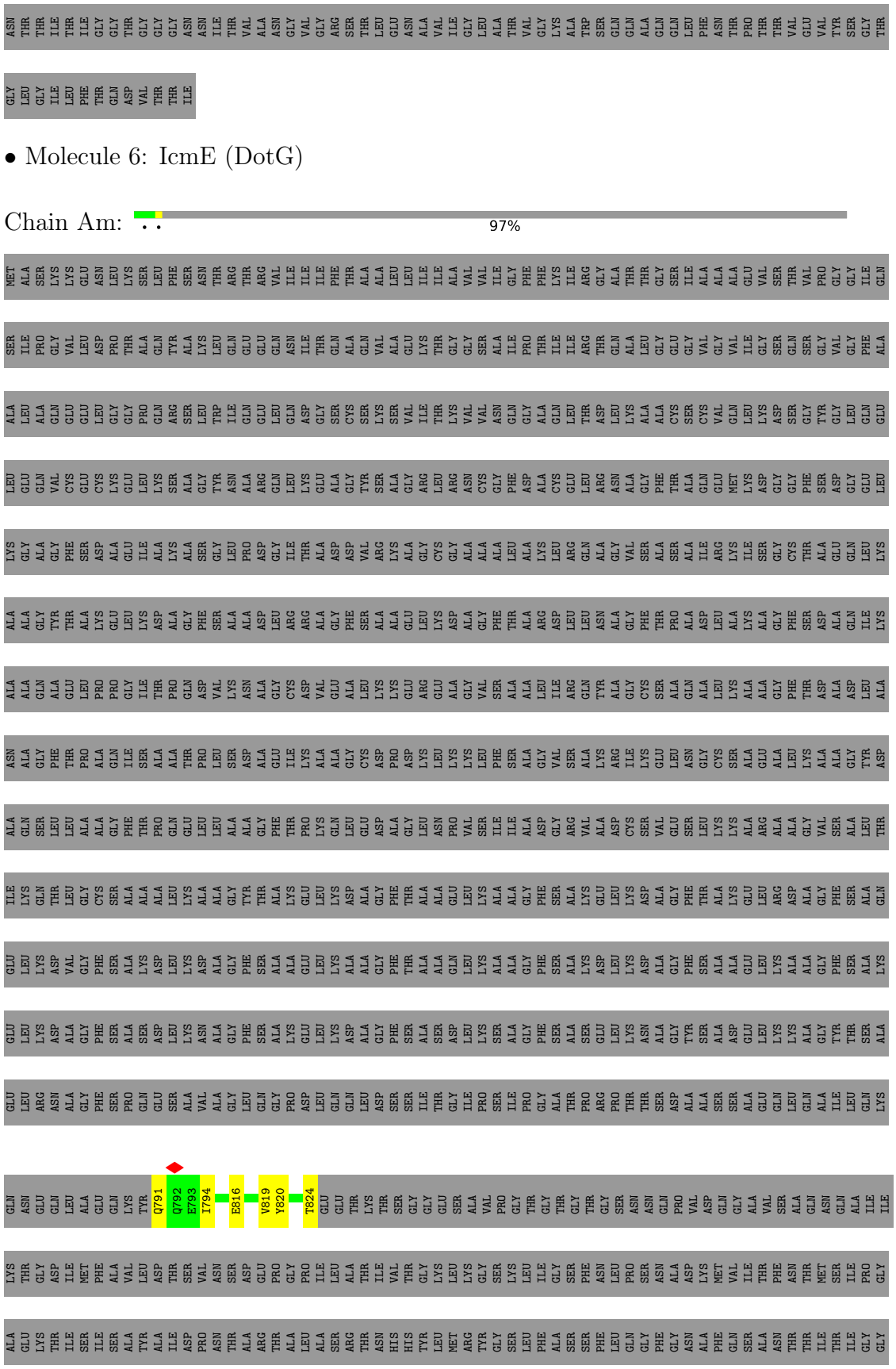
Chain Et: 19% • 77%





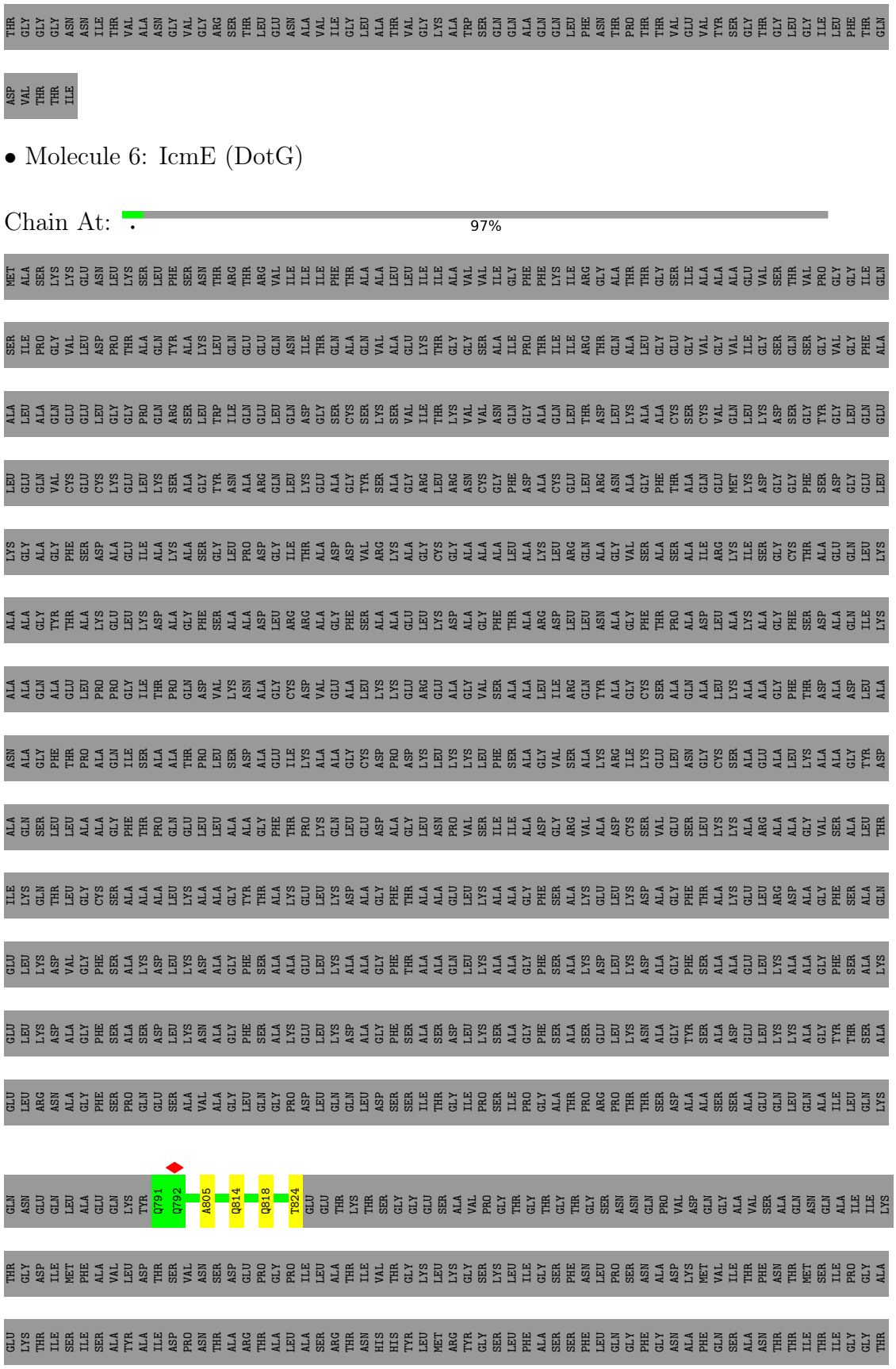
• Molecule 6: IcmE (DotG)

Chain Af: 97%



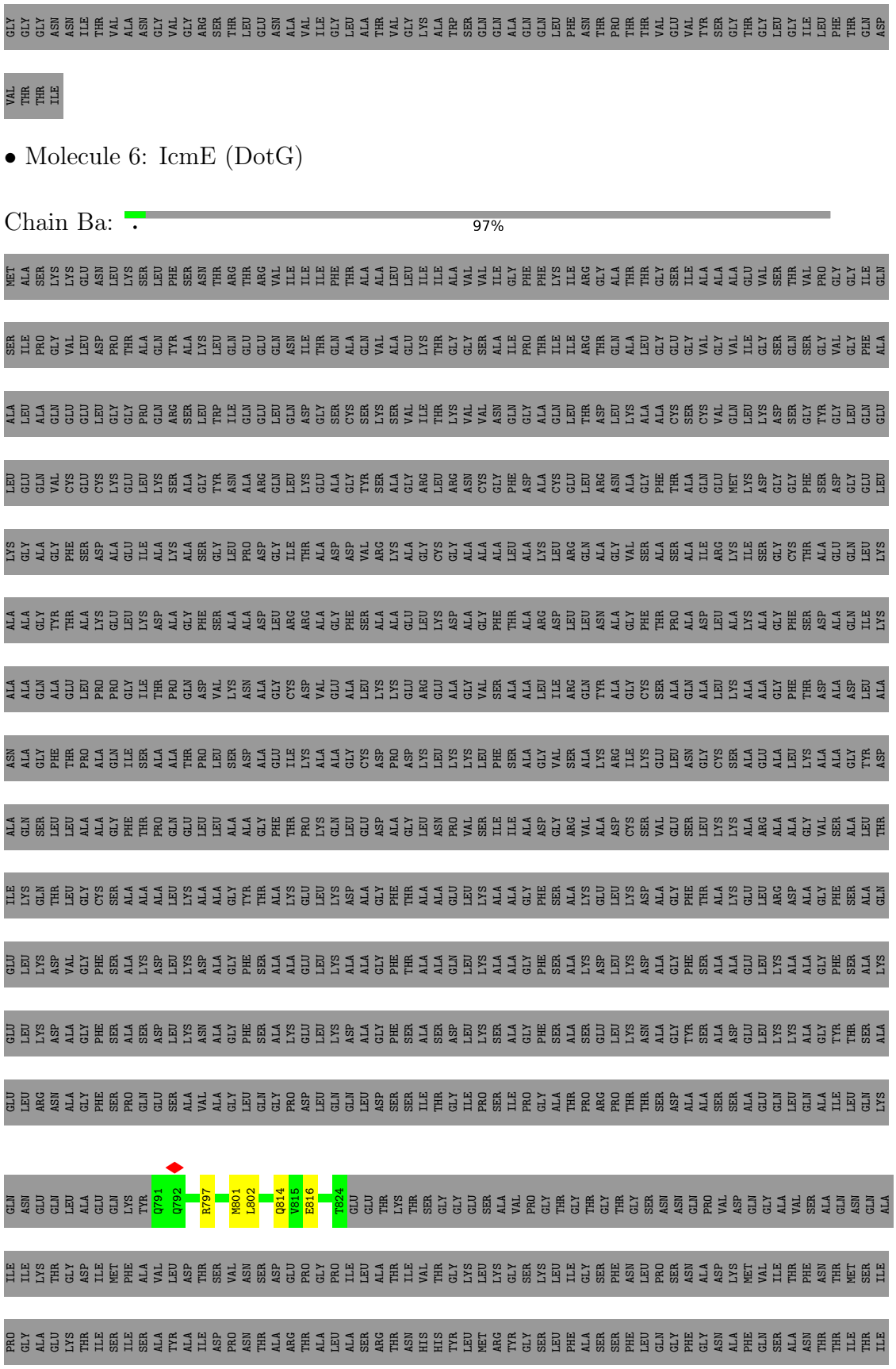
• Molecule 6: IcmE (DotG)

Chain Am: 97%



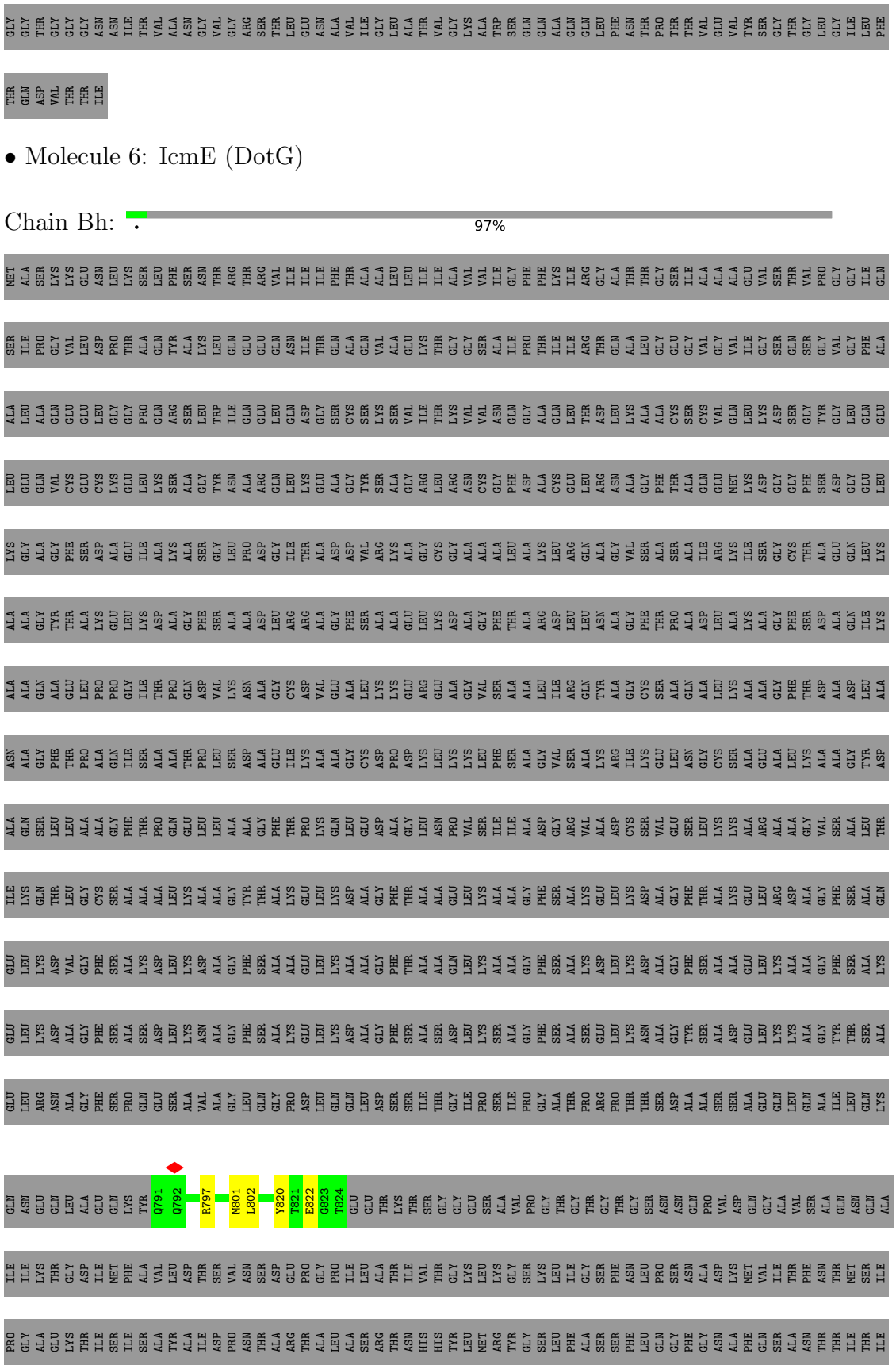
• Molecule 6: IcmE (DotG)

Chain At: . 97%



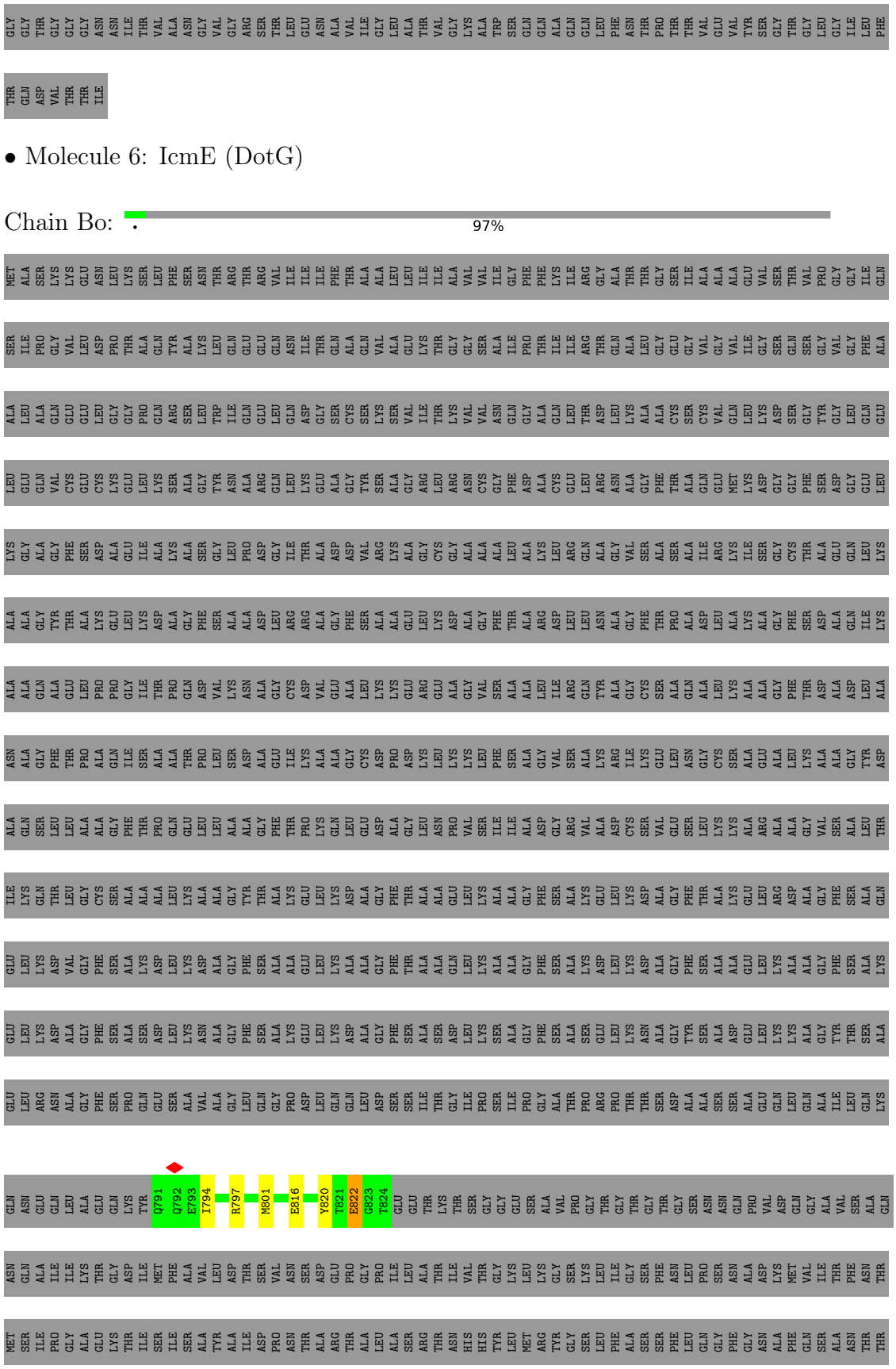
- Molecule 6: IcmE (DotG)

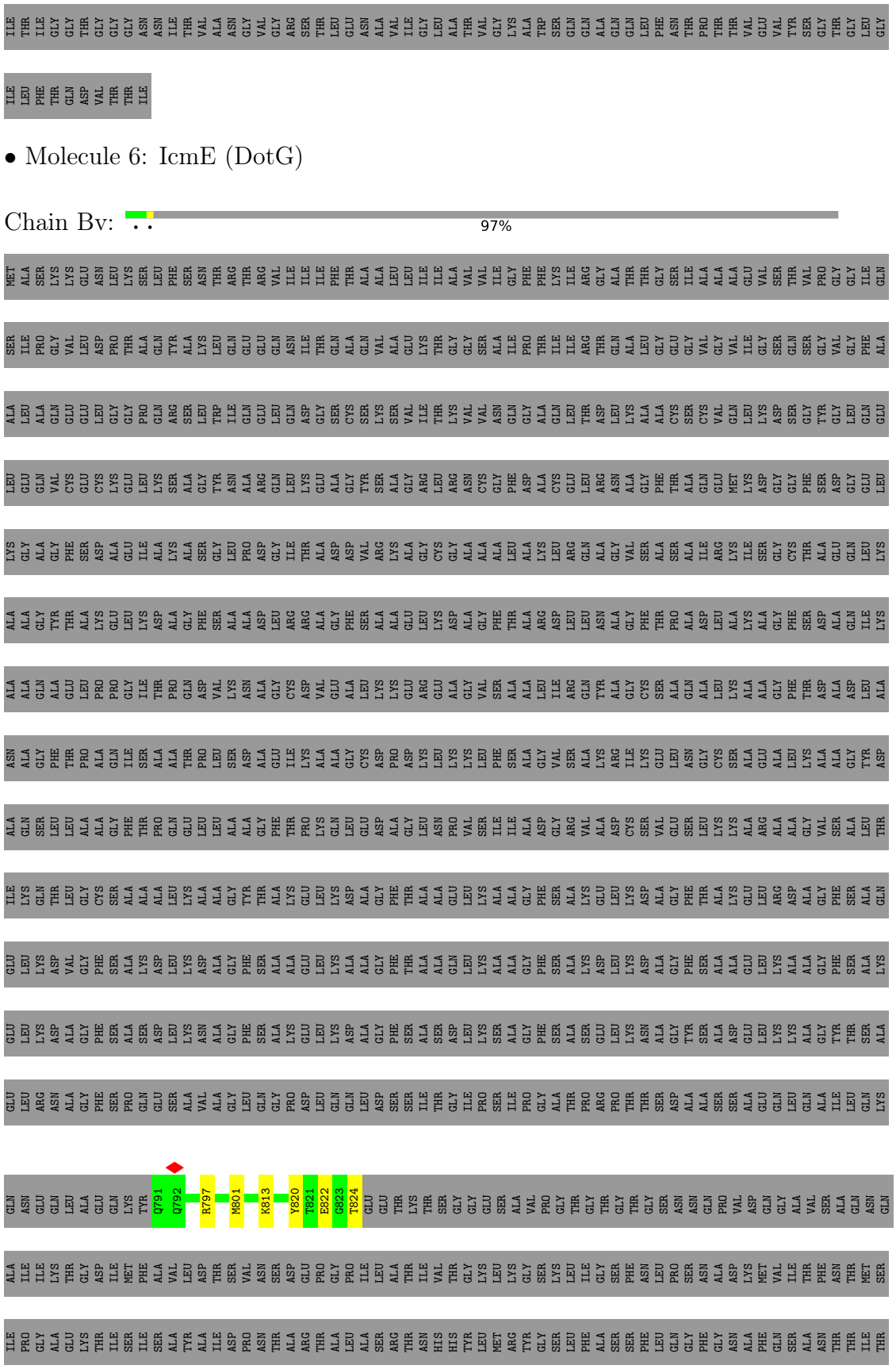
Chain Ba: 97%



- Molecule 6: IcmE (DotG)

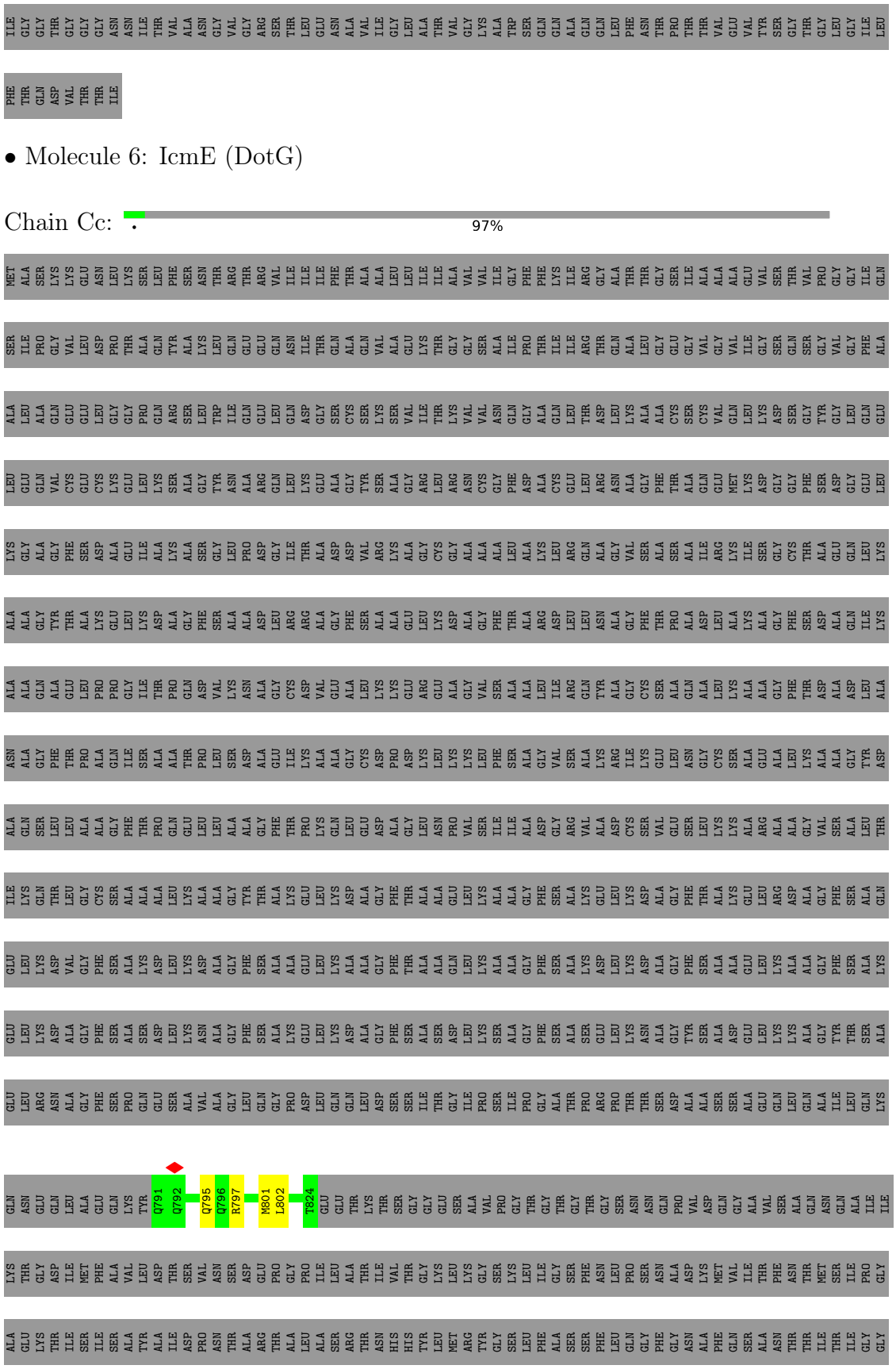
Chain Bh: 97%


GLY GLY THR GLY GLY GLY ASN ASN ILE THR VAL ALA ASN GLY VAL GLY ARG SER THR LEU GLU ASN ALA VAL ILE GLY LEU ALA THR VAL GLY LYS ALA TRP SER GLN GLN ALA GLN GLN LEU PHE ASN THR PRO THR THR VAL GLU VAL TYR SER GLY THR GLY LEU GLY ILE LEU PHE
THR GLN ASP VAL THR THR ILE
• Molecule 6: IcmE (DotG)
Chain Bo:
97%
MET ALA SER LYS LYS GLU ASN LEU LYS SER LEU PHE SER ASN THR ARG THR ARG VAL ILE ILE ILE PHE PHE THR ALA ALA LEU LEU ILE ILE ALA VAL VAL 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 GLN
SER ILE PRO GLY VAL LEU ASP PRO THR ALA GLN TYR ALA LYS LEU GLN GLU GLU GLN ASN ILE THR GLN ALA GLN VAL ALA GLU LYS THR GLY GLY SER ALA ILE PRO THR ILE ILE ARG THR GLN ALA LEU GLY GLU GLY VAL GLY VAL ILE GLY SER GLN SER GLY VAL GLY PHE ALA
ALA LEU ALA GLN GLU GLU LEU GLY GLY PRO GLN ARG SER LEU TRP ILE GLN GLU LEU GLN ASP GLY SER CYS SER LYS SER VAL ILE THR LYS VAL VAL ASN GLN GLY ALA GLN LEU THR ASP LEU LYS ALA ALA CYS SER CYS VAL GLN LEU LYS ASP SER GLY TYR GLY LEU GLN GLU
LEU GLU GLN VAL CYS GLU CYS LYS GLU LEU LYS SER ALA GLY TYR ASN ALA ARG GLN LEU LYS GLU ALA GLY TYR SER ALA GLY ARG LEU ARG ASN CYS GLY PHE ASP ALA CYS GLU LEU ARG ASN ALA GLY PHE THR ALA GLN GLU MET LYS ASP GLY GLY PHE SER ASP GLY GLU LEU
LYS GLY ALA GLY PHE SER ASP ALA GLU ILE ALA LYS ALA SER GLY LEU PRO ASP GLY ILE THR ALA ASP ASP VAL ARG LYS ALA GLY CYS GLY ALA ALA ALA LEU ALA LYS LEU ARG GLN ALA GLY VAL SER ALA SER ALA ILE ARG LYS ILE SER GLY CYS THR ALA GLU GLN LEU LYS
ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA ASP LEU ARG ARG ALA GLY PHE SER ALA ALA GLU LEU LYS ASP ALA GLY PHE THR ALA ARG ASP LEU LEU ASN ALA GLY PHE THR PRO ALA ASP LEU ALA LYS ALA GLY PHE SER ASP ALA GLN ILE LYS
ALA ALA GLN ALA GLU LEU PRO PRO GLY ILE THR PRO GLN ASP VAL LYS ASN ALA GLY CYS ASP VAL GLU ALA LEU LYS LYS GLU ARG GLU ALA GLY VAL SER ALA ALA ALA GLN TYR ALA GLY CYS SER ALA GLN ALA LEU LYS ALA ALA GLY PHE THR ASP ALA ASP LEU ALA
ASN ALA GLY PHE THR PRO ALA GLN ILE SER ALA ALA THR PRO LEU SER ASP ALA GLU ILE LYS ALA ALA GLY CYS ASP PRO ASP LYS LEU LYS LYS LEU PHE SER ALA GLY VAL SER ALA LYS ARG ILE LYS GLU LEU ASN GLY CYS SER ALA GLU ALA LEU LYS ALA GLY TYR ASP
ALA GLN SER LEU LEU ALA ALA GLY PHE THR PRO GLN GLU LEU LEU ALA ALA GLY PHE THR PRO LYS GLN LEU GLU ASP ALA GLY LEU ASN PRO VAL SER ILE ILE ALA ASP GLY ARG VAL ALA ASP CYS SER VAL GLU GLU SER LEU LYS LYS ALA ARG ALA ALA GLY VAL SER ALA LEU THR
ILE LYS GLN THR LEU GLY CYS SER ALA ALA LEU LYS ALA ALA GLY TYR THR ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA LYS GLU ARG ASP ALA ALA GLY PHE SER ALA GLN
GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA ALA GLY PHE SER ALA ALA ALA GLY PHE THR ALA ASP LEU LYS ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS ASP ALA GLY PHE SER ALA LYS
GLU LEU LYS ASP ALA GLY PHE SER ALA SER ASP LEU LYS ASN ALA GLY PHE SER ALA SER GLU LEU LYS ASP ALA GLY PHE SER ALA SER GLU LEU LYS ASN ALA GLY TYR SER ALA ASP GLU LEU LYS ALA ALA GLY TYR THR SER ALA
GLU LEU ARG ASN ALA GLY PHE SER PRO GLN GLU SER ALA VAL ALA GLY LEU GLN GLY PRO ASP LEU GLN GLN LEU ASP SER ILE THR GLY ILE PRO SER ALA GLY ALA THR PRO ARG PRO THR THR SER ASP GLU GLN LEU GLN ALA ILE LEU GLN LYS
GLN ASN GLU GLN LEU ALA GLU GLN LYS TYR Q791 Q792 E793 I794 R797 M801 E816 Y820 T821 E822 G823 T824 GLU GLU THR LYS THR SER GLY GLY GLU SER ALA VAL PRO GLY THR GLY THR GLY SER ASN ASN GLN PRO VAL ASP GLN GLY ALA VAL SER ALA GLN
ASN GLN ALA ILE ILE LYS THR GLY ASP ILE MET PHE ALA VAL LEU ASP THR SER VAL ASN SER ASP GLU PRO GLY PRO ILE LEU ALA THR ILE VAL THR GLY LYS LEU LYS GLY SER PHE ASN LEU PRO SER ASN ALA ASP LYS MET VAL ILE THR PHE ASN THR
MET SER ILE PRO GLY ALA GLU LYS THR ILE SER ILE SER ALA TYR ALA ILE ASP PRO ASN THR ALA ARG THR ALA LEU ALA SER ARG THR ASN HIS HIS TYR LEU MET ARG TYR GLY SER LEU PHE ALA SER SER PHE LEU GLN GLY PHE GLY ASN ALA PHE GLN SER ALA THR



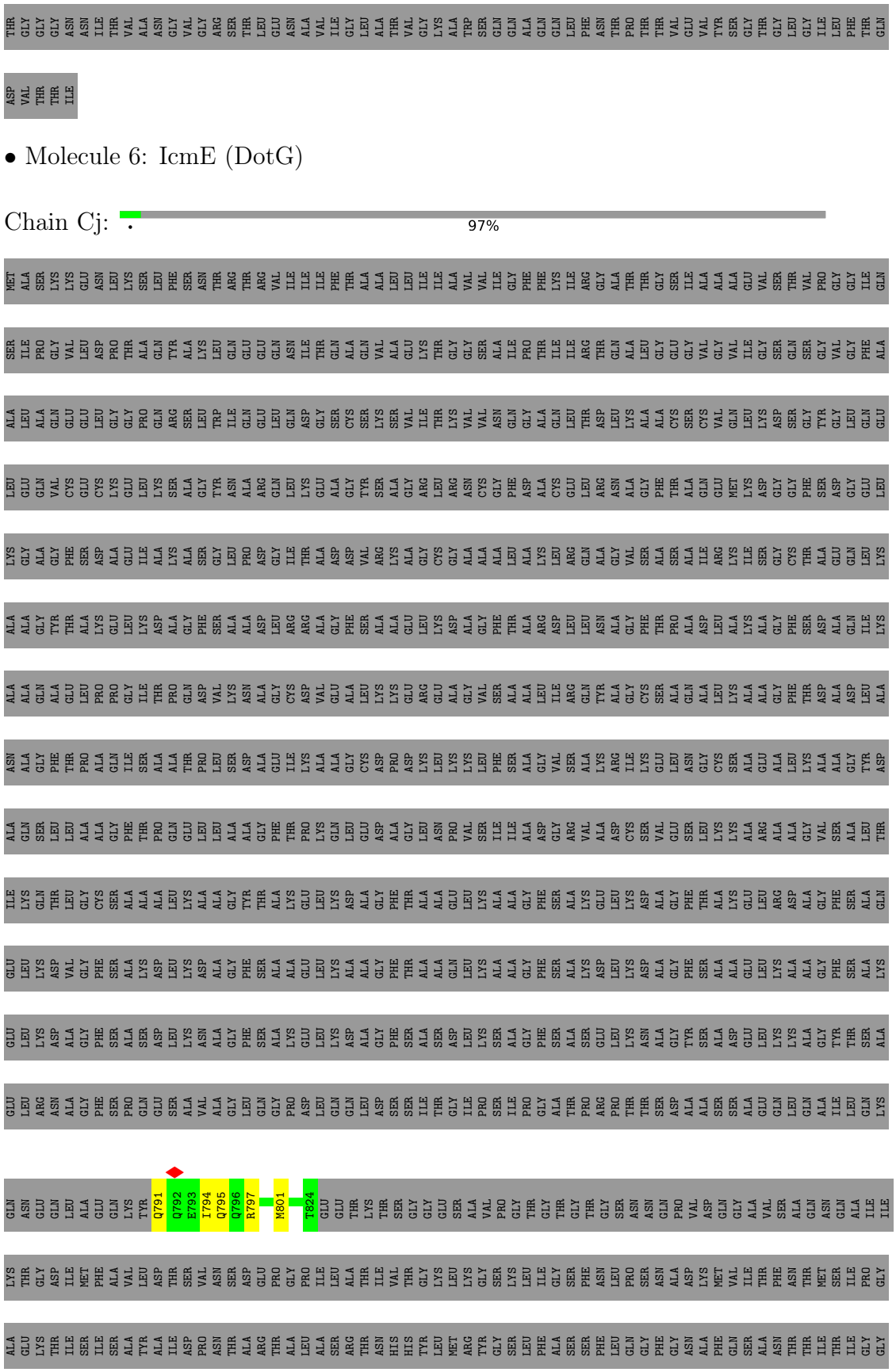
• Molecule 6: IcmE (DotG)

Chain Bv: 97%



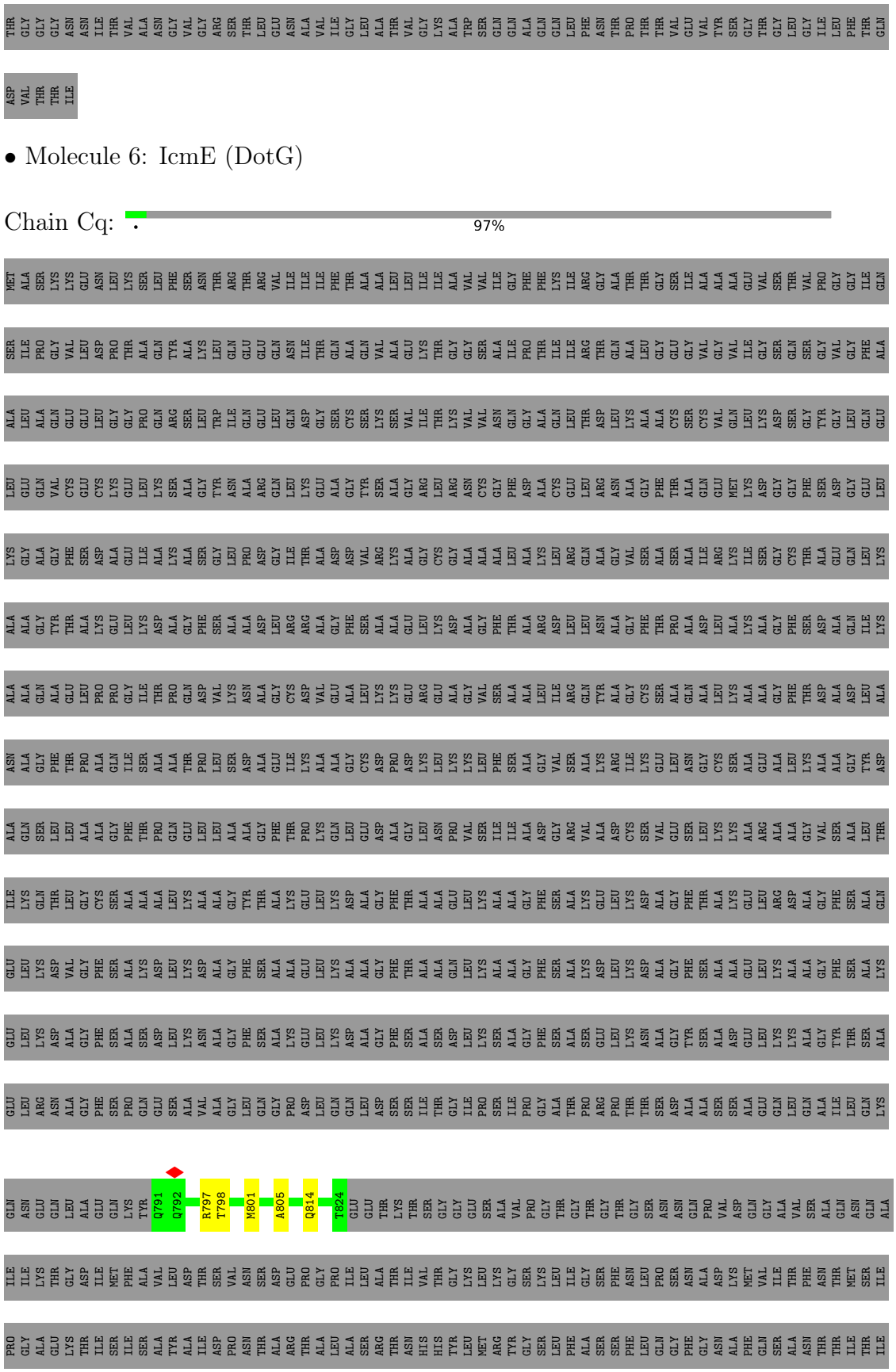
- Molecule 6: IcmE (DotG)

Chain Cc: 97%



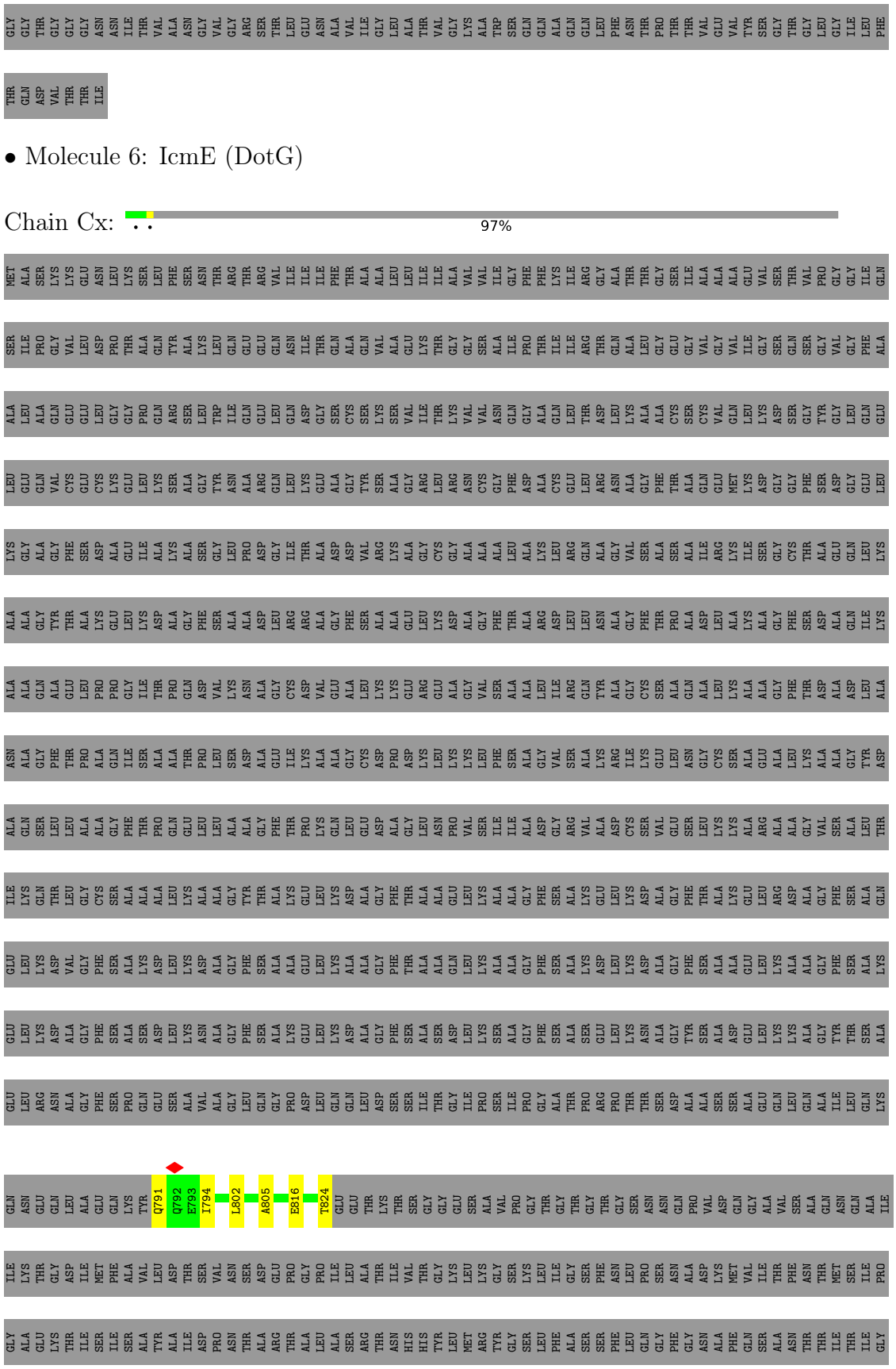
- Molecule 6: IcmE (DotG)

Chain Cj: 97%



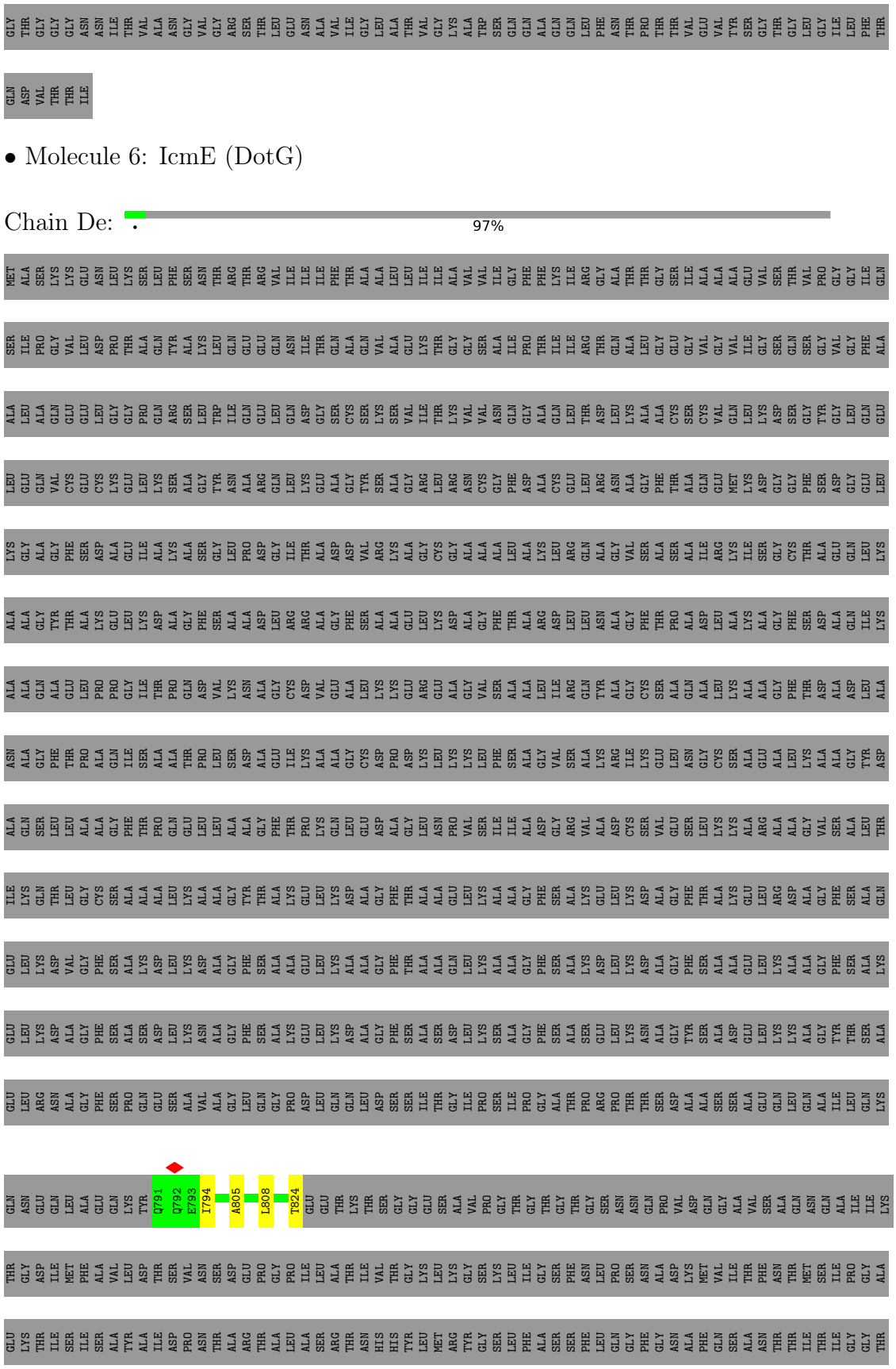
- Molecule 6: IcmE (DotG)

Chain Cq: 97%



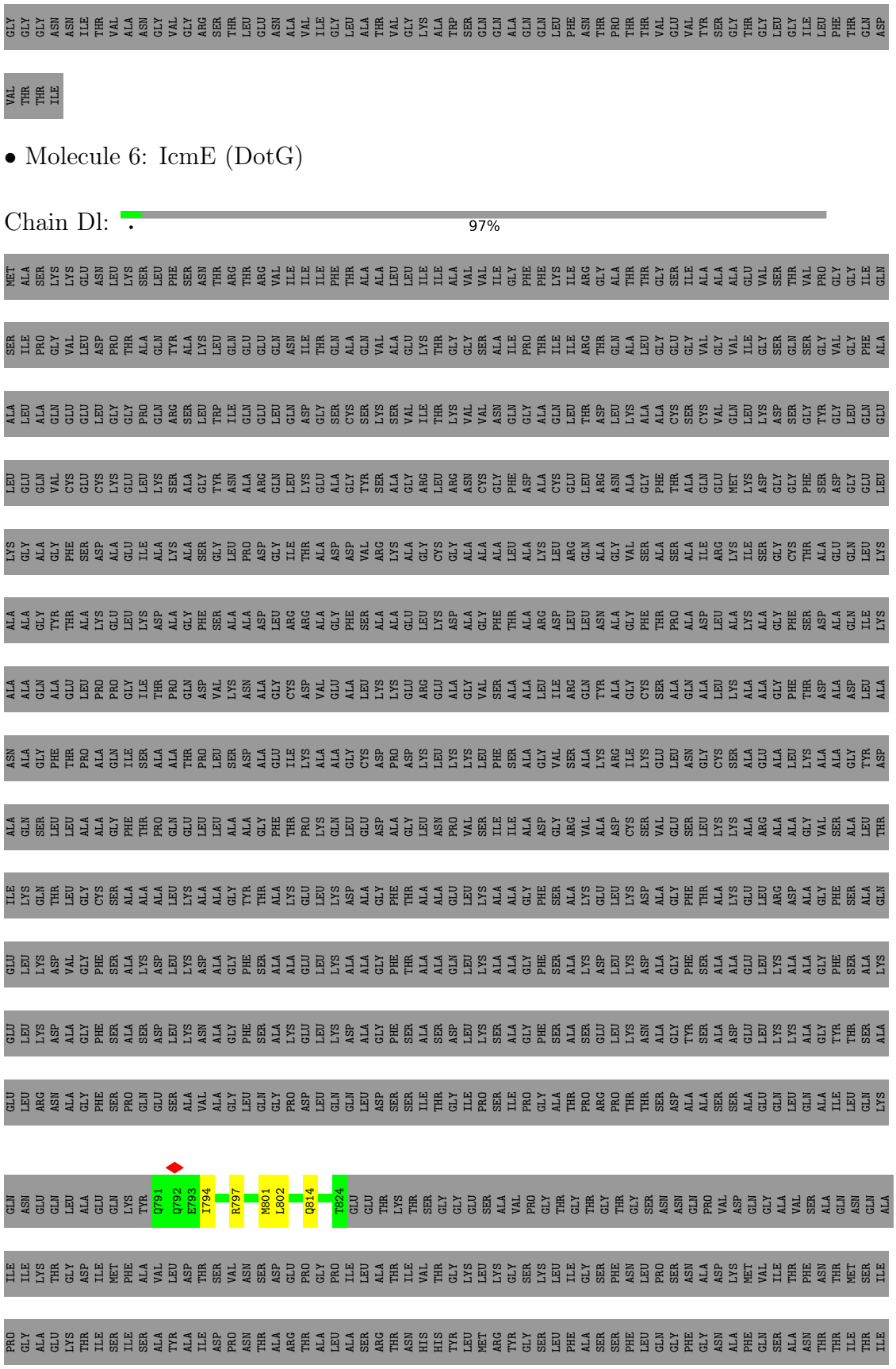
• Molecule 6: IcmE (DotG)

Chain Cx: 97%



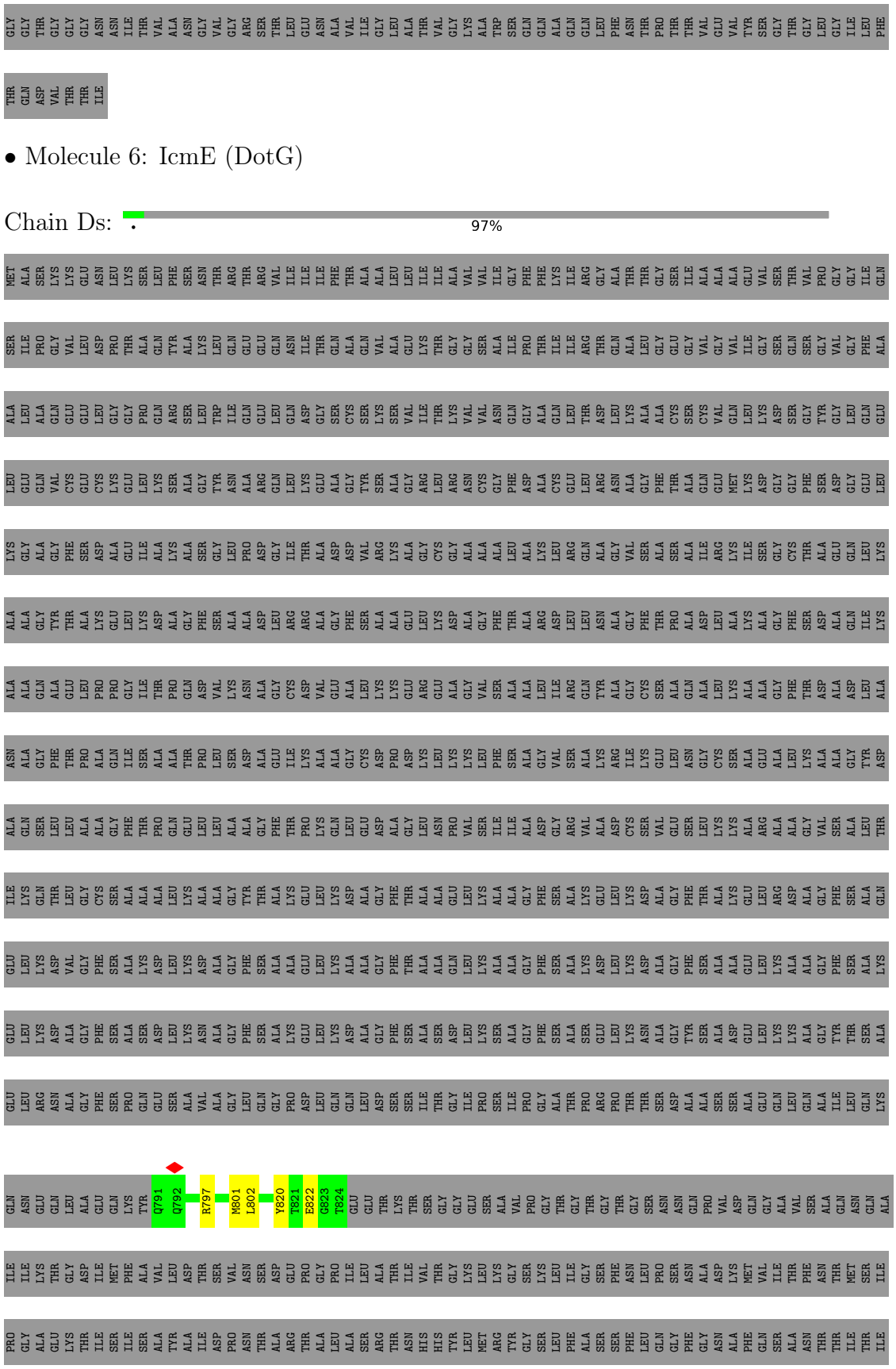
• Molecule 6: IcmE (DotG)

Chain De: 97%



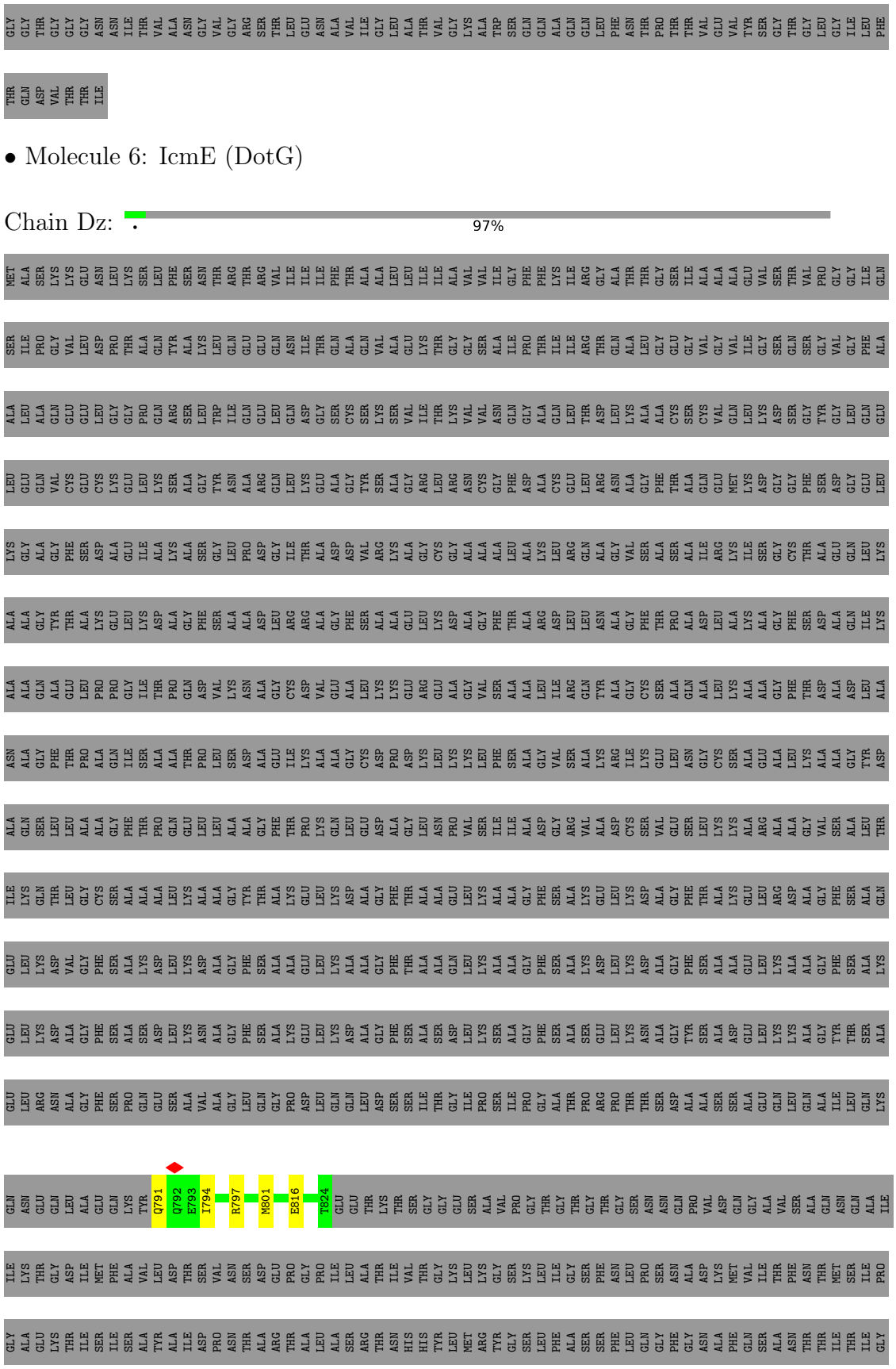
- Molecule 6: IcmE (DotG)

Chain Dl: 97%



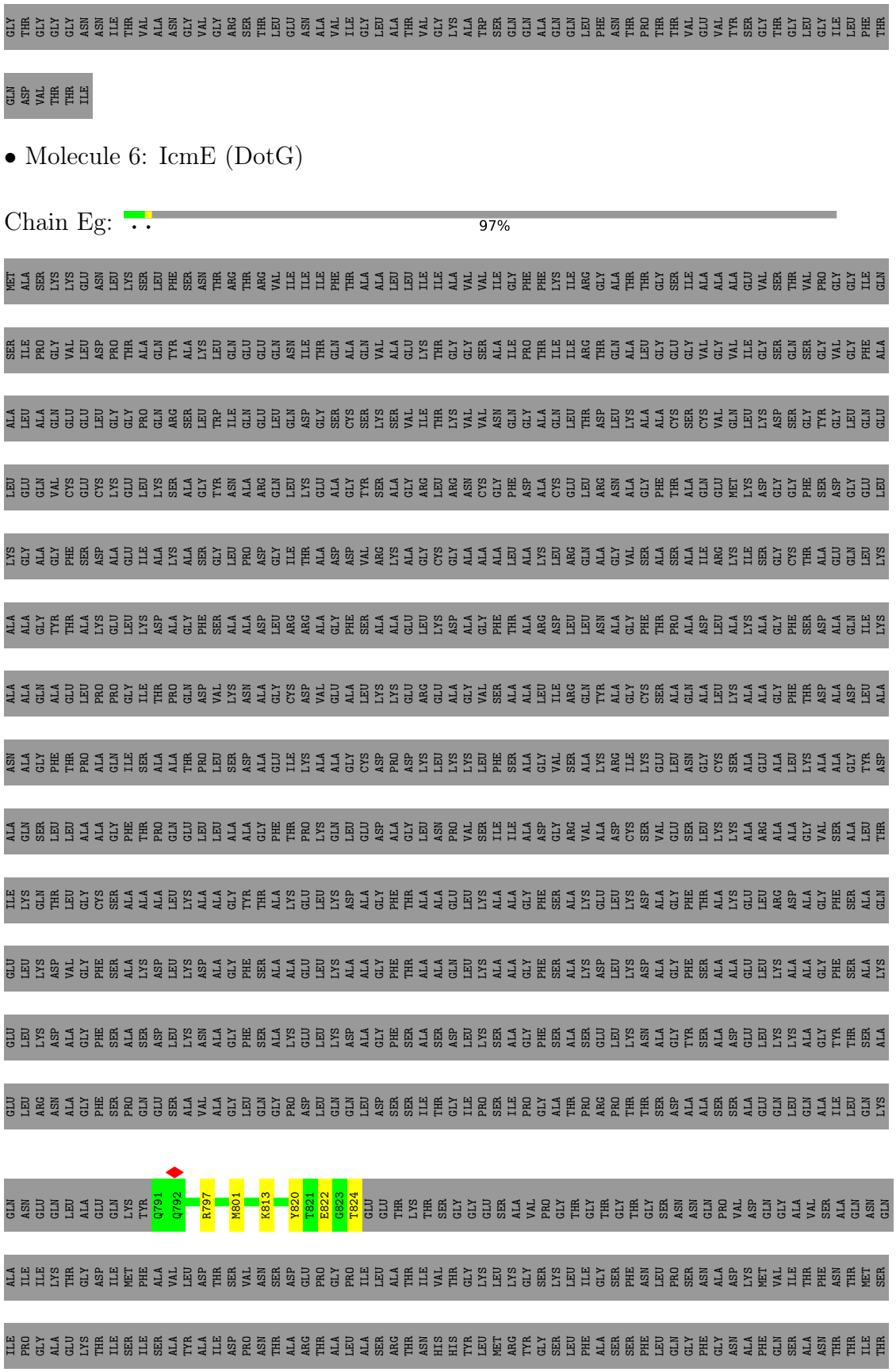
- Molecule 6: IcmE (DotG)

Chain Ds: 97%



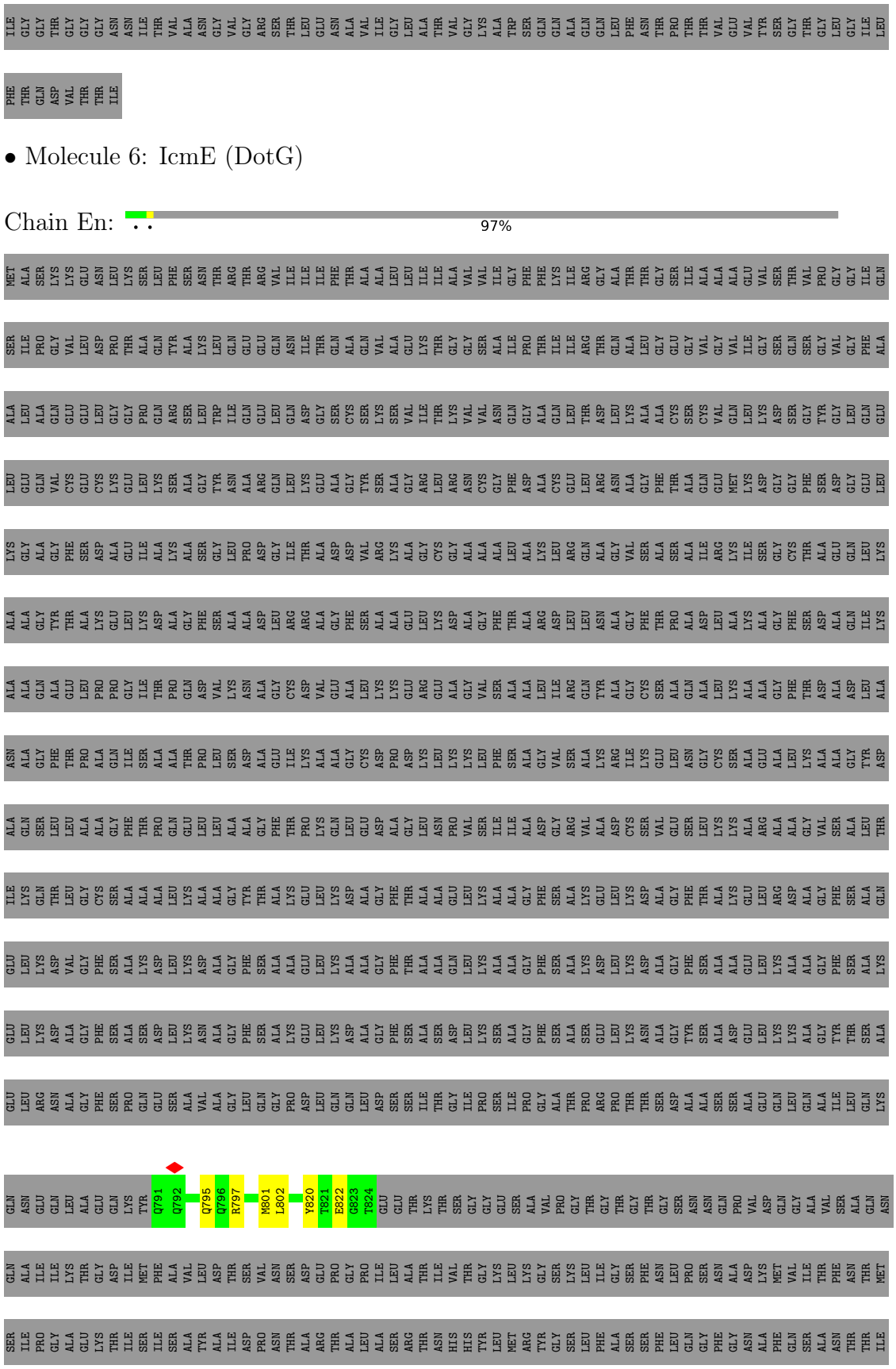
- Molecule 6: IcmE (DotG)

Chain Dz: 97%



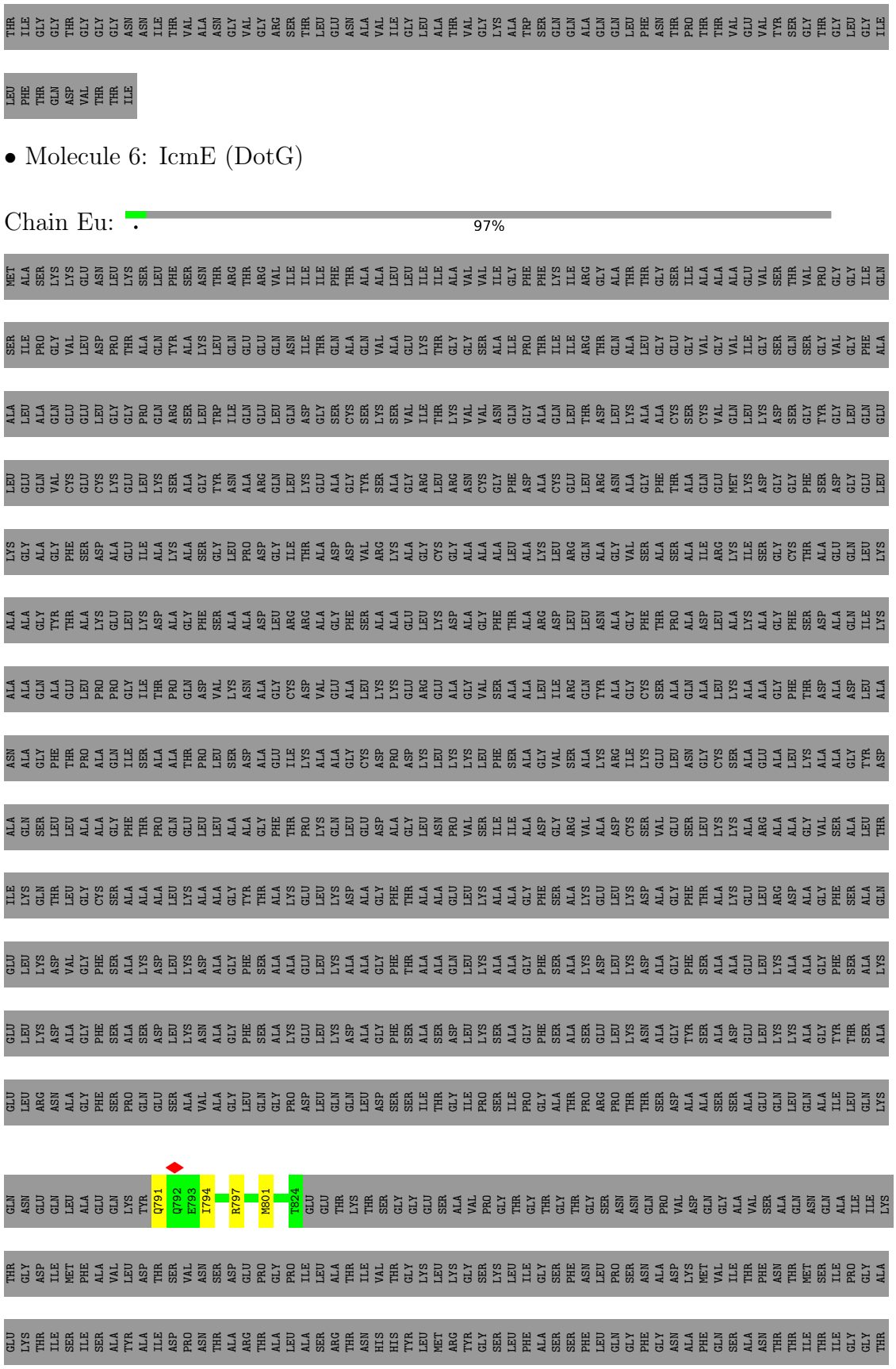
• Molecule 6: IcmE (DotG)

Chain Eg: 97%



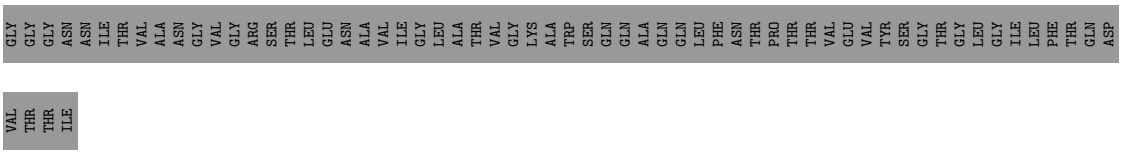
• Molecule 6: IcmE (DotG)

Chain En: 97%



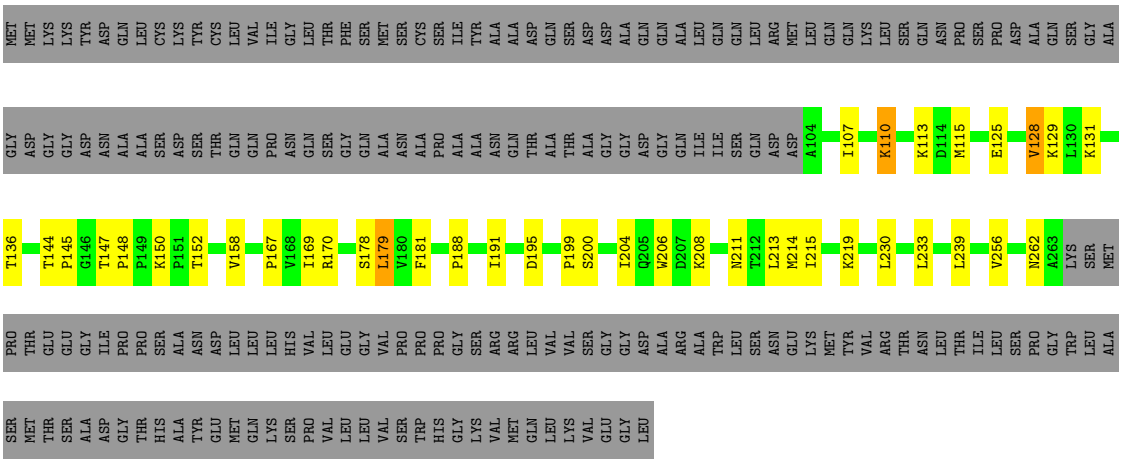
- Molecule 6: IcmE (DotG)

Chain Eu: 97%



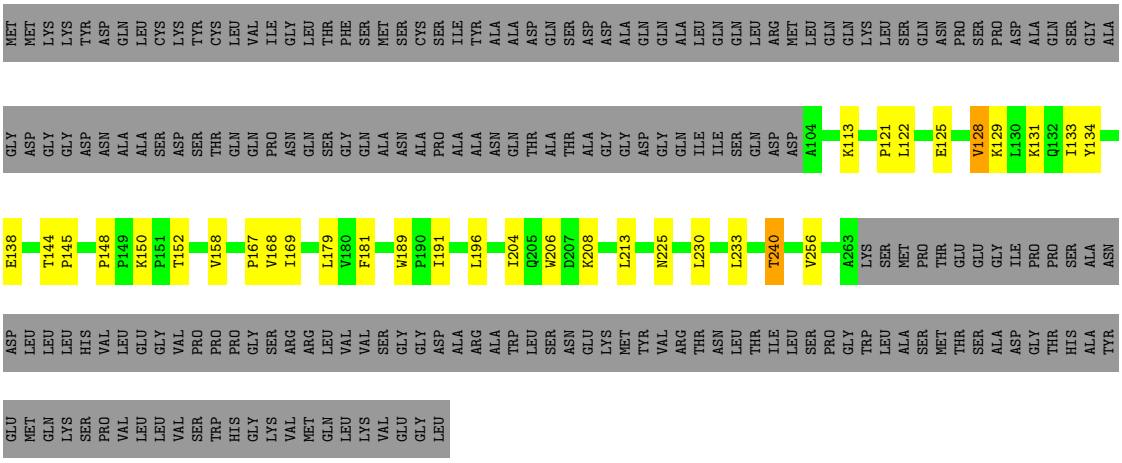
• Molecule 7: IcmK (DotH)

Chain Ag: 33% 10% • 56%



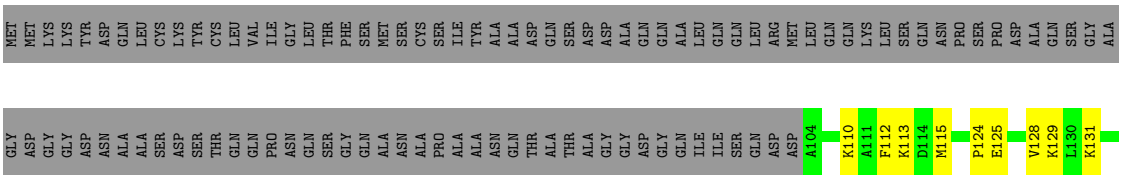
• Molecule 7: IcmK (DotH)

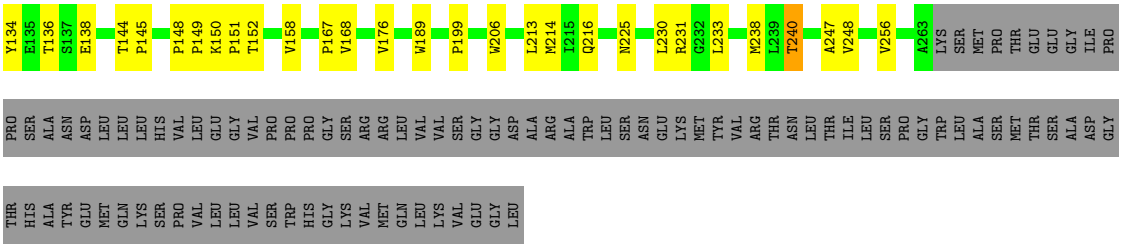
Chain An: 35% 9% • 56%



• Molecule 7: IcmK (DotH)

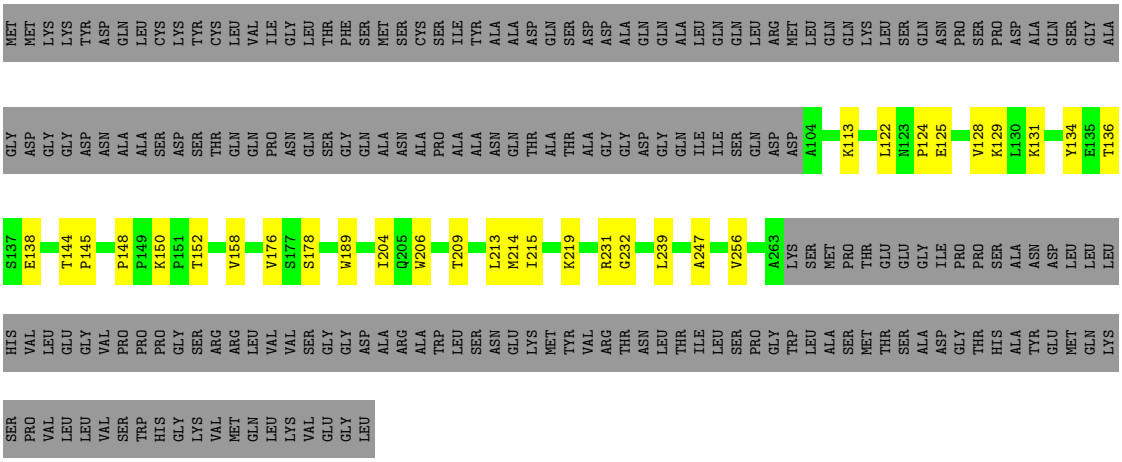
Chain Au: 34% 10% 56%





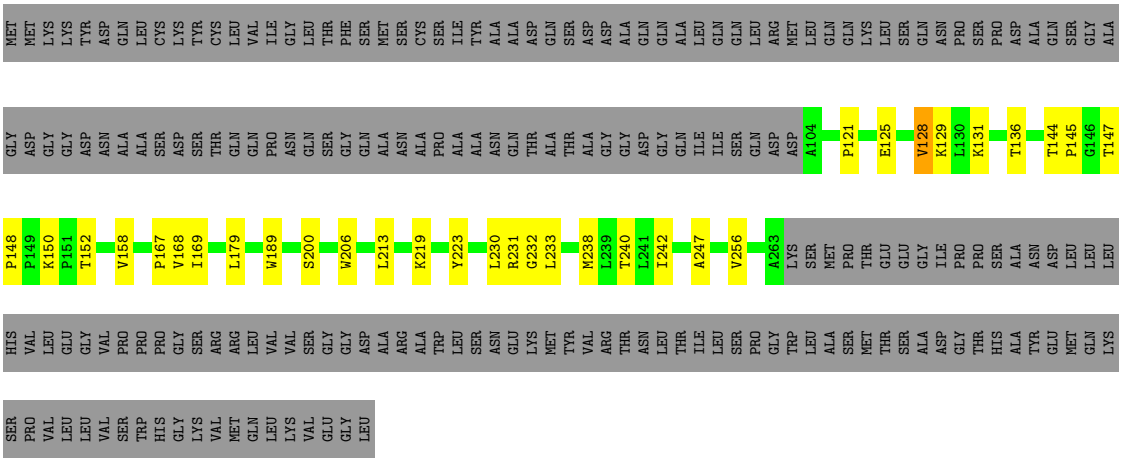
• Molecule 7: IcmK (DotH)

Chain Bb:



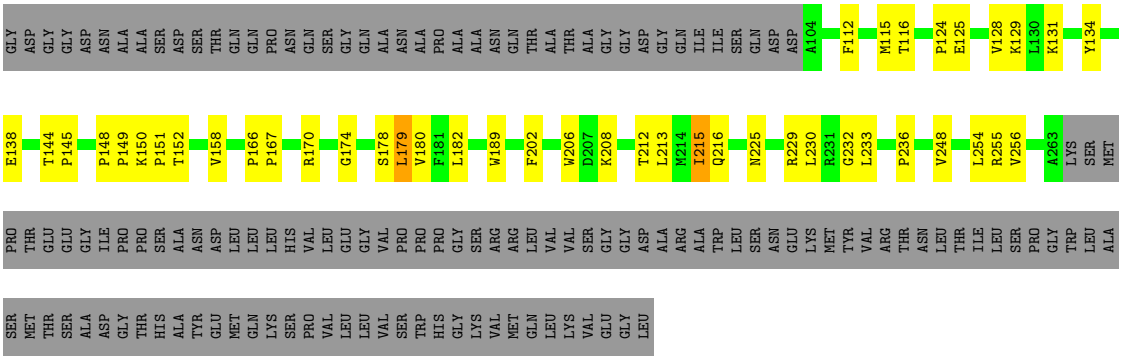
• Molecule 7: IcmK (DotH)

Chain Bi:



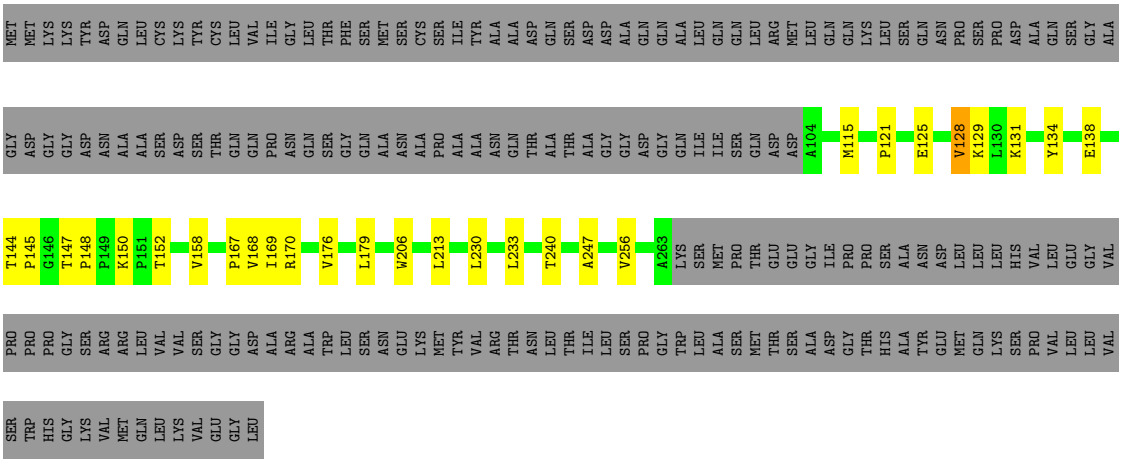
• Molecule 7: IcmK (DotH)

Chain Bp:



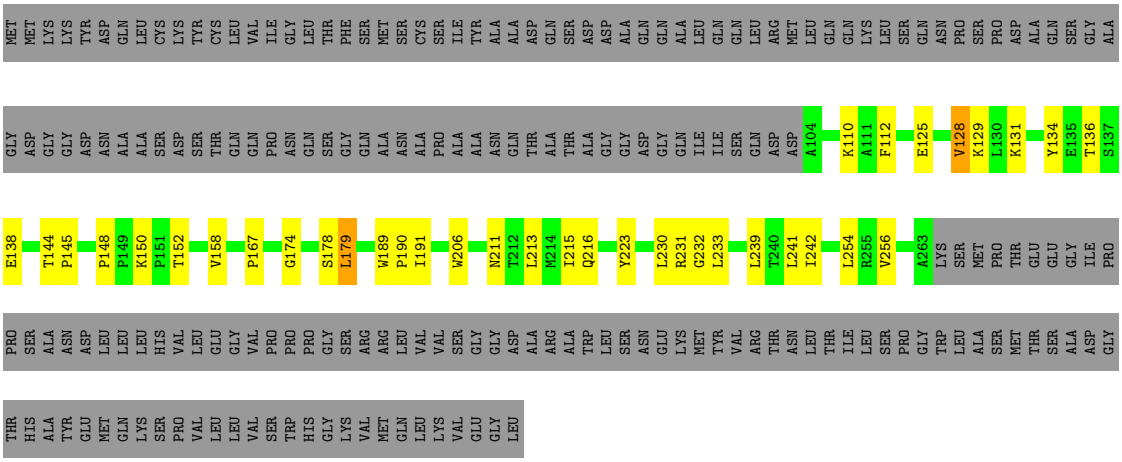
- Molecule 7: IcmK (DotH)

Chain Bw:



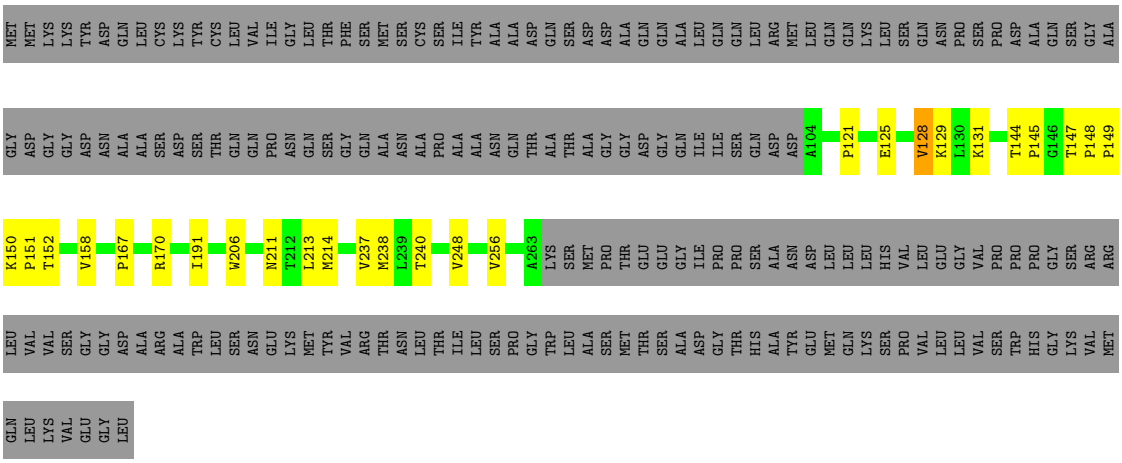
- Molecule 7: IcmK (DotH)

Chain Cd:



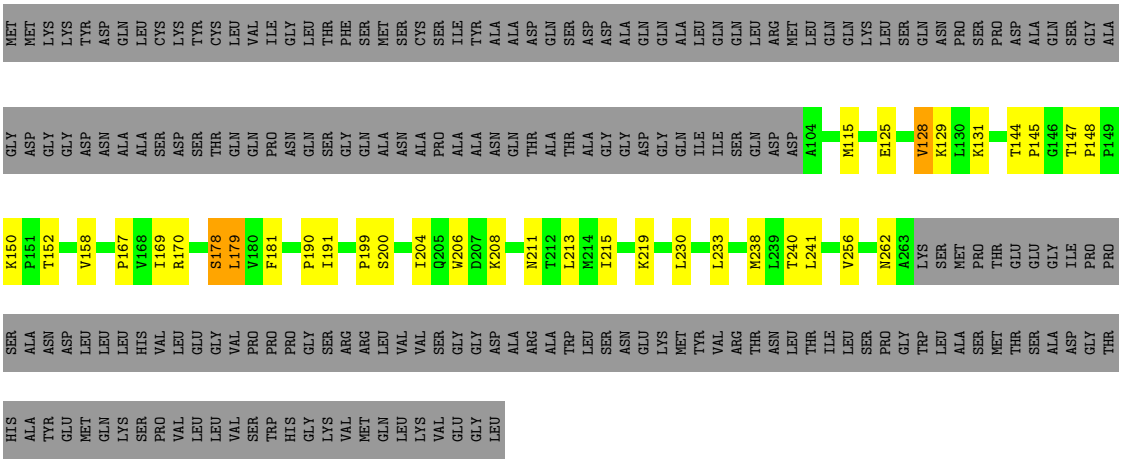
- Molecule 7: IcmK (DotH)

Chain Ck:



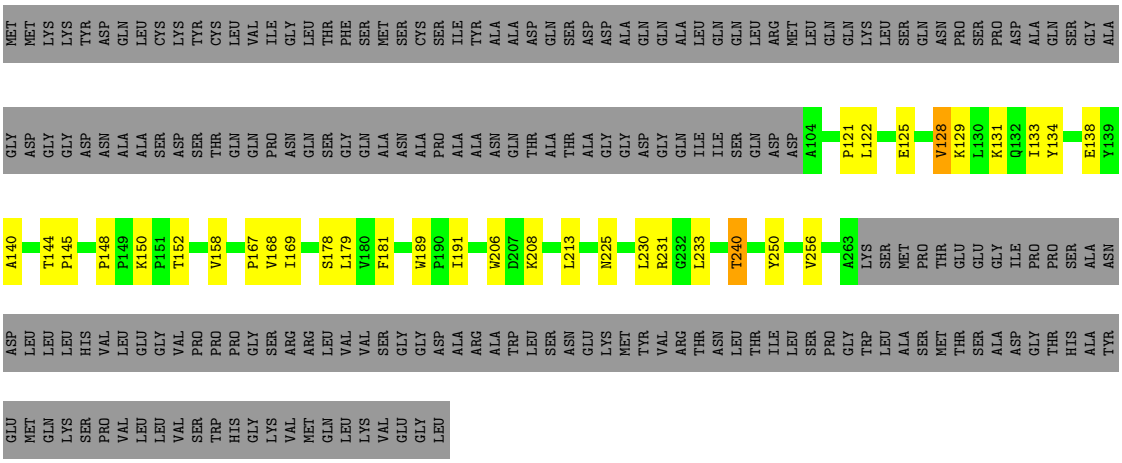
- Molecule 7: IcmK (DotH)

Chain Cr: 34% 9% • 56%



- Molecule 7: IcmK (DotH)

Chain Cy: 35% 9% • 56%



- Molecule 7: IcmK (DotH)

Chain Df: 34% 9% • 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 M115 L122 E125 V128 K129 L130 K131 Y134 E138

T144 P145 P148 P149 K150 P151 T152 V158 P166 P167 V168 V176 F181 W189 P190 I191 D195 W206 L213 M214 N225 L226 L230 L233 M238 L239 T240 A247 V248 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA

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

TYR GLU MET GLN LYS SER PRO VAL LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

• Molecule 7: IcmK (DotH)

Chain Dm: 35% 9% 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 M115 L122 N123 P124 E125 V128 K129 L130 K131 Y134 E135 T136

S137 E138 T144 P145 P148 P149 K150 P151 T152 V158 P166 P167 V176 S177 S178 F181 W189 P190 I191 D195 I204 K208 T209 I215 K219 A227 G232 A247 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA

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

TYR GLU MET GLN LYS SER PRO VAL LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

• Molecule 7: IcmK (DotH)

Chain Dt: 34% 9% • 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 K110 K113 P121 E125 V128 K129 L130 K131 Q132 I133 Y134

E135 T136 S137 E138 T144 P145 G146 T147 P148 P149 K150 P151 T152 V158 P167 V168 W189 S200 W206 L213 K219 Y223 L230 R231 G232 L233 T240 L241 I242 A247 V248 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA

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

TYR GLU MET GLN LYS SER PRO VAL LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

- Molecule 7: IcmK (DotH)

Chain Ea: 31% 13% 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 K110 K113 D114 M115 P124 E125 V128 K129 L130 K131 Y134

E135 T136 S137 E138 T144 P145 P148 P149 K150 P151 T152 V158 P167 R170 G174 S178 L179 V180 F181 L182 W189 L196 N203 I204 Q205 W206 D207 K208 T212 L213 M214 I215 Q216 N225 R229 L230 R231 G232 L233 P236 L241 K246 A247 V248

R251 R255 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA ASN ASP LEU LEU LEU HIS VAL LEU GLU GLY VAL PRO PRO PRO GLY GLY SER ARG ARG LEU VAL VAL SER GLY GLY ASP ALA ARG ALA TRP LEU SER ASN GLU LYS MET TYR VAL ARG THR ASN LEU THR ILE LEU SER PRO GLY TRP LEU ALA SER MET THR SER ALA ASP GLY THR HIS ALA TYR

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

- Molecule 7: IcmK (DotH)

Chain Eh: 35% 9% 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 K113 D114 M115 P124 E125 V128 K129 L130 K131 Y134 E135 T136

S137 E138 T144 P145 P148 P149 K150 P151 T152 V158 P167 V168 I169 R170 V176 L179 A192 W206 T209 L213 M214 L230 R231 G232 L233 M238 L239 T240 A247 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA ASN

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

GLU MET GLN LYS SER PRO VAL LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

- Molecule 7: IcmK (DotH)

Chain Eo: 34% 10% 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 K113 P121 E125 V128 K129 L130 K131 Y134 E135 T136 S137

E138 T144 P145 P148 P149 K150 P151 T152 V158 P167 R170 S178 L179 W189 P190 I191 W206 N211 T212 L213 M214 I215 L230 R231 G232 L233 L239 T240 L241 V248 L254 R255 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER

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

ALA TYR GLU MET GLN LYS SER PRO VAL LEU LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

- Molecule 7: IcmK (DotH)

Chain Ev: 36% 8% 56%

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

GLY ASP GLY GLY ASP ASN ALA ALA SER ASP SER THR GLN GLN PRO ASN GLN SER GLY GLN ALA ASN ALA PRO ALA ALA ASN GLN THR ALA THR ALA GLY GLY ASP GLY GLN ILE ILE SER GLN ASP ASP A104 K113 P121 E125 V128 K129 L130 K131 T136 T144 P145

G146 T147 P148 P149 K150 P151 T152 V158 P167 R170 W189 P190 I191 D195 W206 N211 T212 L213 R231 G232 L233 N234 V237 M238 L239 T240 V248 V256 A263 LYS SER MET PRO THR GLU GLU GLY ILE PRO PRO SER ALA ASN ASP LEU LEU LEU HIS

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

PRO VAL LEU LEU VAL SER TRP HIS GLY LYS VAL MET GLN LEU LYS VAL GLU GLY LEU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76406	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 ($e^-/Å^2$)	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	2.503	Depositor
Minimum map value	-1.764	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	598.08, 598.08, 598.08	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.335, 1.335, 1.335	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	Aa	0.10	0/118	0.26	0/158
1	Ah	0.09	0/118	0.23	0/158
1	Ao	0.09	0/118	0.26	0/158
1	Av	0.07	0/118	0.21	0/158
1	Bc	0.07	0/118	0.22	0/158
1	Bj	0.07	0/118	0.22	0/158
1	Bq	0.06	0/118	0.20	0/158
1	Bx	0.08	0/118	0.23	0/158
1	Ce	0.08	0/118	0.23	0/158
1	Cl	0.08	0/118	0.21	0/158
1	Cs	0.07	0/118	0.21	0/158
1	Cz	0.07	0/118	0.23	0/158
1	Dg	0.07	0/118	0.21	0/158
1	Dn	0.07	0/118	0.20	0/158
1	Du	0.13	0/118	0.32	0/158
1	Eb	0.06	0/118	0.22	0/158
1	Ei	0.08	0/118	0.24	0/158
1	Ep	0.10	0/118	0.24	0/158
2	Ab	0.10	0/60	0.26	0/76
2	Ai	0.07	0/60	0.23	0/76
2	Ap	0.09	0/60	0.30	0/76
2	Aw	0.09	0/60	0.29	0/76
2	Bd	0.10	0/60	0.32	0/76
2	Bk	0.12	0/60	0.45	0/76
2	Br	0.11	0/60	0.25	0/76
2	By	0.12	0/60	0.39	0/76
2	Cf	0.11	0/60	0.36	0/76
2	Cm	0.09	0/60	0.27	0/76
2	Ct	0.11	0/60	0.27	0/76
2	Da	0.08	0/60	0.30	0/76
2	Dh	0.08	0/60	0.30	0/76
2	Do	0.08	0/60	0.26	0/76
2	Dv	0.17	0/60	0.56	0/76
2	Ec	0.11	0/60	0.27	0/76

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	Ej	0.08	0/60	0.31	0/76
2	Eq	0.09	0/60	0.29	0/76
3	Ac	0.15	0/126	0.39	0/167
3	Aj	0.09	0/126	0.31	0/167
3	Aq	0.10	0/126	0.35	0/167
3	Ax	0.09	0/126	0.30	0/167
3	Be	0.10	0/126	0.31	0/167
3	Bl	0.12	0/126	0.35	0/167
3	Bs	0.12	0/126	0.31	0/167
3	Bz	0.14	0/126	0.37	0/167
3	Cg	0.12	0/126	0.36	0/167
3	Cn	0.12	0/126	0.40	0/167
3	Cu	0.10	0/126	0.36	0/167
3	Db	0.10	0/126	0.37	0/167
3	Di	0.08	0/126	0.29	0/167
3	Dp	0.14	0/126	0.34	0/167
3	Dw	0.13	0/126	0.32	0/167
3	Ed	0.12	0/126	0.31	0/167
3	Ek	0.13	0/126	0.37	0/167
3	Er	0.11	0/126	0.37	0/167
4	Ad	0.14	0/37	0.25	0/47
4	Ak	0.07	0/37	0.16	0/47
4	Ar	0.09	0/37	0.23	0/47
4	Ay	0.09	0/37	0.23	0/47
4	Bf	0.07	0/37	0.17	0/47
4	Bm	0.08	0/37	0.27	0/47
4	Bt	0.06	0/37	0.17	0/47
4	Ca	0.07	0/37	0.18	0/47
4	Ch	0.08	0/37	0.23	0/47
4	Co	0.08	0/37	0.27	0/47
4	Cv	0.06	0/37	0.17	0/47
4	Dc	0.07	0/37	0.22	0/47
4	Dj	0.09	0/37	0.23	0/47
4	Dq	0.07	0/37	0.18	0/47
4	Dx	0.09	0/37	0.22	0/47
4	Ee	0.06	0/37	0.17	0/47
4	El	0.07	0/37	0.19	0/47
4	Es	0.07	0/37	0.19	0/47
5	Ae	0.11	0/491	0.27	0/660
5	Al	0.19	0/491	0.35	0/660
5	As	0.11	0/491	0.27	0/660
5	Az	0.11	0/491	0.30	0/660
5	Bg	0.10	0/491	0.27	0/660

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
5	Bn	0.11	0/491	0.32	0/660
5	Bu	0.11	0/491	0.27	0/660
5	Cb	0.12	0/491	0.30	0/660
5	Ci	0.13	0/491	0.31	0/660
5	Cp	0.11	0/491	0.29	0/660
5	Cw	0.11	0/491	0.29	0/660
5	Dd	0.11	0/491	0.29	0/660
5	Dk	0.12	0/491	0.31	0/660
5	Dr	0.11	0/491	0.27	0/660
5	Dy	0.11	0/491	0.31	0/660
5	Ef	0.11	0/491	0.27	0/660
5	Em	0.12	0/491	0.29	0/660
5	Et	0.12	0/491	0.30	0/660
6	Af	0.13	0/278	0.29	0/377
6	Am	0.10	0/278	0.24	0/377
6	At	0.13	0/278	0.33	0/377
6	Ba	0.10	0/278	0.23	0/377
6	Bh	0.10	0/278	0.20	0/377
6	Bo	0.11	0/278	0.25	0/377
6	Bv	0.11	0/278	0.23	0/377
6	Cc	0.10	0/278	0.23	0/377
6	Cj	0.12	0/278	0.24	0/377
6	Cq	0.12	0/278	0.26	0/377
6	Cx	0.11	0/278	0.26	0/377
6	De	0.11	0/278	0.29	0/377
6	Dl	0.10	0/278	0.26	0/377
6	Ds	0.11	0/278	0.23	0/377
6	Dz	0.11	0/278	0.21	0/377
6	Eg	0.10	0/278	0.24	0/377
6	En	0.09	0/278	0.23	0/377
6	Eu	0.11	0/278	0.25	0/377
7	Ag	0.15	0/1269	0.29	0/1734
7	An	0.13	0/1269	0.31	0/1734
7	Au	0.12	0/1269	0.27	0/1734
7	Bb	0.12	0/1269	0.29	0/1734
7	Bi	0.13	0/1269	0.28	0/1734
7	Bp	0.15	0/1269	0.31	0/1734
7	Bw	0.13	0/1269	0.33	0/1734
7	Cd	0.12	0/1269	0.28	0/1734
7	Ck	0.13	0/1269	0.30	0/1734
7	Cr	0.13	0/1269	0.29	0/1734
7	Cy	0.13	0/1269	0.30	0/1734
7	Df	0.13	0/1269	0.27	0/1734

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
7	Dm	0.14	0/1269	0.31	0/1734
7	Dt	0.13	0/1269	0.28	0/1734
7	Ea	0.14	0/1269	0.29	0/1734
7	Eh	0.13	0/1269	0.32	0/1734
7	Eo	0.12	0/1269	0.28	0/1734
7	Ev	0.14	0/1269	0.30	0/1734
All	All	0.12	0/42822	0.29	0/57942

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Aa	117	0	111	4	0
1	Ah	117	0	111	3	0
1	Ao	117	0	111	4	0
1	Av	117	0	111	3	0
1	Bc	117	0	111	3	0
1	Bj	117	0	111	5	0
1	Bq	117	0	111	3	0
1	Bx	117	0	111	2	0
1	Ce	117	0	111	4	0
1	Cl	117	0	111	4	0
1	Cs	117	0	111	4	0
1	Cz	117	0	111	4	0
1	Dg	117	0	111	4	0
1	Dn	117	0	111	3	0
1	Du	117	0	111	3	0
1	Eb	117	0	111	4	0
1	Ei	117	0	111	2	0
1	Ep	117	0	111	6	0
2	Ab	61	0	65	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ai	61	0	65	3	0
2	Ap	61	0	65	5	0
2	Aw	61	0	65	4	0
2	Bd	61	0	65	2	0
2	Bk	61	0	65	2	0
2	Br	61	0	65	3	0
2	By	61	0	65	3	0
2	Cf	61	0	65	2	0
2	Cm	61	0	65	5	0
2	Ct	61	0	65	6	0
2	Da	61	0	65	4	0
2	Dh	61	0	65	6	0
2	Do	61	0	65	5	0
2	Dv	61	0	65	7	0
2	Ec	61	0	65	3	0
2	Ej	61	0	65	7	0
2	Eq	61	0	65	4	0
3	Ac	125	0	126	4	0
3	Aj	125	0	126	3	0
3	Aq	125	0	126	5	0
3	Ax	125	0	126	4	0
3	Be	125	0	126	4	0
3	Bl	125	0	126	7	0
3	Bs	125	0	126	3	0
3	Bz	125	0	126	6	0
3	Cg	125	0	126	5	0
3	Cn	125	0	126	4	0
3	Cu	125	0	126	7	0
3	Db	125	0	126	6	0
3	Di	125	0	126	5	0
3	Dp	125	0	126	6	0
3	Dw	125	0	126	6	0
3	Ed	125	0	126	5	0
3	Ek	125	0	126	7	0
3	Er	125	0	126	7	0
4	Ad	36	0	30	3	0
4	Ak	36	0	30	1	0
4	Ar	36	0	30	3	0
4	Ay	36	0	30	2	0
4	Bf	36	0	30	1	0
4	Bm	36	0	30	1	0
4	Bt	36	0	30	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Ca	36	0	30	1	0
4	Ch	36	0	30	1	0
4	Co	36	0	30	2	0
4	Cv	36	0	30	1	0
4	Dc	36	0	30	2	0
4	Dj	36	0	30	4	0
4	Dq	36	0	30	1	0
4	Dx	36	0	30	1	0
4	Ee	36	0	30	1	0
4	El	36	0	30	2	0
4	Es	36	0	30	1	0
5	Ae	484	0	502	11	0
5	Al	484	0	502	11	0
5	As	484	0	502	14	0
5	Az	484	0	502	13	0
5	Bg	484	0	502	10	0
5	Bn	484	0	502	12	0
5	Bu	484	0	502	11	0
5	Cb	484	0	502	13	0
5	Ci	484	0	502	13	0
5	Cp	484	0	502	12	0
5	Cw	484	0	502	13	0
5	Dd	484	0	502	13	0
5	Dk	484	0	502	13	0
5	Dr	484	0	502	11	0
5	Dy	484	0	502	14	0
5	Ef	484	0	502	12	0
5	Em	484	0	502	14	0
5	Et	484	0	502	14	0
6	Af	276	0	263	7	0
6	Am	276	0	263	6	0
6	At	276	0	263	3	0
6	Ba	276	0	263	4	0
6	Bh	276	0	263	4	0
6	Bo	276	0	263	6	0
6	Bv	276	0	263	4	0
6	Cc	276	0	263	4	0
6	Cj	276	0	263	3	0
6	Cq	276	0	263	4	0
6	Cx	276	0	263	6	0
6	De	276	0	263	4	0
6	Dl	276	0	263	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Ds	276	0	263	4	0
6	Dz	276	0	263	3	0
6	Eg	276	0	263	5	0
6	En	276	0	263	6	0
6	Eu	276	0	263	2	0
7	Ag	1238	0	1252	36	0
7	An	1238	0	1252	28	0
7	Au	1238	0	1252	35	0
7	Bb	1238	0	1252	24	0
7	Bi	1238	0	1252	26	0
7	Bp	1238	0	1252	38	0
7	Bw	1238	0	1252	24	0
7	Cd	1238	0	1252	29	0
7	Ck	1238	0	1252	22	0
7	Cr	1238	0	1252	30	0
7	Cy	1238	0	1252	30	0
7	Df	1238	0	1252	31	0
7	Dm	1238	0	1252	27	0
7	Dt	1238	0	1252	29	0
7	Ea	1238	0	1252	40	0
7	Eh	1238	0	1252	28	0
7	Eo	1238	0	1252	29	0
7	Ev	1238	0	1252	29	0
All	All	42066	0	42282	794	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 794 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Ec:5:ILE:HD11	7:Eo:136:THR:HG23	1.61	0.82
2:Br:5:ILE:HD11	7:Cd:136:THR:HG23	1.61	0.82
7:Ag:136:THR:HG23	2:Eq:5:ILE:HD11	1.62	0.81
2:Ai:5:ILE:HD11	7:Au:136:THR:HG23	1.66	0.77
2:Dv:5:ILE:HD11	7:Eh:136:THR:HG23	1.67	0.76

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	Ah	14/16 (88%)	14 (100%)	0	0	100	100
1	Ao	14/16 (88%)	14 (100%)	0	0	100	100
1	Av	14/16 (88%)	14 (100%)	0	0	100	100
1	Bc	14/16 (88%)	14 (100%)	0	0	100	100
1	Bj	14/16 (88%)	14 (100%)	0	0	100	100
1	Bq	14/16 (88%)	14 (100%)	0	0	100	100
1	Bx	14/16 (88%)	14 (100%)	0	0	100	100
1	Ce	14/16 (88%)	14 (100%)	0	0	100	100
1	Cl	14/16 (88%)	14 (100%)	0	0	100	100
1	Cs	14/16 (88%)	14 (100%)	0	0	100	100
1	Cz	14/16 (88%)	14 (100%)	0	0	100	100
1	Dg	14/16 (88%)	14 (100%)	0	0	100	100
1	Dn	14/16 (88%)	14 (100%)	0	0	100	100
1	Du	14/16 (88%)	14 (100%)	0	0	100	100
1	Eb	14/16 (88%)	14 (100%)	0	0	100	100
1	Ei	14/16 (88%)	14 (100%)	0	0	100	100
1	Ep	14/16 (88%)	14 (100%)	0	0	100	100
2	Ab	7/9 (78%)	7 (100%)	0	0	100	100
2	Ai	7/9 (78%)	7 (100%)	0	0	100	100
2	Ap	7/9 (78%)	7 (100%)	0	0	100	100
2	Aw	7/9 (78%)	7 (100%)	0	0	100	100
2	Bd	7/9 (78%)	7 (100%)	0	0	100	100
2	Bk	7/9 (78%)	7 (100%)	0	0	100	100
2	Br	7/9 (78%)	7 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	By	7/9 (78%)	7 (100%)	0	0	100	100
2	Cf	7/9 (78%)	7 (100%)	0	0	100	100
2	Cm	7/9 (78%)	7 (100%)	0	0	100	100
2	Ct	7/9 (78%)	7 (100%)	0	0	100	100
2	Da	7/9 (78%)	7 (100%)	0	0	100	100
2	Dh	7/9 (78%)	7 (100%)	0	0	100	100
2	Do	7/9 (78%)	7 (100%)	0	0	100	100
2	Dv	7/9 (78%)	7 (100%)	0	0	100	100
2	Ec	7/9 (78%)	7 (100%)	0	0	100	100
2	Ej	7/9 (78%)	7 (100%)	0	0	100	100
2	Eq	7/9 (78%)	7 (100%)	0	0	100	100
3	Ac	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Aj	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Aq	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ax	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Be	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Bl	14/16 (88%)	12 (86%)	2 (14%)	0	100	100
3	Bs	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Bz	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cg	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cn	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Cu	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Db	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Di	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Dp	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Dw	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ed	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Ek	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
3	Er	14/16 (88%)	13 (93%)	1 (7%)	0	100	100
4	Ad	3/5 (60%)	3 (100%)	0	0	100	100
4	Ak	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ar	3/5 (60%)	3 (100%)	0	0	100	100
4	Ay	3/5 (60%)	3 (100%)	0	0	100	100
4	Bf	3/5 (60%)	3 (100%)	0	0	100	100
4	Bm	3/5 (60%)	3 (100%)	0	0	100	100
4	Bt	3/5 (60%)	3 (100%)	0	0	100	100
4	Ca	3/5 (60%)	3 (100%)	0	0	100	100
4	Ch	3/5 (60%)	3 (100%)	0	0	100	100
4	Co	3/5 (60%)	3 (100%)	0	0	100	100
4	Cv	3/5 (60%)	3 (100%)	0	0	100	100
4	Dc	3/5 (60%)	3 (100%)	0	0	100	100
4	Dj	3/5 (60%)	3 (100%)	0	0	100	100
4	Dq	3/5 (60%)	3 (100%)	0	0	100	100
4	Dx	3/5 (60%)	3 (100%)	0	0	100	100
4	Ee	3/5 (60%)	3 (100%)	0	0	100	100
4	El	3/5 (60%)	3 (100%)	0	0	100	100
4	Es	3/5 (60%)	3 (100%)	0	0	100	100
5	Ae	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Al	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	As	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Az	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Bg	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Bn	61/269 (23%)	61 (100%)	0	0	100	100
5	Bu	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Cb	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Ci	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Cp	61/269 (23%)	58 (95%)	3 (5%)	0	100	100
5	Cw	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Dd	61/269 (23%)	61 (100%)	0	0	100	100
5	Dk	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Dr	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Dy	61/269 (23%)	60 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Ef	61/269 (23%)	59 (97%)	2 (3%)	0	100	100
5	Em	61/269 (23%)	60 (98%)	1 (2%)	0	100	100
5	Et	61/269 (23%)	61 (100%)	0	0	100	100
6	Af	32/1048 (3%)	32 (100%)	0	0	100	100
6	Am	32/1048 (3%)	32 (100%)	0	0	100	100
6	At	32/1048 (3%)	32 (100%)	0	0	100	100
6	Ba	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bh	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bo	32/1048 (3%)	32 (100%)	0	0	100	100
6	Bv	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cc	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cj	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cq	32/1048 (3%)	32 (100%)	0	0	100	100
6	Cx	32/1048 (3%)	32 (100%)	0	0	100	100
6	De	32/1048 (3%)	32 (100%)	0	0	100	100
6	Dl	32/1048 (3%)	32 (100%)	0	0	100	100
6	Ds	32/1048 (3%)	32 (100%)	0	0	100	100
6	Dz	32/1048 (3%)	32 (100%)	0	0	100	100
6	Eg	32/1048 (3%)	32 (100%)	0	0	100	100
6	En	32/1048 (3%)	32 (100%)	0	0	100	100
6	Eu	32/1048 (3%)	32 (100%)	0	0	100	100
7	Ag	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	An	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Au	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bb	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bi	158/361 (44%)	154 (98%)	4 (2%)	0	100	100
7	Bp	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Bw	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Cd	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ck	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Cr	158/361 (44%)	155 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Cy	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Df	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Dm	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Dt	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ea	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Eh	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Eo	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
7	Ev	158/361 (44%)	155 (98%)	3 (2%)	0	100	100
All	All	5202/31032 (17%)	5105 (98%)	97 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Aa	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Ah	11/11 (100%)	11 (100%)	0	100	100
1	Ao	11/11 (100%)	9 (82%)	2 (18%)	2	8
1	Av	11/11 (100%)	11 (100%)	0	100	100
1	Bc	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Bj	11/11 (100%)	11 (100%)	0	100	100
1	Bq	11/11 (100%)	11 (100%)	0	100	100
1	Bx	11/11 (100%)	11 (100%)	0	100	100
1	Ce	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Cl	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Cs	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Cz	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Dg	11/11 (100%)	11 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Dn	11/11 (100%)	10 (91%)	1 (9%)	9	31
1	Du	11/11 (100%)	11 (100%)	0	100	100
1	Eb	11/11 (100%)	11 (100%)	0	100	100
1	Ei	11/11 (100%)	11 (100%)	0	100	100
1	Ep	11/11 (100%)	11 (100%)	0	100	100
2	Ab	7/7 (100%)	6 (86%)	1 (14%)	3	14
2	Ai	7/7 (100%)	7 (100%)	0	100	100
2	Ap	7/7 (100%)	6 (86%)	1 (14%)	3	14
2	Aw	7/7 (100%)	7 (100%)	0	100	100
2	Bd	7/7 (100%)	7 (100%)	0	100	100
2	Bk	7/7 (100%)	7 (100%)	0	100	100
2	Br	7/7 (100%)	7 (100%)	0	100	100
2	By	7/7 (100%)	7 (100%)	0	100	100
2	Cf	7/7 (100%)	7 (100%)	0	100	100
2	Cm	7/7 (100%)	6 (86%)	1 (14%)	3	14
2	Ct	7/7 (100%)	7 (100%)	0	100	100
2	Da	7/7 (100%)	6 (86%)	1 (14%)	3	14
2	Dh	7/7 (100%)	6 (86%)	1 (14%)	3	14
2	Do	7/7 (100%)	7 (100%)	0	100	100
2	Dv	7/7 (100%)	7 (100%)	0	100	100
2	Ec	7/7 (100%)	7 (100%)	0	100	100
2	Ej	7/7 (100%)	5 (71%)	2 (29%)	0	2
2	Eq	7/7 (100%)	7 (100%)	0	100	100
3	Ac	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Aj	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Aq	13/13 (100%)	9 (69%)	4 (31%)	0	1
3	Ax	13/13 (100%)	11 (85%)	2 (15%)	2	12
3	Be	13/13 (100%)	12 (92%)	1 (8%)	12	37
3	Bl	13/13 (100%)	12 (92%)	1 (8%)	12	37
3	Bs	13/13 (100%)	12 (92%)	1 (8%)	12	37
3	Bz	13/13 (100%)	12 (92%)	1 (8%)	12	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Cg	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Cn	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Cu	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Db	13/13 (100%)	9 (69%)	4 (31%)	0	1
3	Di	13/13 (100%)	11 (85%)	2 (15%)	2	12
3	Dp	13/13 (100%)	10 (77%)	3 (23%)	1	4
3	Dw	13/13 (100%)	11 (85%)	2 (15%)	2	12
3	Ed	13/13 (100%)	12 (92%)	1 (8%)	12	37
3	Ek	13/13 (100%)	11 (85%)	2 (15%)	2	12
3	Er	13/13 (100%)	11 (85%)	2 (15%)	2	12
4	Ad	3/3 (100%)	3 (100%)	0	100	100
4	Ak	3/3 (100%)	3 (100%)	0	100	100
4	Ar	3/3 (100%)	3 (100%)	0	100	100
4	Ay	3/3 (100%)	3 (100%)	0	100	100
4	Bf	3/3 (100%)	3 (100%)	0	100	100
4	Bm	3/3 (100%)	3 (100%)	0	100	100
4	Bt	3/3 (100%)	3 (100%)	0	100	100
4	Ca	3/3 (100%)	3 (100%)	0	100	100
4	Ch	3/3 (100%)	3 (100%)	0	100	100
4	Co	3/3 (100%)	3 (100%)	0	100	100
4	Cv	3/3 (100%)	3 (100%)	0	100	100
4	Dc	3/3 (100%)	3 (100%)	0	100	100
4	Dj	3/3 (100%)	3 (100%)	0	100	100
4	Dq	3/3 (100%)	3 (100%)	0	100	100
4	Dx	3/3 (100%)	3 (100%)	0	100	100
4	Ee	3/3 (100%)	3 (100%)	0	100	100
4	El	3/3 (100%)	3 (100%)	0	100	100
4	Es	3/3 (100%)	3 (100%)	0	100	100
5	Ae	53/237 (22%)	53 (100%)	0	100	100
5	Al	53/237 (22%)	53 (100%)	0	100	100
5	As	53/237 (22%)	53 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	Az	53/237 (22%)	52 (98%)	1 (2%)	50	73
5	Bg	53/237 (22%)	52 (98%)	1 (2%)	50	73
5	Bn	53/237 (22%)	53 (100%)	0	100	100
5	Bu	53/237 (22%)	52 (98%)	1 (2%)	50	73
5	Cb	53/237 (22%)	53 (100%)	0	100	100
5	Ci	53/237 (22%)	51 (96%)	2 (4%)	29	60
5	Cp	53/237 (22%)	52 (98%)	1 (2%)	50	73
5	Cw	53/237 (22%)	53 (100%)	0	100	100
5	Dd	53/237 (22%)	53 (100%)	0	100	100
5	Dk	53/237 (22%)	53 (100%)	0	100	100
5	Dr	53/237 (22%)	52 (98%)	1 (2%)	50	73
5	Dy	53/237 (22%)	53 (100%)	0	100	100
5	Ef	53/237 (22%)	53 (100%)	0	100	100
5	Em	53/237 (22%)	53 (100%)	0	100	100
5	Et	53/237 (22%)	52 (98%)	1 (2%)	50	73
6	Af	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Am	31/765 (4%)	31 (100%)	0	100	100
6	At	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Ba	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Bh	31/765 (4%)	31 (100%)	0	100	100
6	Bo	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Bv	31/765 (4%)	31 (100%)	0	100	100
6	Cc	31/765 (4%)	31 (100%)	0	100	100
6	Cj	31/765 (4%)	31 (100%)	0	100	100
6	Cq	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Cx	31/765 (4%)	31 (100%)	0	100	100
6	De	31/765 (4%)	31 (100%)	0	100	100
6	Dl	31/765 (4%)	30 (97%)	1 (3%)	34	64
6	Ds	31/765 (4%)	31 (100%)	0	100	100
6	Dz	31/765 (4%)	31 (100%)	0	100	100
6	Eg	31/765 (4%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	En	31/765 (4%)	31 (100%)	0	100	100
6	Eu	31/765 (4%)	31 (100%)	0	100	100
7	Ag	137/300 (46%)	132 (96%)	5 (4%)	31	62
7	An	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Au	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Bb	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Bi	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Bp	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Bw	137/300 (46%)	134 (98%)	3 (2%)	45	71
7	Cd	137/300 (46%)	134 (98%)	3 (2%)	45	71
7	Ck	137/300 (46%)	134 (98%)	3 (2%)	45	71
7	Cr	137/300 (46%)	130 (95%)	7 (5%)	21	52
7	Cy	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Df	137/300 (46%)	134 (98%)	3 (2%)	45	71
7	Dm	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Dt	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Ea	137/300 (46%)	135 (98%)	2 (2%)	57	77
7	Eh	137/300 (46%)	133 (97%)	4 (3%)	37	67
7	Eo	137/300 (46%)	134 (98%)	3 (2%)	45	71
7	Ev	137/300 (46%)	135 (98%)	2 (2%)	57	77
All	All	4590/24048 (19%)	4464 (97%)	126 (3%)	40	68

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	Ci	249	SER
7	Eh	168	VAL
7	Cr	219	LYS
3	Ed	3	SER
7	Eo	128	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
7	Dt	126	GLN
7	Eo	126	GLN
7	Dt	222	ASN
7	Eh	126	GLN
7	Ev	234	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

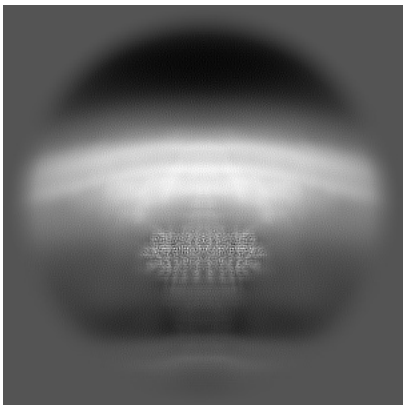
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-49394. These allow visual inspection of the internal detail of the map and identification of artifacts.

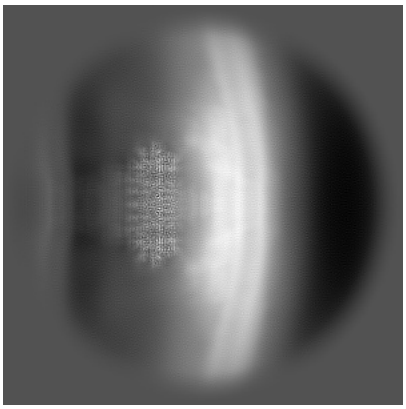
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

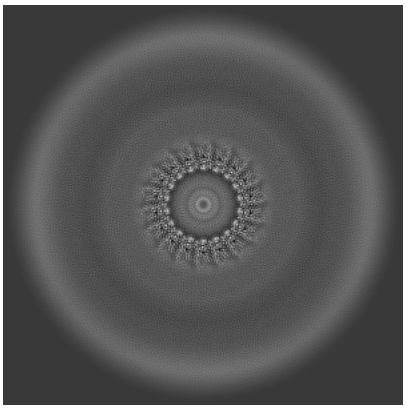
6.1.1 Primary map



X

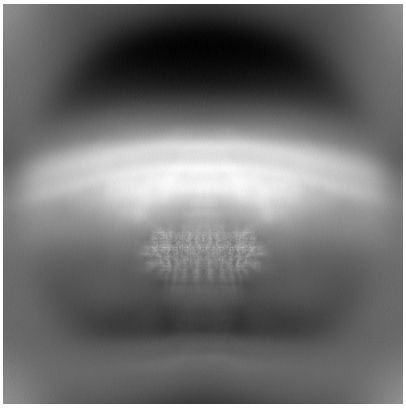


Y

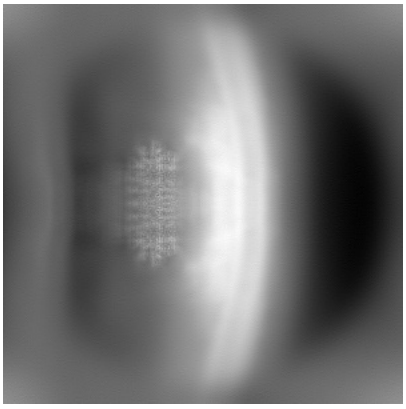


Z

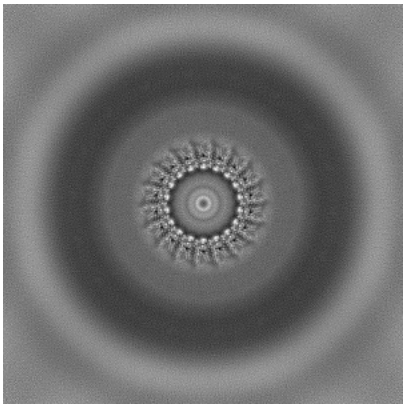
6.1.2 Raw map



X



Y

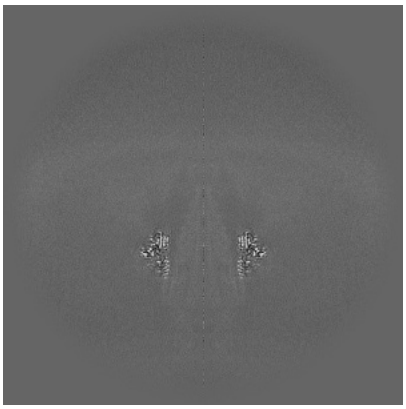


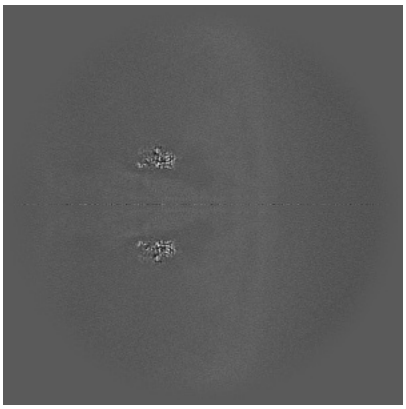
Z

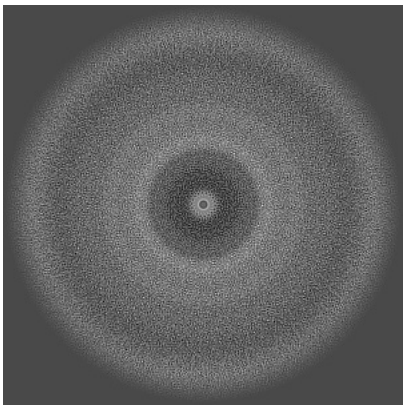
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

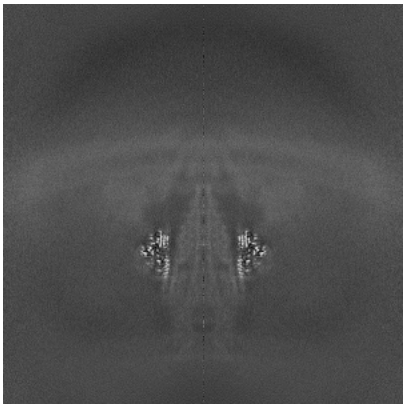
6.2.1 Primary map

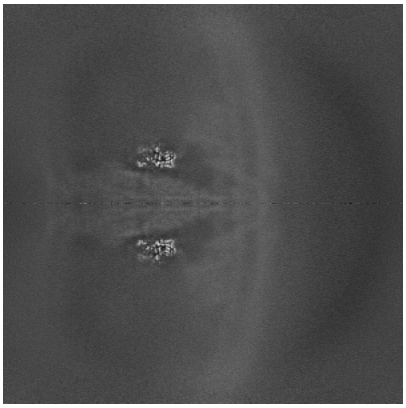

X Index: 224

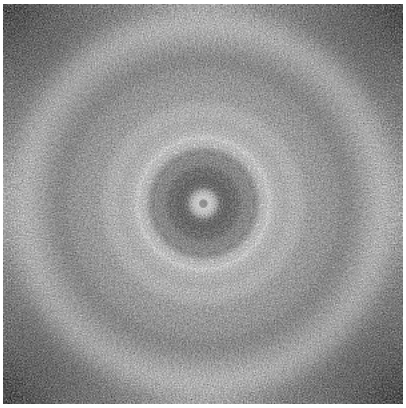

Y Index: 224


Z Index: 224

6.2.2 Raw map


X Index: 224

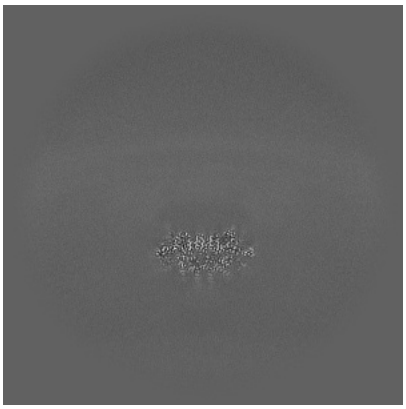

Y Index: 224


Z Index: 224

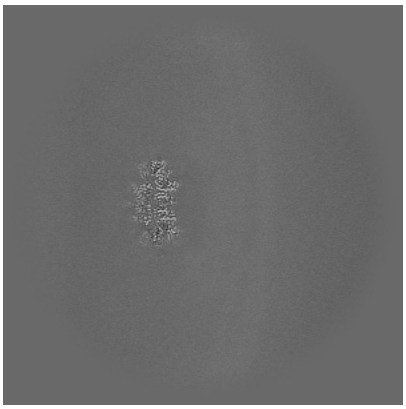
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

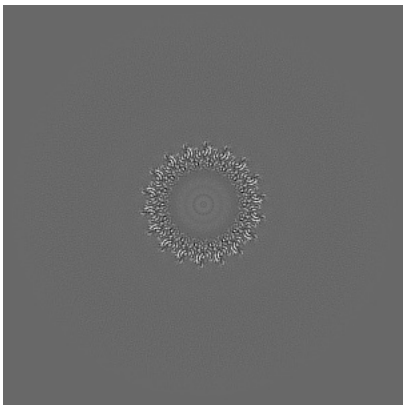
6.3.1 Primary map



X Index: 181

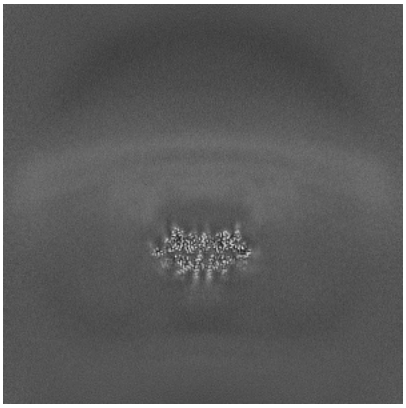


Y Index: 269

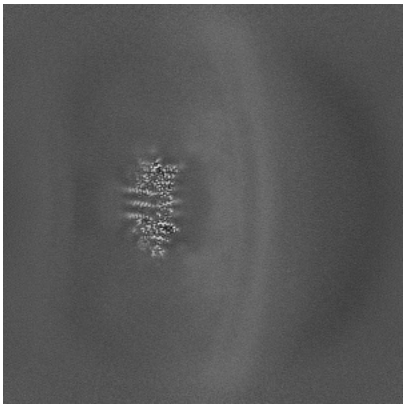


Z Index: 174

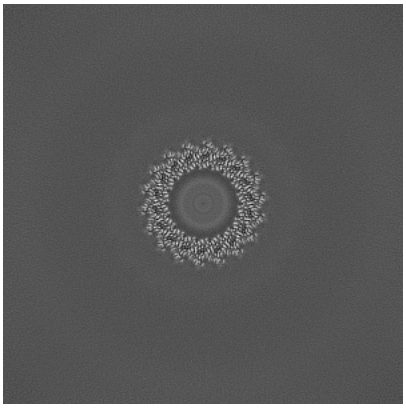
6.3.2 Raw map



X Index: 266



Y Index: 264

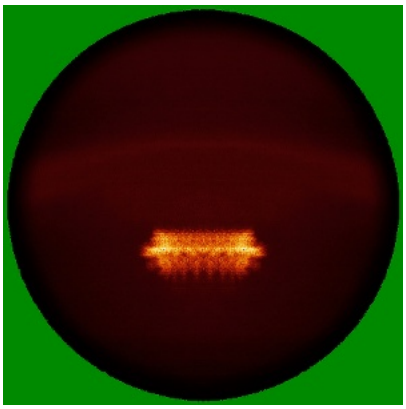


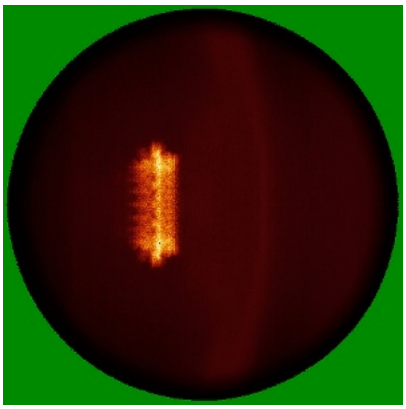
Z Index: 175

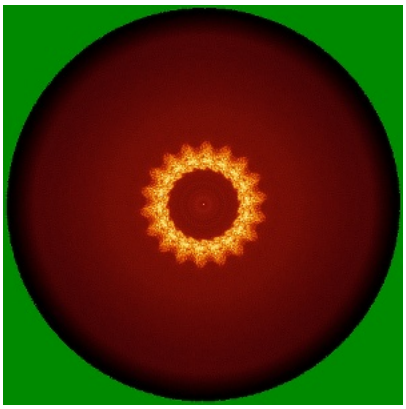
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

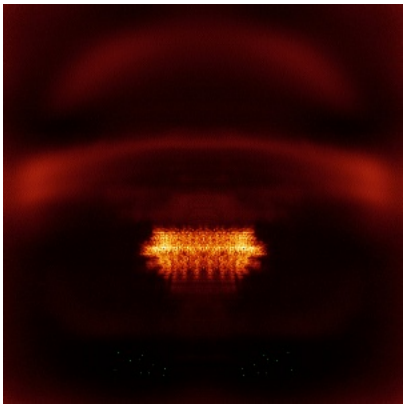
6.4.1 Primary map

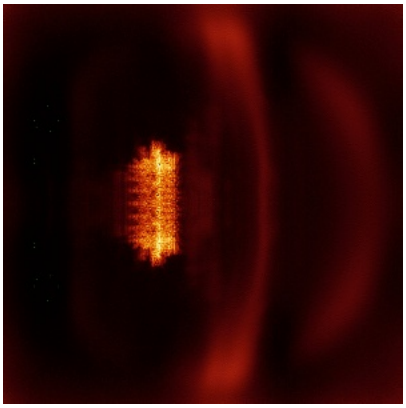

X

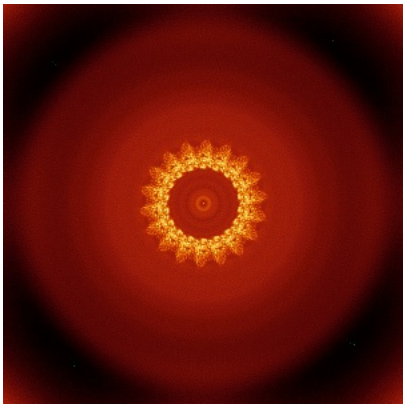

Y


Z

6.4.2 Raw map


X

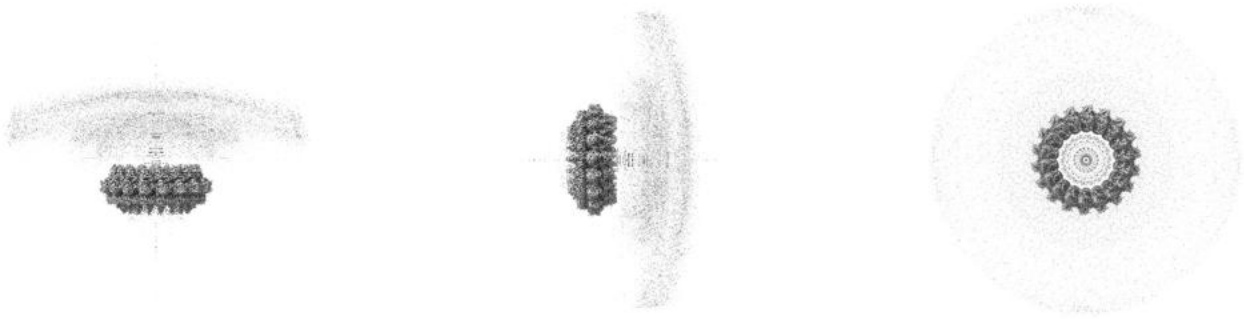

Y


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



X Y Z

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

6.5.2 Raw map

X Y Z

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

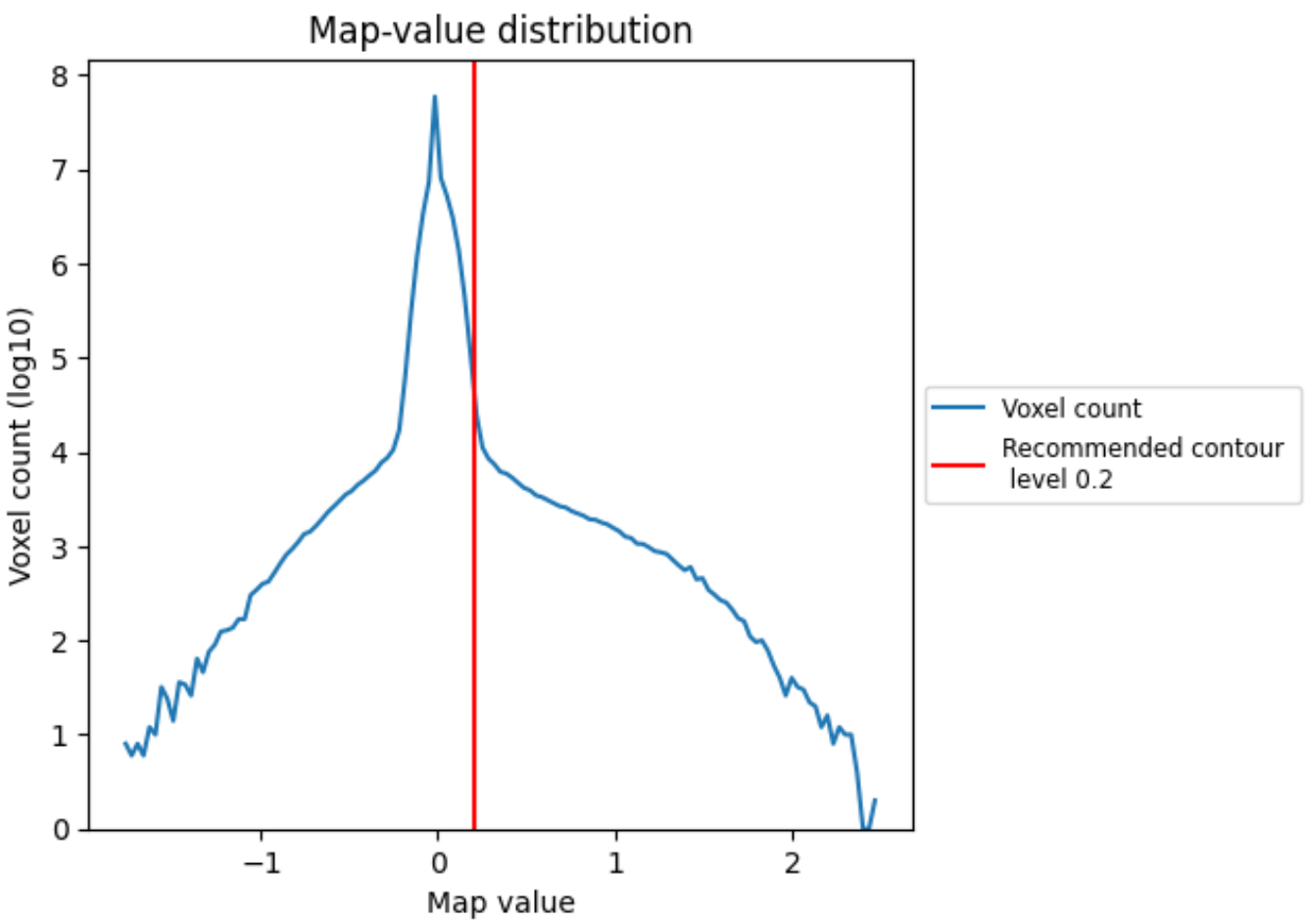
6.6 Mask visualisation (i)

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

7 Map analysis (i)

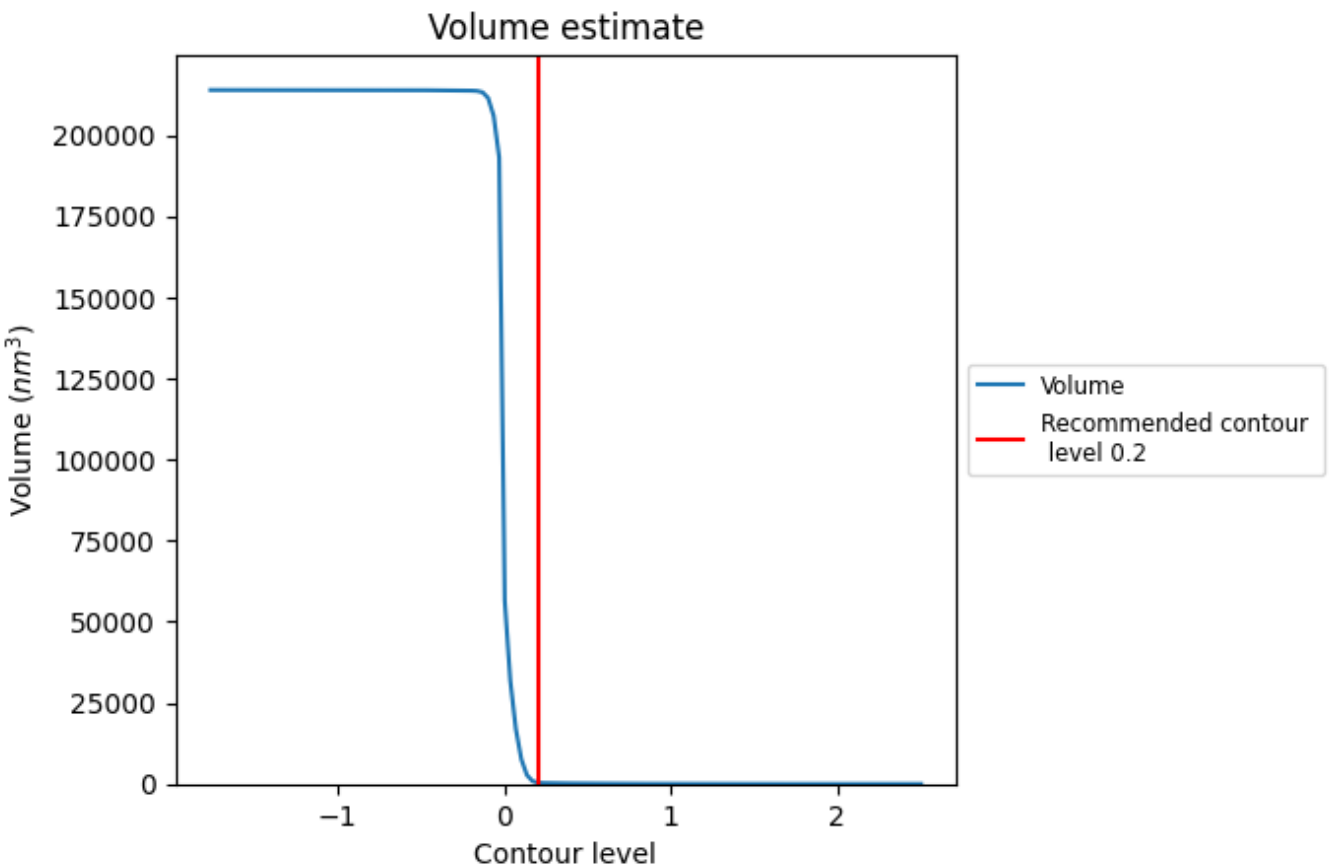
This section contains the results of statistical analysis of the map.

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.

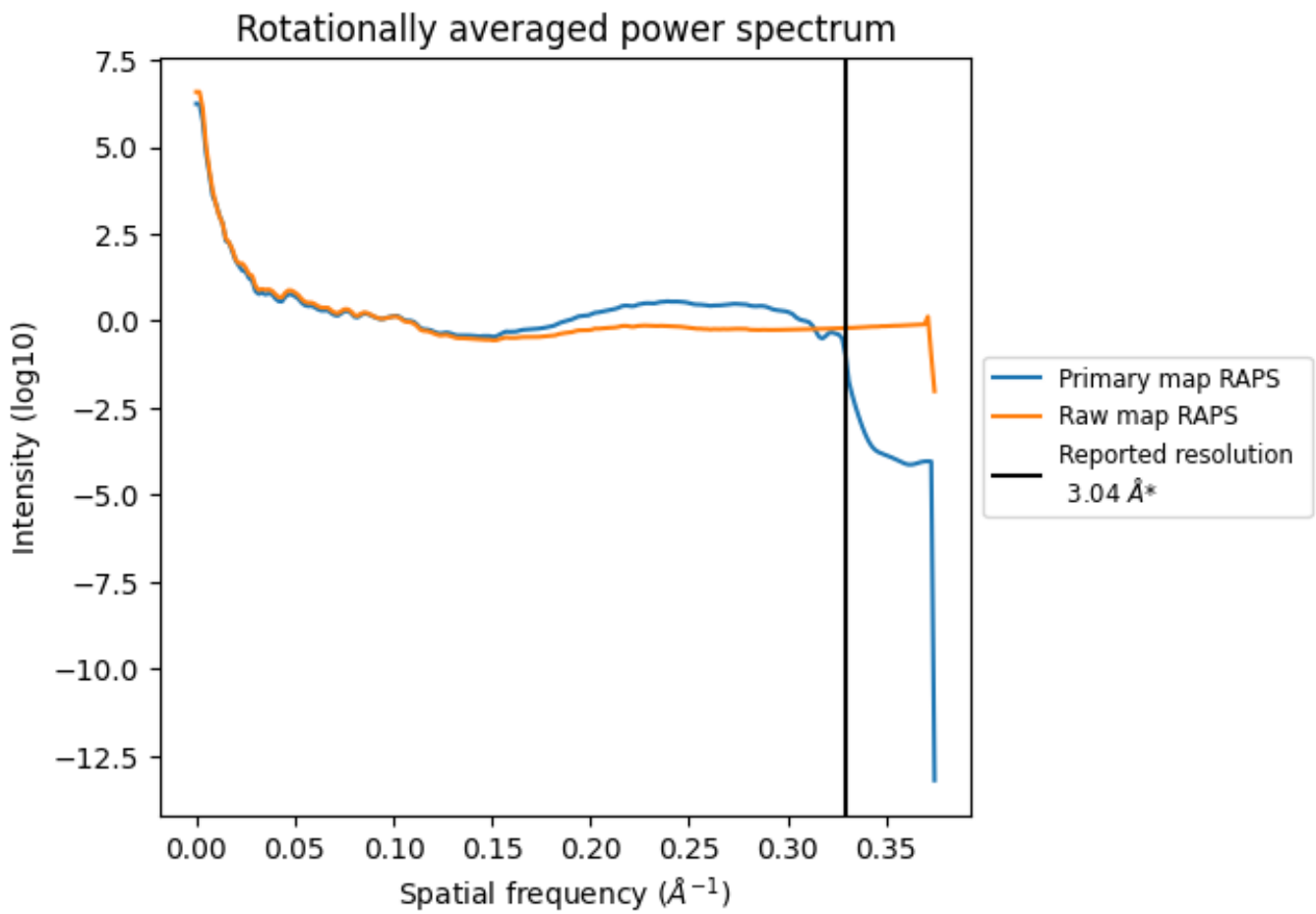
7.2 Volume estimate (i)



The volume at the recommended contour level is 428 nm^3; this corresponds to an approximate mass of 387 kDa.

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

7.3 Rotationally averaged power spectrum (i)

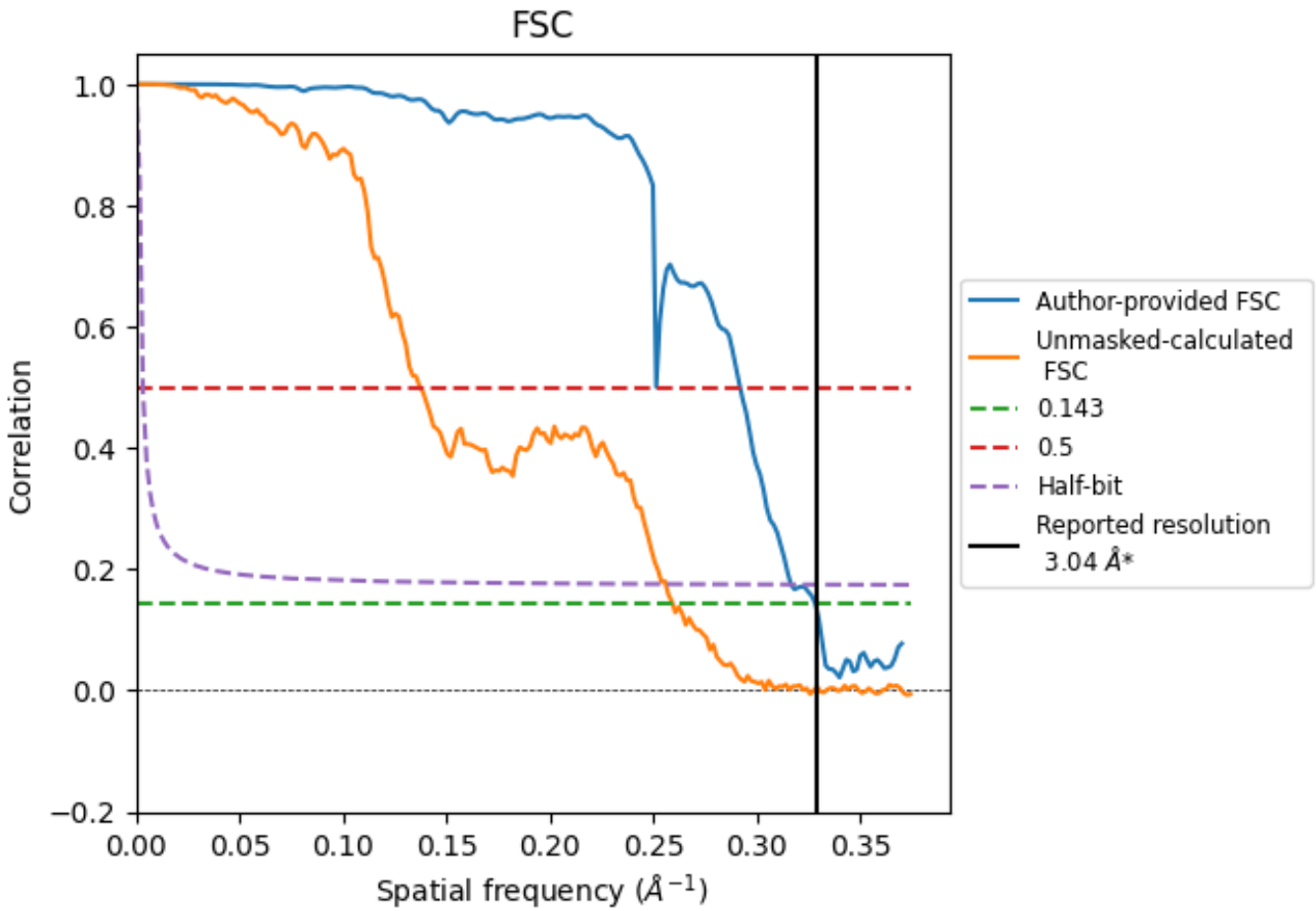


*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

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 0.329 Å^{-1}

8.2 Resolution estimates (i)

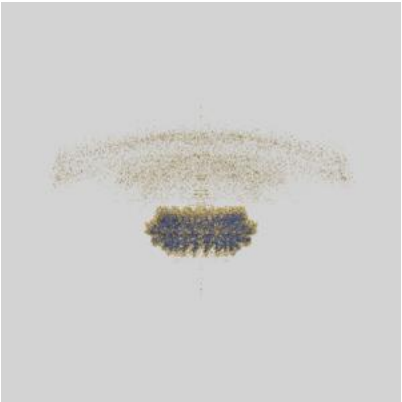
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.42	3.16
Unmasked-calculated*	3.85	7.28	3.90

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.85 differs from the reported value 3.04 by more than 10 %

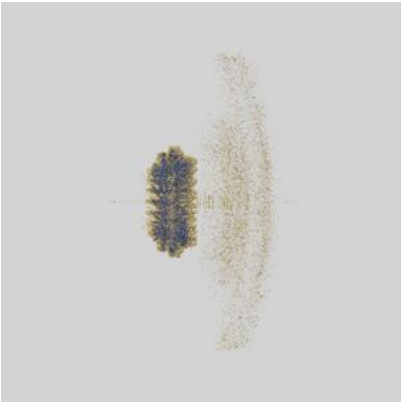
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-49394 and PDB model 9NGV. Per-residue inclusion information can be found in section 3 on page 15.

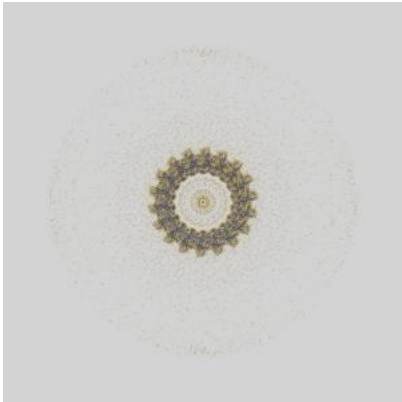
9.1 Map-model overlay (i)



X



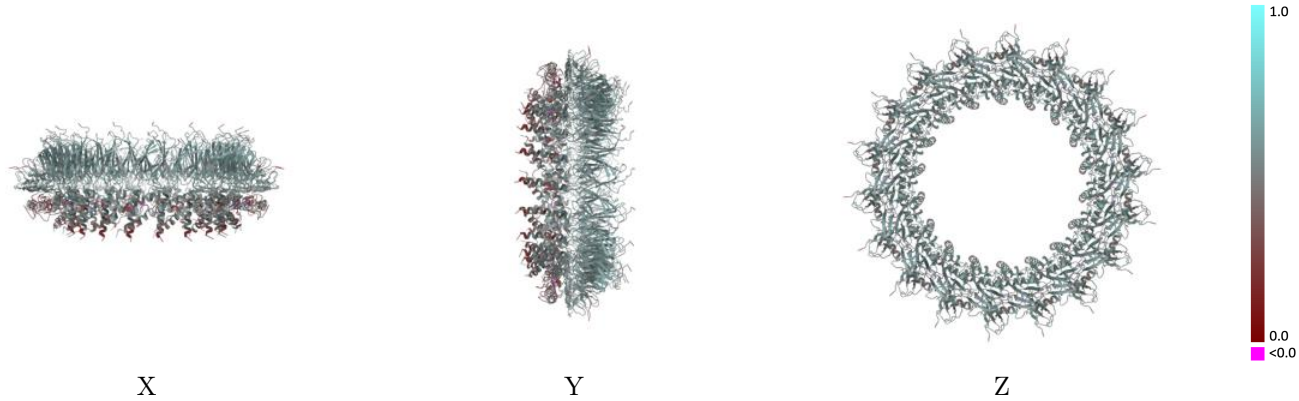
Y



Z

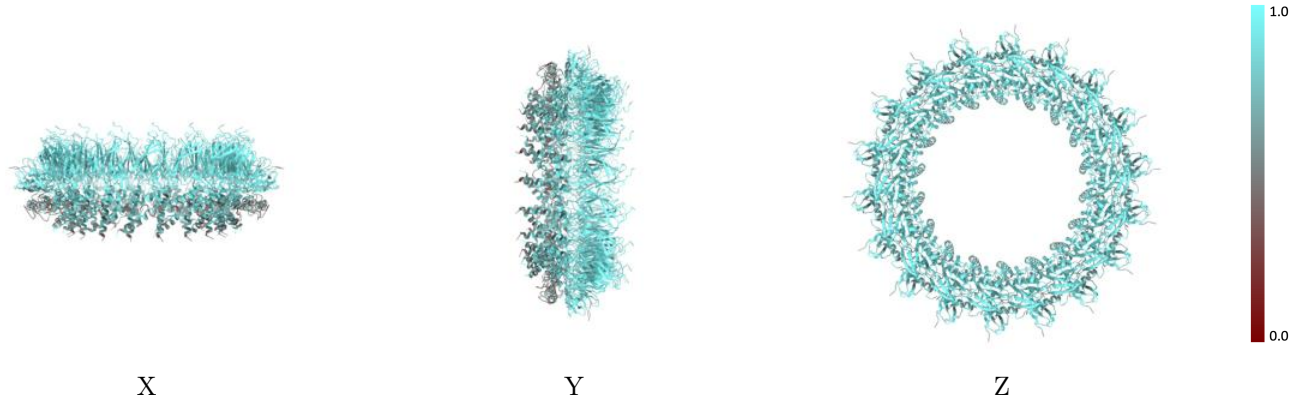
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



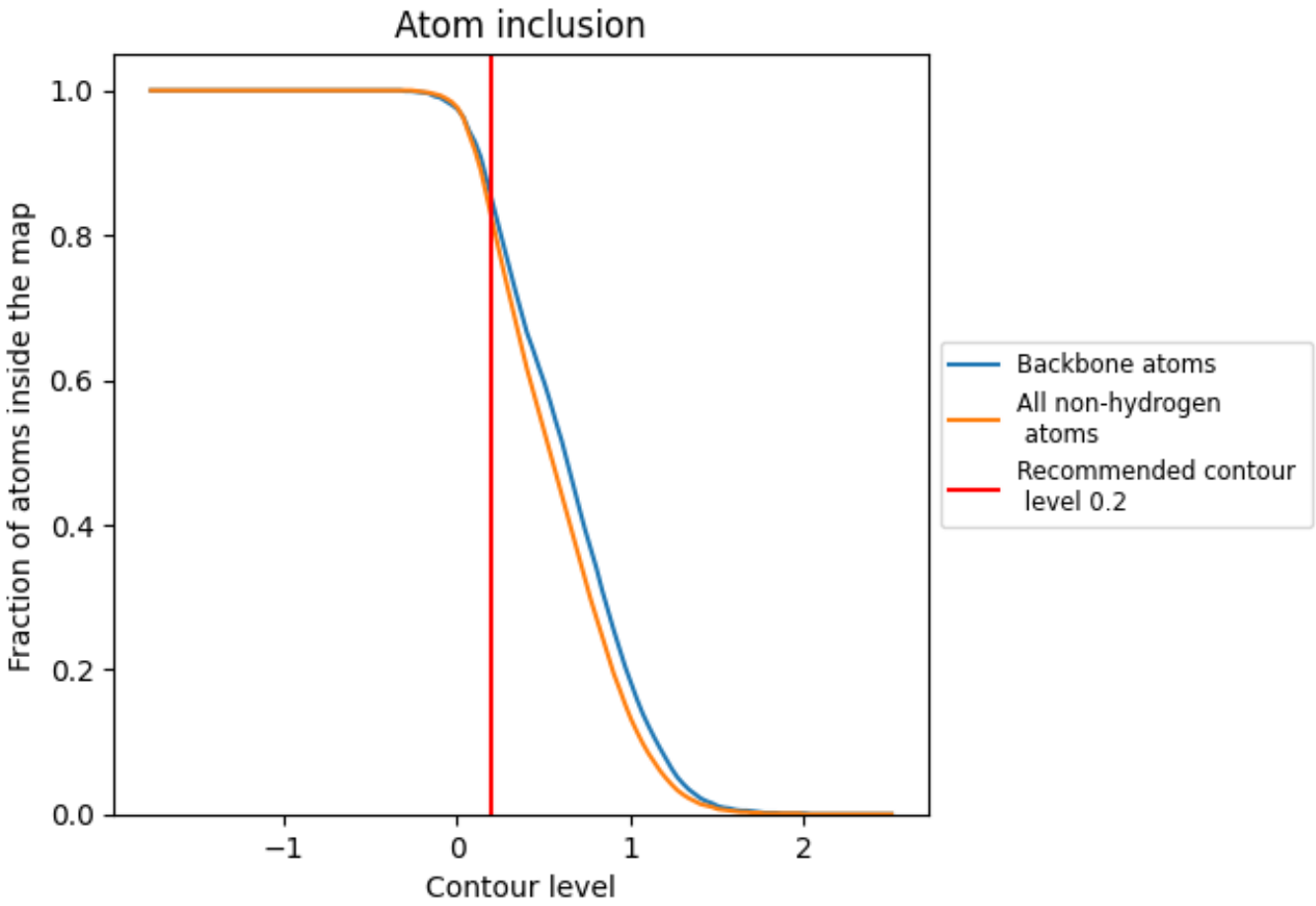
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.5110
Aa	0.5950	0.4440
Ab	0.6100	0.3260
Ac	0.4380	0.2980
Ad	0.2780	0.1990
Ae	0.8410	0.5190
Af	0.7900	0.5080
Ag	0.9090	0.5550
Ah	0.5950	0.4260
Ai	0.6610	0.3410
Aj	0.4380	0.3090
Ak	0.3330	0.2090
Al	0.8620	0.5210
Am	0.7900	0.5070
An	0.9060	0.5560
Ao	0.5520	0.4530
Ap	0.6270	0.3520
Aq	0.4460	0.3000
Ar	0.3060	0.1960
As	0.8560	0.5210
At	0.7980	0.5060
Au	0.9070	0.5550
Av	0.5690	0.4400
Aw	0.6780	0.3570
Ax	0.4300	0.3060
Ay	0.3330	0.1840
Az	0.8500	0.5180
Ba	0.7980	0.4970
Bb	0.9040	0.5540
Bc	0.5860	0.4370
Bd	0.6440	0.3430
Be	0.4460	0.3240
Bf	0.3330	0.1970
Bg	0.8430	0.5170
Bh	0.7760	0.4920

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Chain	Atom inclusion	Q-score
Bi	0.8960	0.5530
Bj	0.5950	0.4470
Bk	0.6270	0.3460
Bl	0.4460	0.3210
Bm	0.2500	0.1680
Bn	0.8500	0.5150
Bo	0.8160	0.5030
Bp	0.8960	0.5540
Bq	0.5780	0.4310
Br	0.6780	0.3610
Bs	0.4130	0.3090
Bt	0.3060	0.2320
Bu	0.8410	0.5190
Bv	0.8200	0.5050
Bw	0.8990	0.5540
Bx	0.5600	0.4370
By	0.6440	0.3440
Bz	0.4550	0.3000
Ca	0.3330	0.1850
Cb	0.8430	0.5160
Cc	0.7870	0.5030
Cd	0.8960	0.5510
Ce	0.5950	0.4420
Cf	0.6100	0.3350
Cg	0.4460	0.3070
Ch	0.3060	0.2080
Ci	0.8540	0.5190
Cj	0.7830	0.5040
Ck	0.9000	0.5550
Cl	0.5860	0.4370
Cm	0.6100	0.3360
Cn	0.4380	0.2910
Co	0.3060	0.1780
Cp	0.8350	0.5170
Cq	0.7980	0.5000
Cr	0.9050	0.5550
Cs	0.6210	0.4420
Ct	0.6440	0.3340
Cu	0.4460	0.3040
Cv	0.3330	0.2120
Cw	0.8620	0.5220
Cx	0.7980	0.5050

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Chain	Atom inclusion	Q-score
Cy	0.9090	0.5560
Cz	0.5690	0.4530
Da	0.6610	0.3470
Db	0.4550	0.3060
Dc	0.3060	0.1860
Dd	0.8560	0.5190
De	0.7940	0.5060
Df	0.9050	0.5560
Dg	0.5600	0.4330
Dh	0.6610	0.3490
Di	0.4300	0.3110
Dj	0.2780	0.1890
Dk	0.8500	0.5240
Dl	0.8010	0.4980
Dm	0.9050	0.5540
Dn	0.6030	0.4280
Do	0.6100	0.3410
Dp	0.4710	0.3130
Dq	0.3330	0.1920
Dr	0.8410	0.5180
Ds	0.7760	0.4950
Dt	0.9000	0.5550
Du	0.6120	0.4330
Dv	0.6100	0.3440
Dw	0.4550	0.3160
Dx	0.3060	0.1690
Dy	0.8450	0.5180
Dz	0.8120	0.5120
Ea	0.9000	0.5550
Eb	0.5690	0.4170
Ec	0.6440	0.3610
Ed	0.4130	0.3100
Ee	0.3060	0.2330
Ef	0.8390	0.5190
Eg	0.8160	0.5120
Eh	0.8960	0.5550
Ei	0.5780	0.4320
Ej	0.6950	0.3560
Ek	0.4630	0.3050
El	0.3060	0.2070
Em	0.8450	0.5200
En	0.7900	0.5050

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Chain	Atom inclusion	Q-score
Eo	0.8960	0.5530
Ep	0.5950	0.4380
Eq	0.6440	0.3420
Er	0.4550	0.3100
Es	0.3060	0.2300
Et	0.8540	0.5190
Eu	0.7830	0.5020
Ev	0.9000	0.5560