wwPDB X-ray Structure Validation Summary Report (i)

May 18, 2020 – 11:49 am BST

PDB ID	:	4O9Y
Title	:	Crystal Structure of TcdA1
Authors	:	Meusch, D.; Gatsogiannis, C.; Efremov, R.G.; Lang, A.E.; Hofnagel, O.; Vetter, I.R.; Aktories, K.; Raunser, S.
Deposited on	:	2014-01-03
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

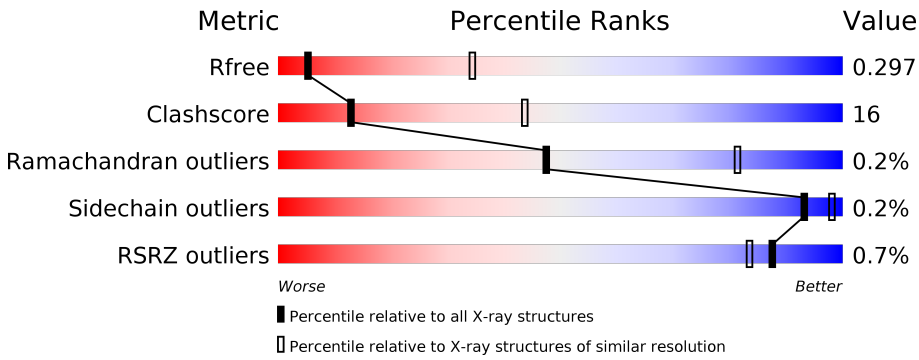
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2516	63% 35% •
1	B	2516	64% 35% •
1	C	2516	% 64% 35% •
1	D	2516	65% 34% •
1	E	2516	% 64% 34% •
1	F	2516	% 64% 35% •

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Mol	Chain	Length	Quality of chain
1	G	2516	% 65% 33% •
1	H	2516	% 66% 33% •
1	I	2516	% 64% 35% •
1	J	2516	% 63% 35% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 197663 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 TcdA1.

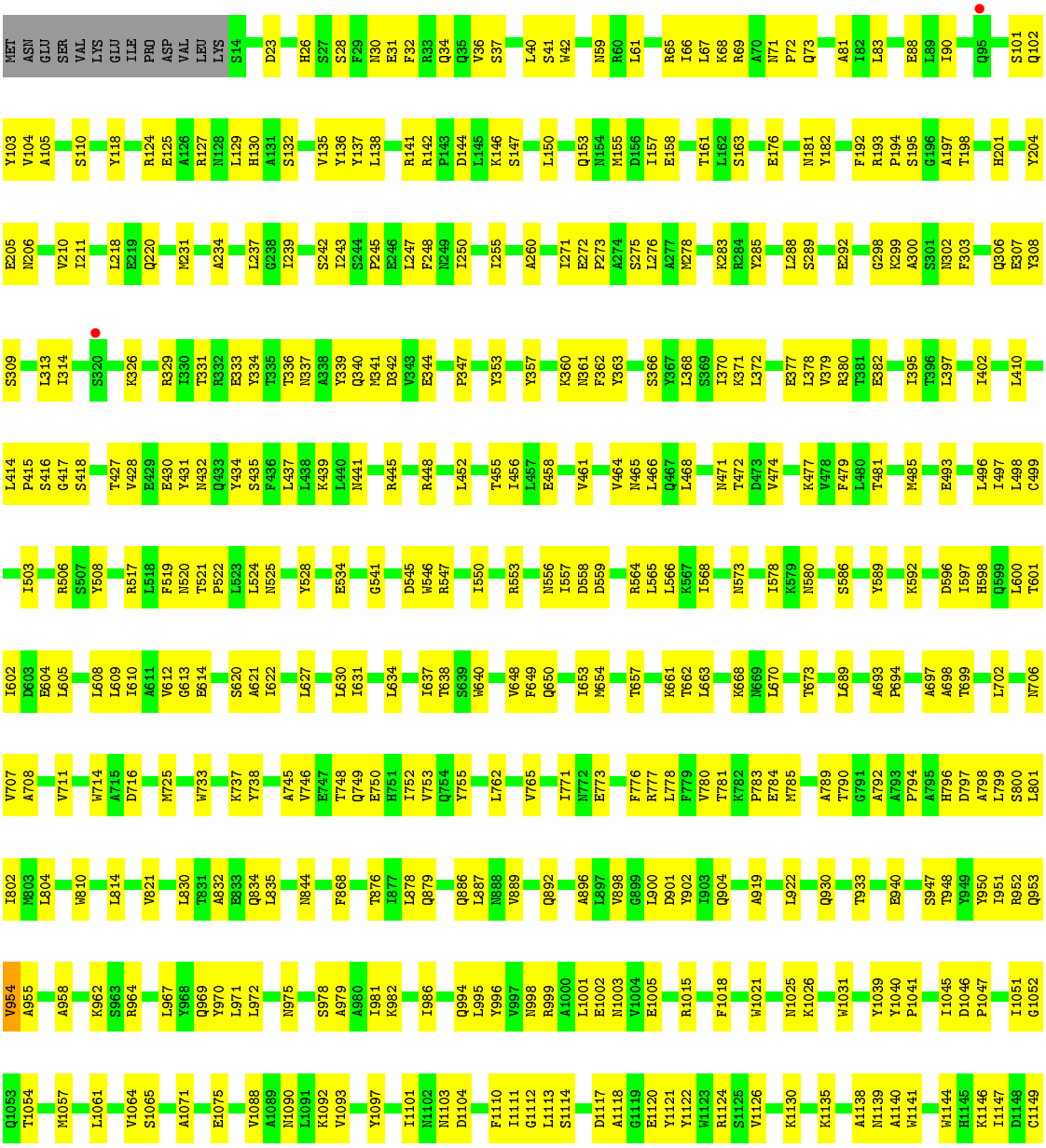
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	2490	19768	12508	3364	3833	63	0	0	0
1	B	2490	19768	12508	3364	3833	63	0	0	0
1	C	2490	19768	12508	3364	3833	63	0	0	0
1	D	2490	19768	12508	3364	3833	63	0	0	0
1	E	2490	19768	12508	3364	3833	63	0	0	0
1	F	2490	19768	12508	3364	3833	63	0	0	0
1	G	2488	19751	12499	3359	3830	63	0	0	0
1	H	2490	19768	12508	3364	3833	63	0	0	0
1	I	2490	19768	12508	3364	3833	63	0	0	0
1	J	2490	19768	12508	3364	3833	63	0	0	0

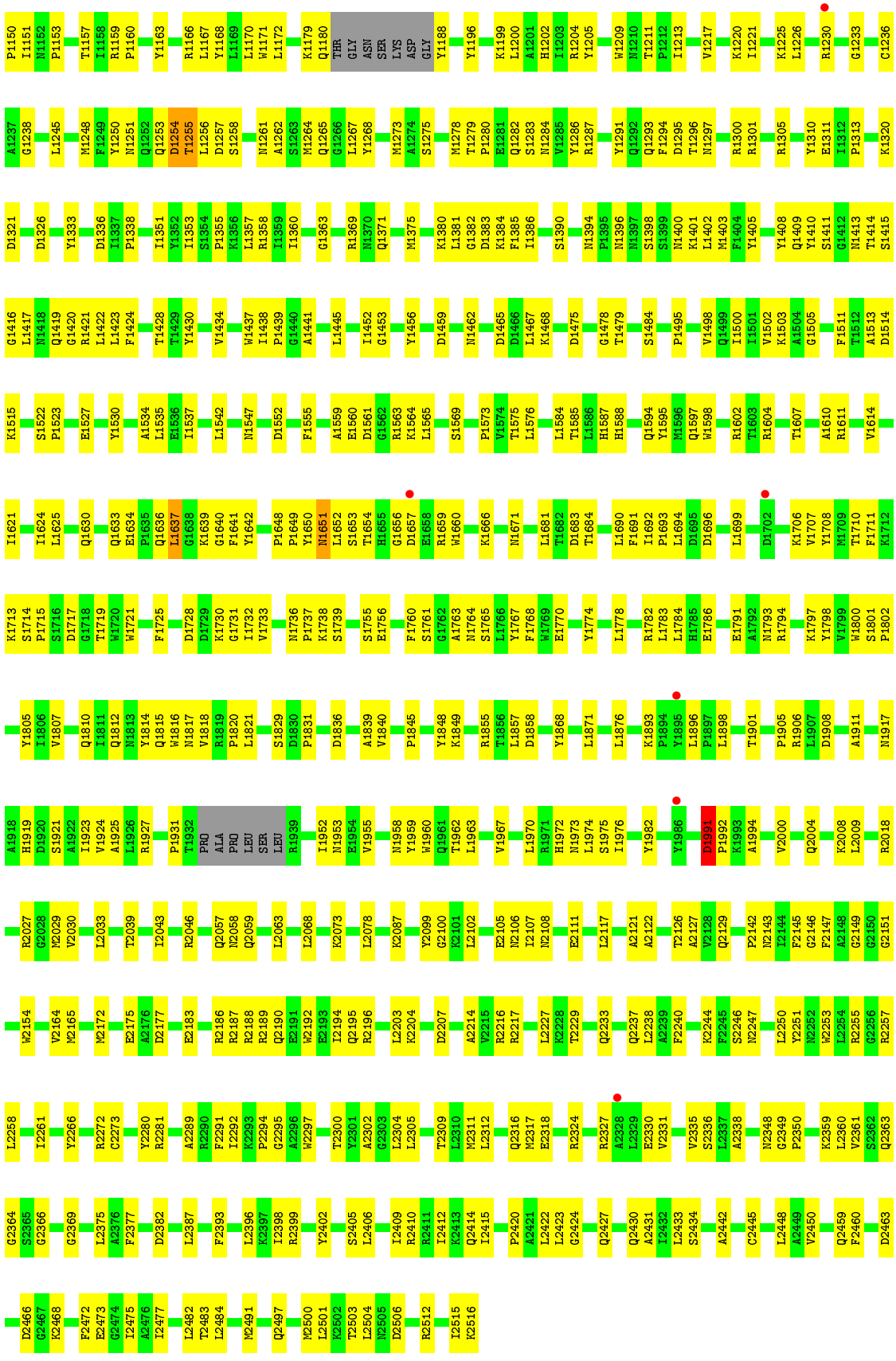
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: TcdA1

Chain A: 63% 35%





- Molecule 1: TcdA1

Chain B: 64% 35%

MET ASN GLU SER VAL LYS GLU ILE PRO ASP VAL LEU LYS S14 Q15 C16 G17 H26 F29 N30 E31 F32 R33 Q34 Q35 V36 L40 S41 W42 S43 E44 Y49 K57 L61 Q73 A81 I90 Q95 R99 A100 S101 Q102 Y103 V104 T108 R124 E125

A126 R127 H130 V135 Y136 Y137 L138 R141 R142 P143 K146 S147 L150 Q153 N154 M155 D156 I157 E158 L159 S160 T161 L162 S163 L170 E176 N181 Y182 V185 L189 F192 R193 P194 S195 G196 A197 T198 H201 Y204 E205 R208 E209 V210 I211

E219 Q220 A223 S224 M231 H232 Q233 L237 G238 I239 E246 L247 I250 L251 A260 N267 I271 E272 P273 A274 S275 L276 A277 M278 Y281 L282 K283 R284 Y285 L288 S289 E292 F296 I297 G298 K299 A300 Q306 E307 Y308 S309 I313 I314 T315 V318

N319 G323 T324 V325 R329 I330 T331 T336 N337 A338 Y339 Q340 M341 D342 P347 F348 Y353 R354 N361 F362 Y363 S366 I370 K371 L372 N373 E377 L378 V379 R380 T381 E382 I395 N398 I402 F406 L410 L414 P415 S416 G417 S418 T427

Y434 L437 N441 I444 R445 R448 A449 T450 S453 I456 V461 V464 N465 N471 T472 D473 V474 K477 V478 F479 K482 M485 Y488 T494 A495 L496 I497 L498 N520 T521 P522 L523 L524 N525 G526 Q527 Y528 T531 E534 D537 L538 N539

S540 G541 S542 K548 T549 I550 L551 K552 R553 N556 I557 D558 D559 R564 L565 L566 K567 I568 N573 I578 K579 N580 S586 Y589 I590 G591 K592 L593 L594 A595 D596 I597 H598 Q599 L600 T601 I602 D603 E604 L605 L608 L609 V612 G613 E614 G615 K616 S620 A621

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A979 A980 I981 K982 T983 T984 R985 I986 A987 Q994 L995 Y996 V997 N998 R999 E1002 E1005 N1009 V1012 I1013 S1014 R1015 Q1016 F1017 F1018 W1021 Y1024 N1025 K1026 Y1034 L1061 L1069 F1085 N1090 L1091 K1092 V1093 Y1097 H1098 I1101 N1102 N1103 D1104 I1111 G1112

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R1204 T1208 W1209 N1210 T1211 P1212 I1213 K1220 I1221 K1225 R1230 C1236 A1237 G1238 L1245 M1248 F1249 Y1250 N1251 Q1252 Q1253 D1254 T1255 L1256 D1257 S1258 Y1259 K1260 N1261 Q1265 G1266 L1267 Y1268 I1269 M1273 A1274 S1275 T1279 P1280 E1281 Q1282 S1283 N1284 V1285 Y1286 R1287 D1288 N1289 S1290 Y1291

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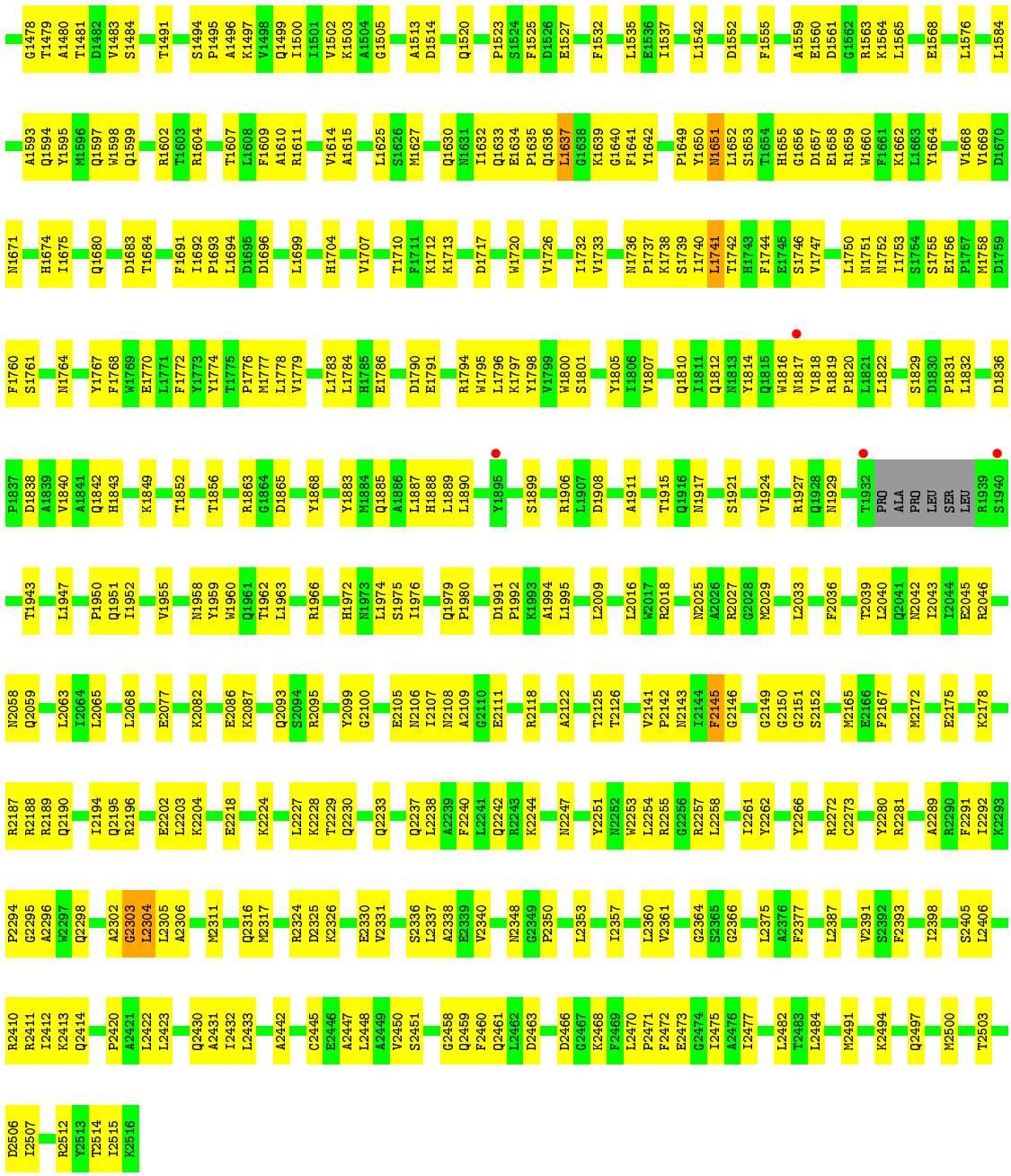
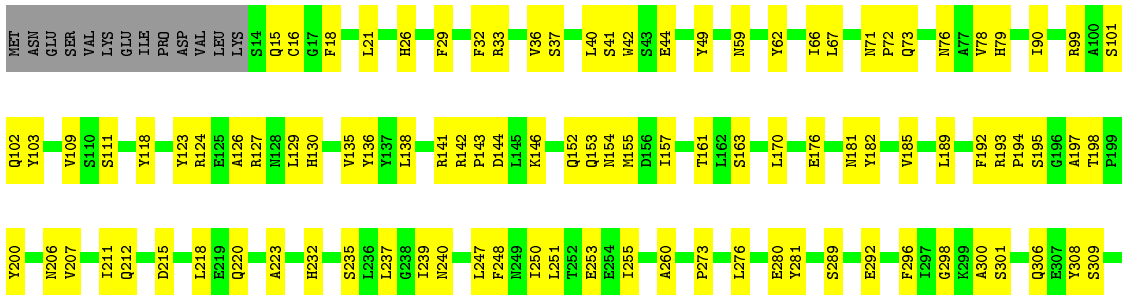
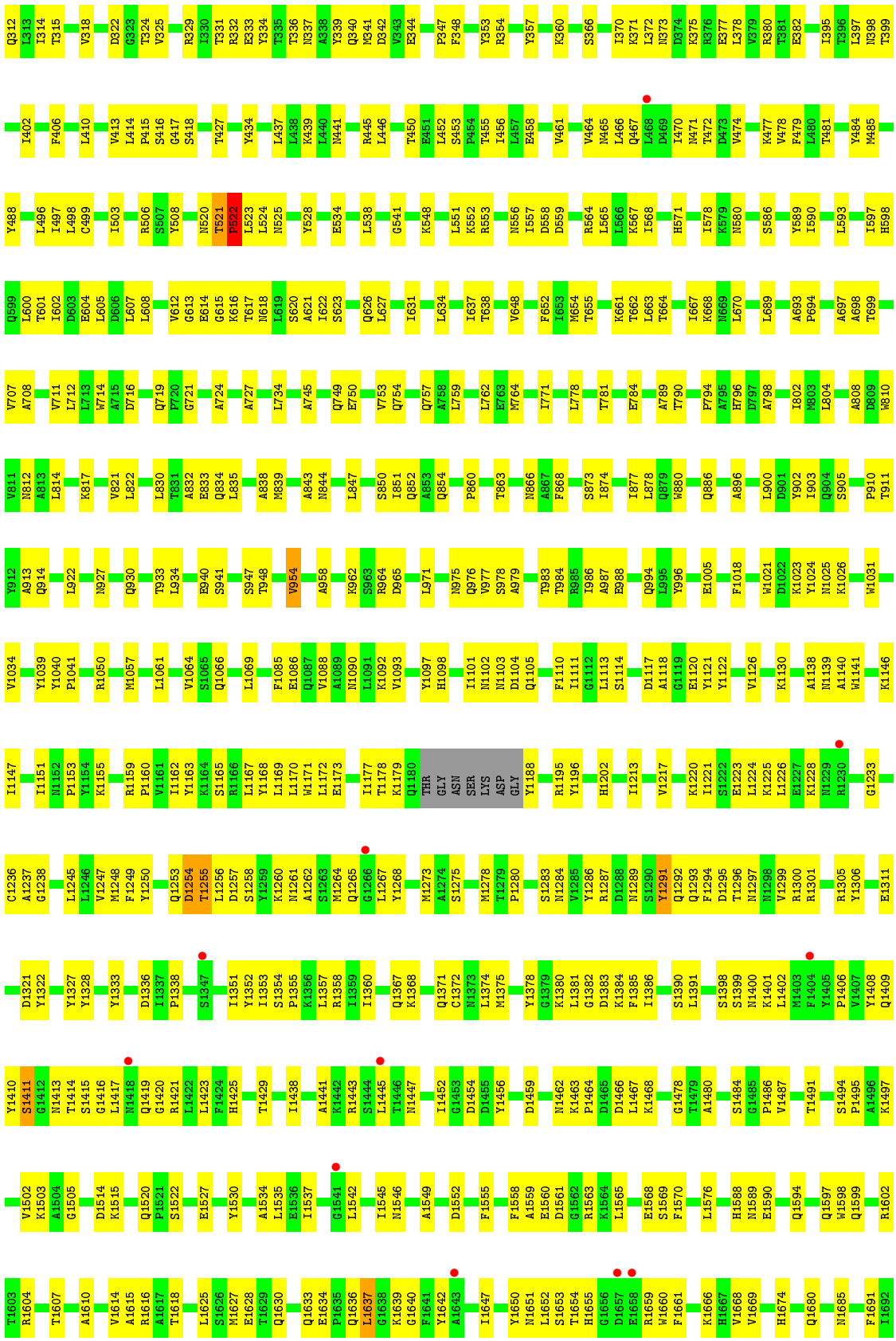


- Molecule 1: TcdA1

Chain C:

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I402 F406 L410 V413 L414 P415 S416 G417 S418 T427 Y434 L437 L438 K439 L440 N441 R445 L446 T450 E451 L452 S453 P454 T455 I456 L457 E458 V461 V464 N465 L466 Q467 L468 D469 I470 N471 T472 D473 V474 K477 V478 F479 L480 T481 Y484 M485
Y488 L496 I497 L498 C499 I503 R506 S507 Y508 N520 T521 P522 L523 L524 N525 Y528 E534 L538 G541 K548 L551 K552 R553 N556 I557 D558 D559 R564 L565 L566 K567 I568 H571 L578 K579 N580 S586 Y589 I590 L593 I597 H598
Q599 L600 T601 I602 D603 E604 L605 D606 L607 L608 V612 G613 E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 Q626 L627 I631 L634 I637 T638 V648 F652 I653 M654 T655 K661 T662 L663 T664 I667 K668 N669 L670 L689 A693 P694 A697 A698 T699
V707 A708 V711 L712 L713 W714 A715 D716 Q719 F720 G721 A724 A727 L734 A745 Q749 E750 V753 Q754 Q757 A758 L759 L762 E763 M764 I771 L778 T781 E784 A789 T790 P794 A795 H796 D797 A798 I802 M803 L804 A808 D809 W810
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V1502 K1503 A1504 G1505 D1514 K1515 Q1520 P1521 S1522 E1527 Y1530 A1534 L1535 E1536 I1537 G1541 L1542 I1545 N1546 A1549 D1552 F1555 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 E1568 S1569 F1570 L1576 H1588 N1589 E1590 Q1594 Q1597 W1598 Q1599 R1602
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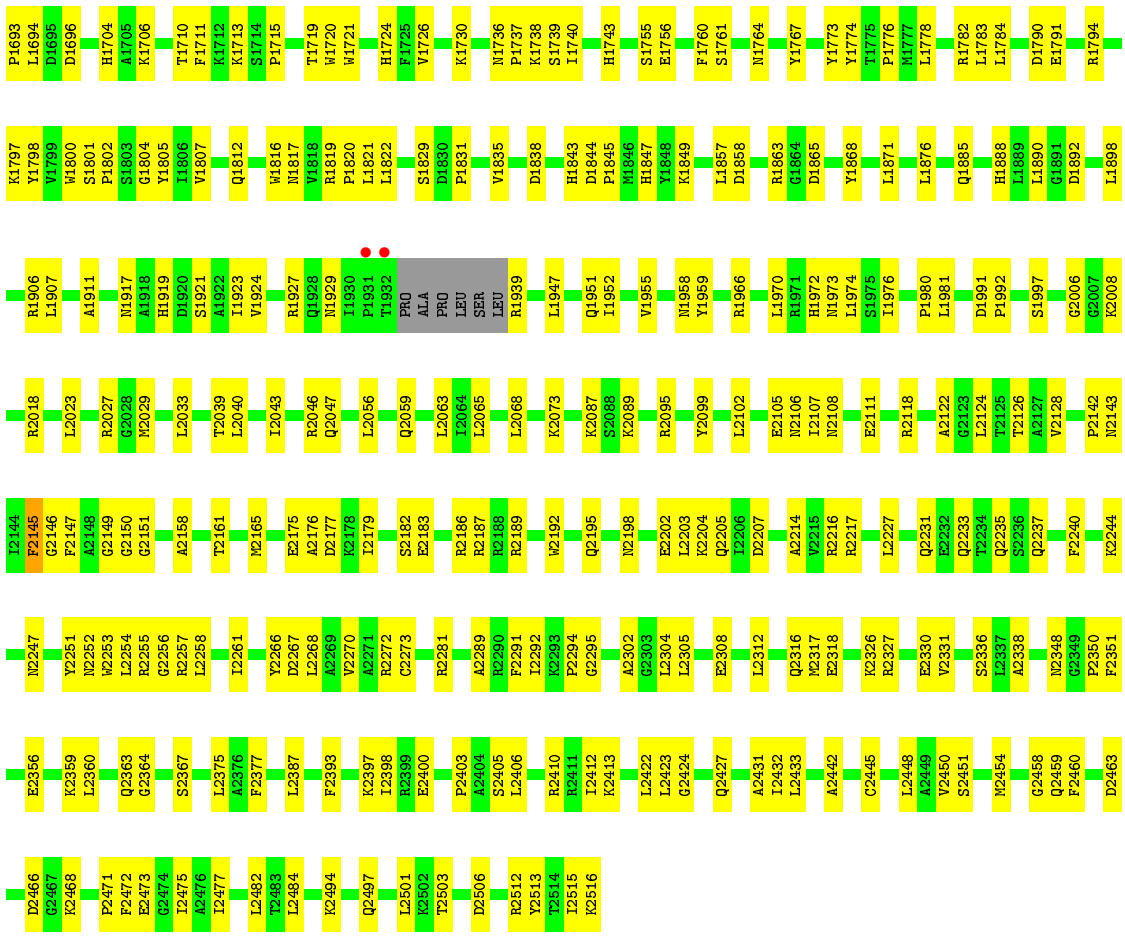
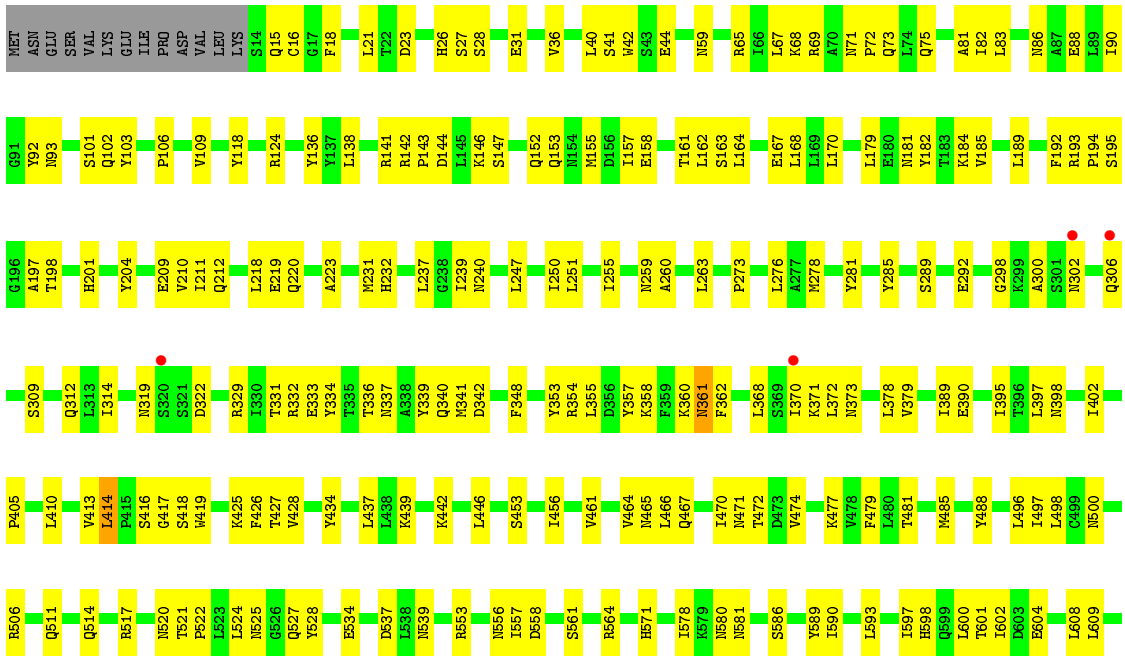
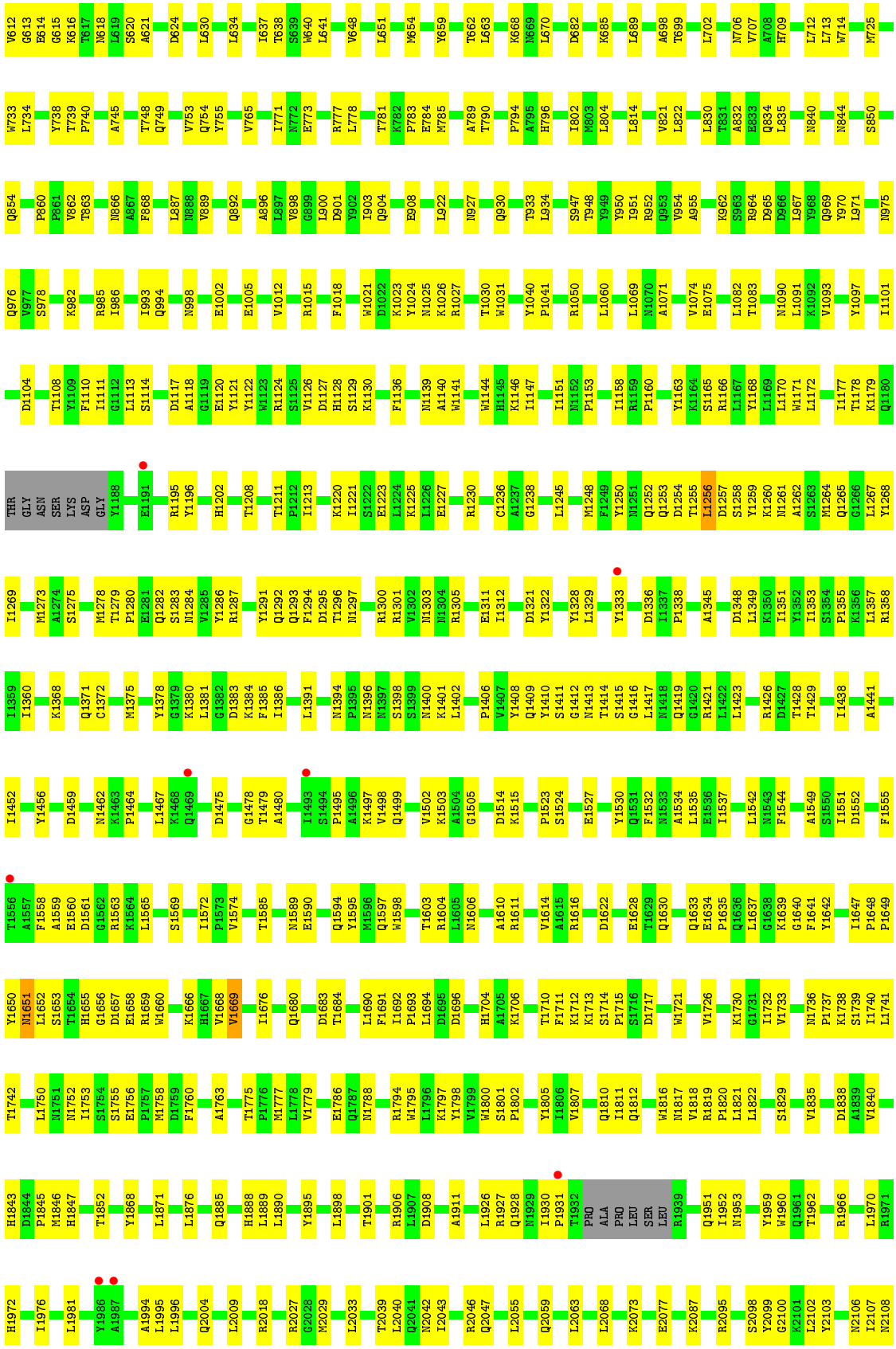


- Molecule 1: TcdA1

Chain D:

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D1104 T1108 Y1109 F1110 I1111 G1112 L1113 S1114 D1117 A1118 G1119 E1120 Y1121 Y1122 W1123 R1124 S1125 V1126 D1127 H1128 S1129 K1130 F1136 N1139 A1140 W1141 W1144 H1145 K1146 I1147 I1151 N1152 P1153 I1158 R1159 P1160 Y1163 K1164 S1165 R1166 L1167 Y1168 L1169 L1170 W1171 L1172 I1177 T1178 K1179 Q1180
THR GLY ASN SER LYS ASP GLY Y1188 E1191 R1195 Y1196 H1202 T1208 T1211 P1212 I1213 K1220 I1221 S1222 E1223 L1224 K1225 L1226 E1227 R1230 C1236 A1237 G1238 L1245 M1248 F1249 Y1250 M1251 Q1252 Q1253 D1254 T1255 L1256 D1257 S1258 Y1259 K1260 M1261 A1262 S1263 M1264 Q1265 G1266 L1267 Y1268
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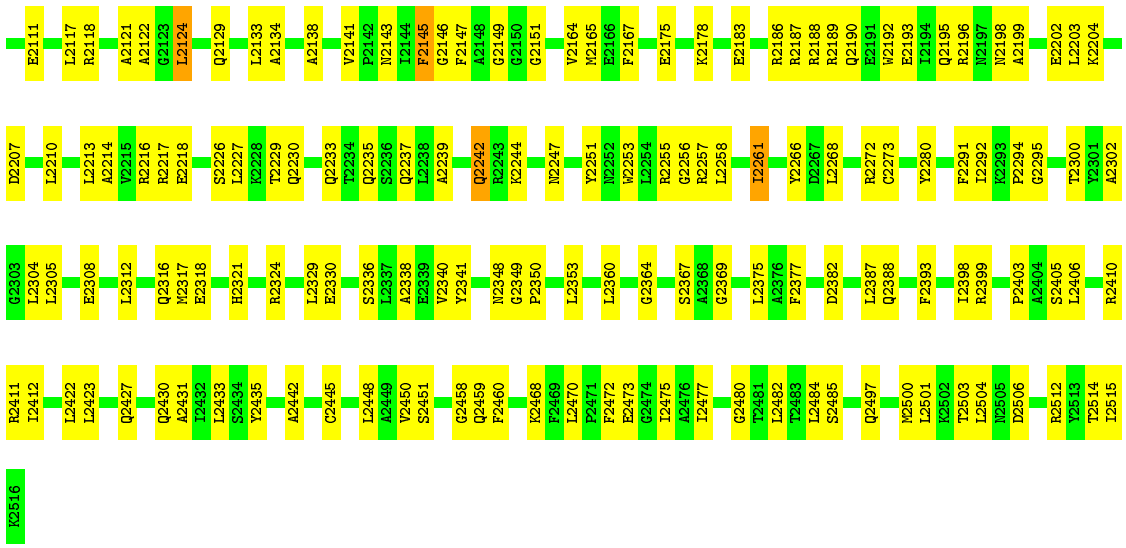
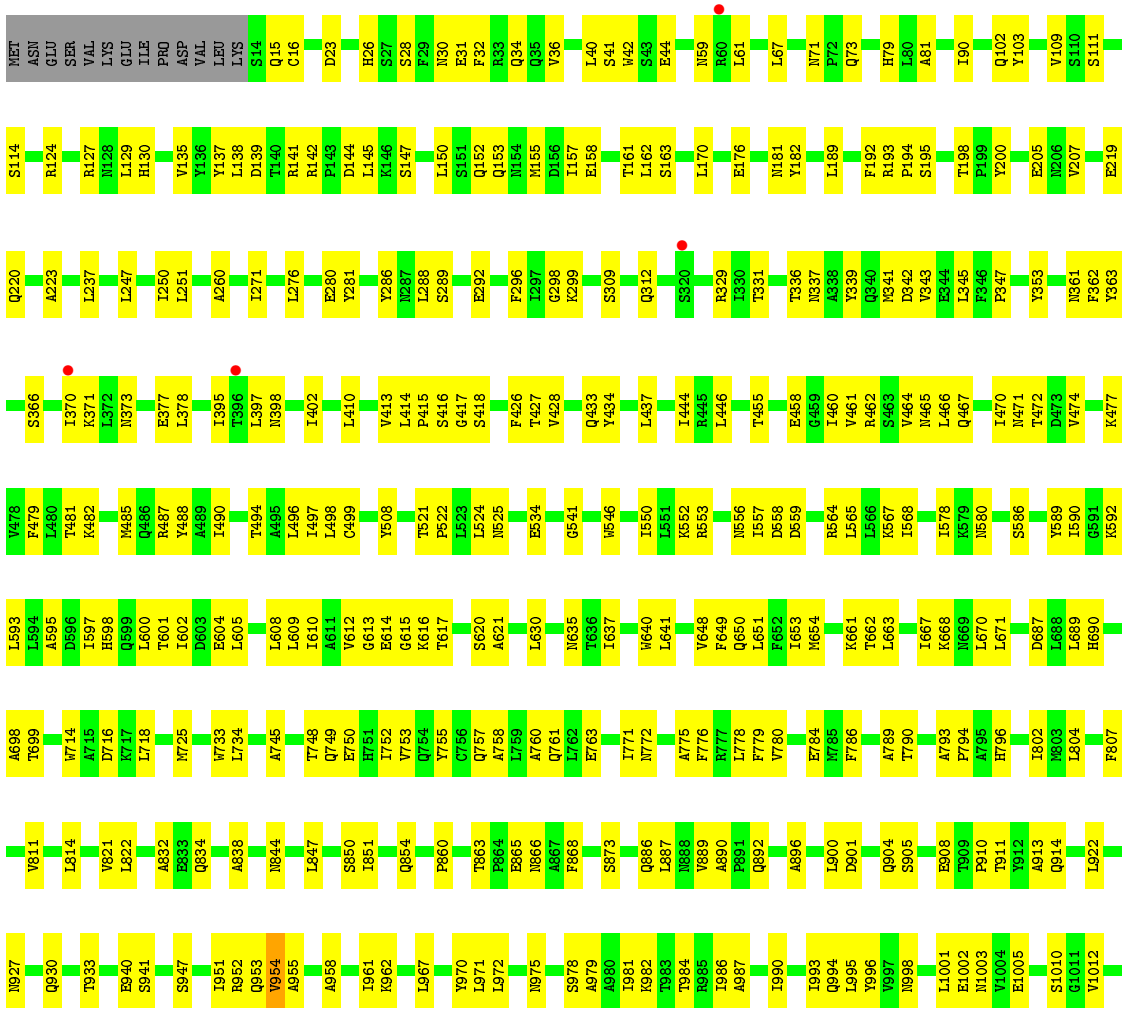
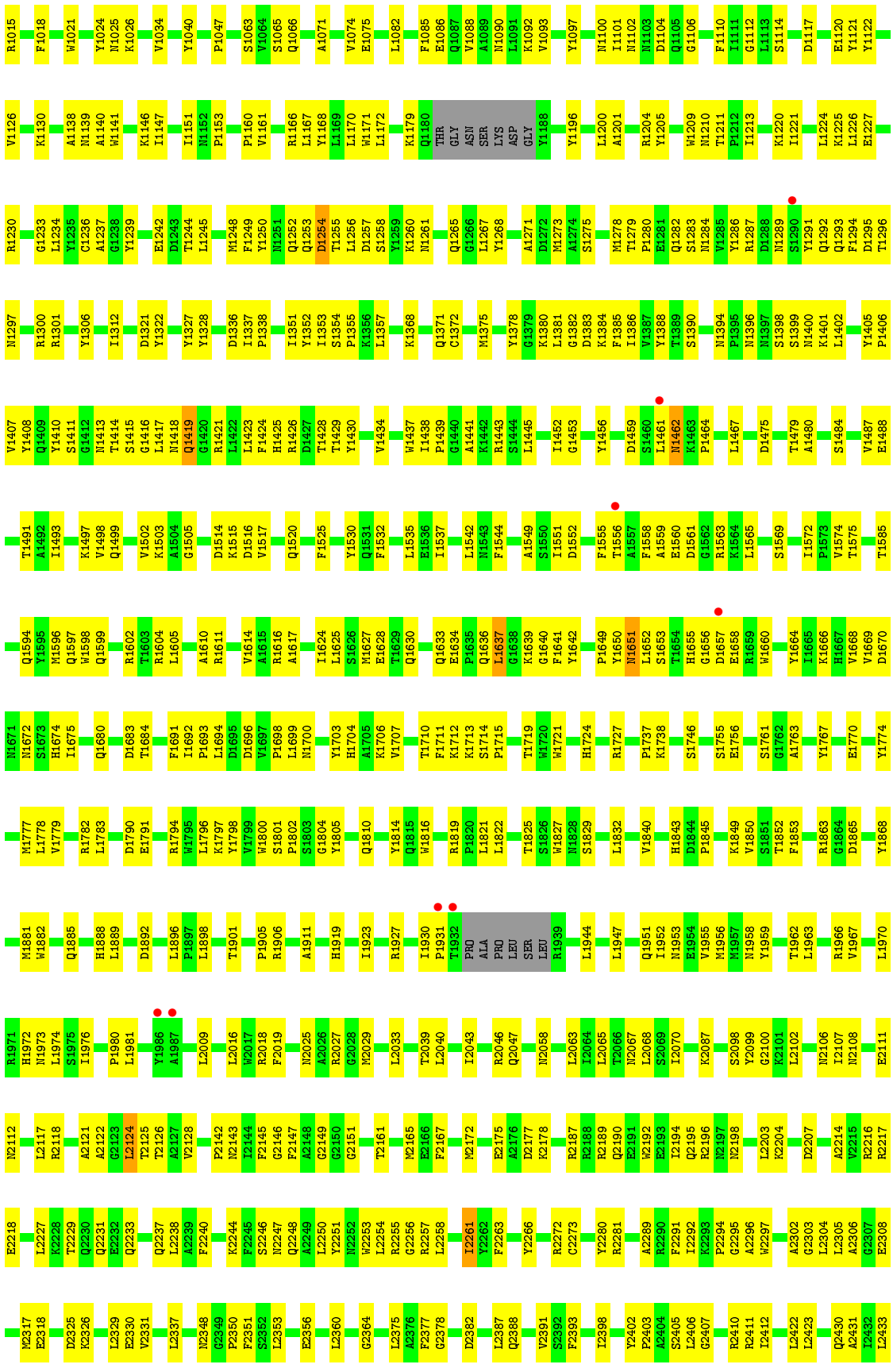


- Molecule 1: TcdA1

Chain E:

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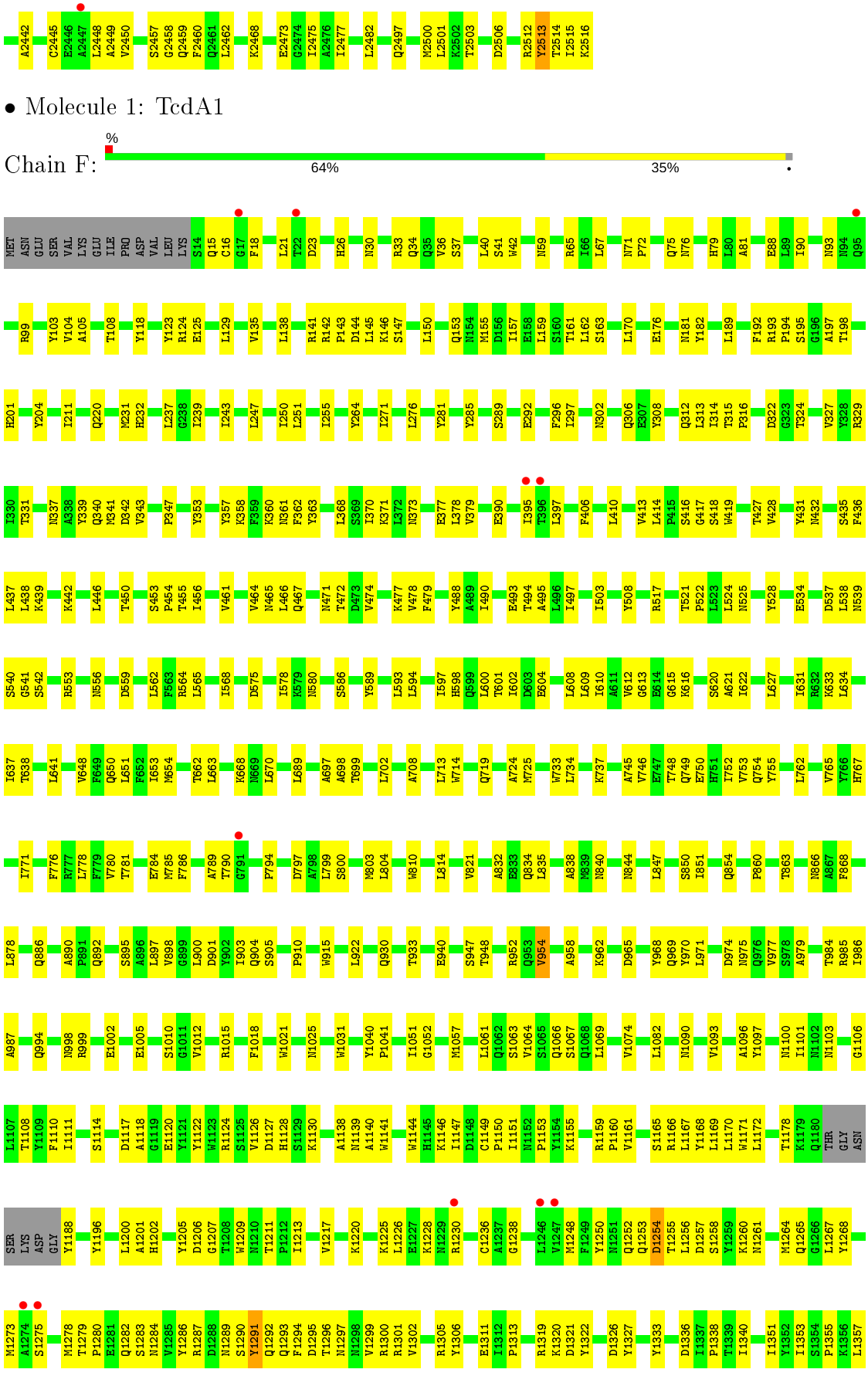
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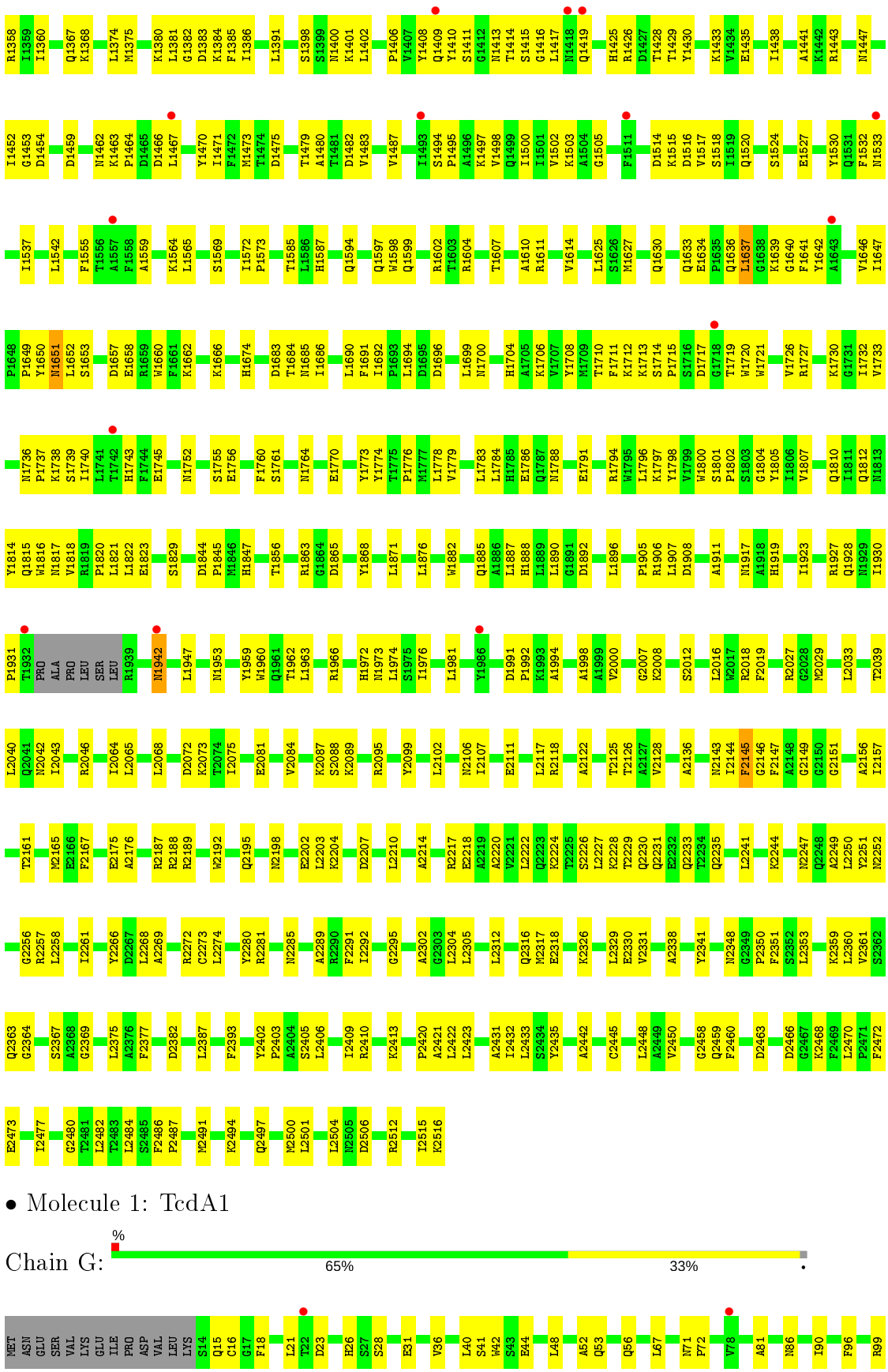

- Molecule 1: TcdA1

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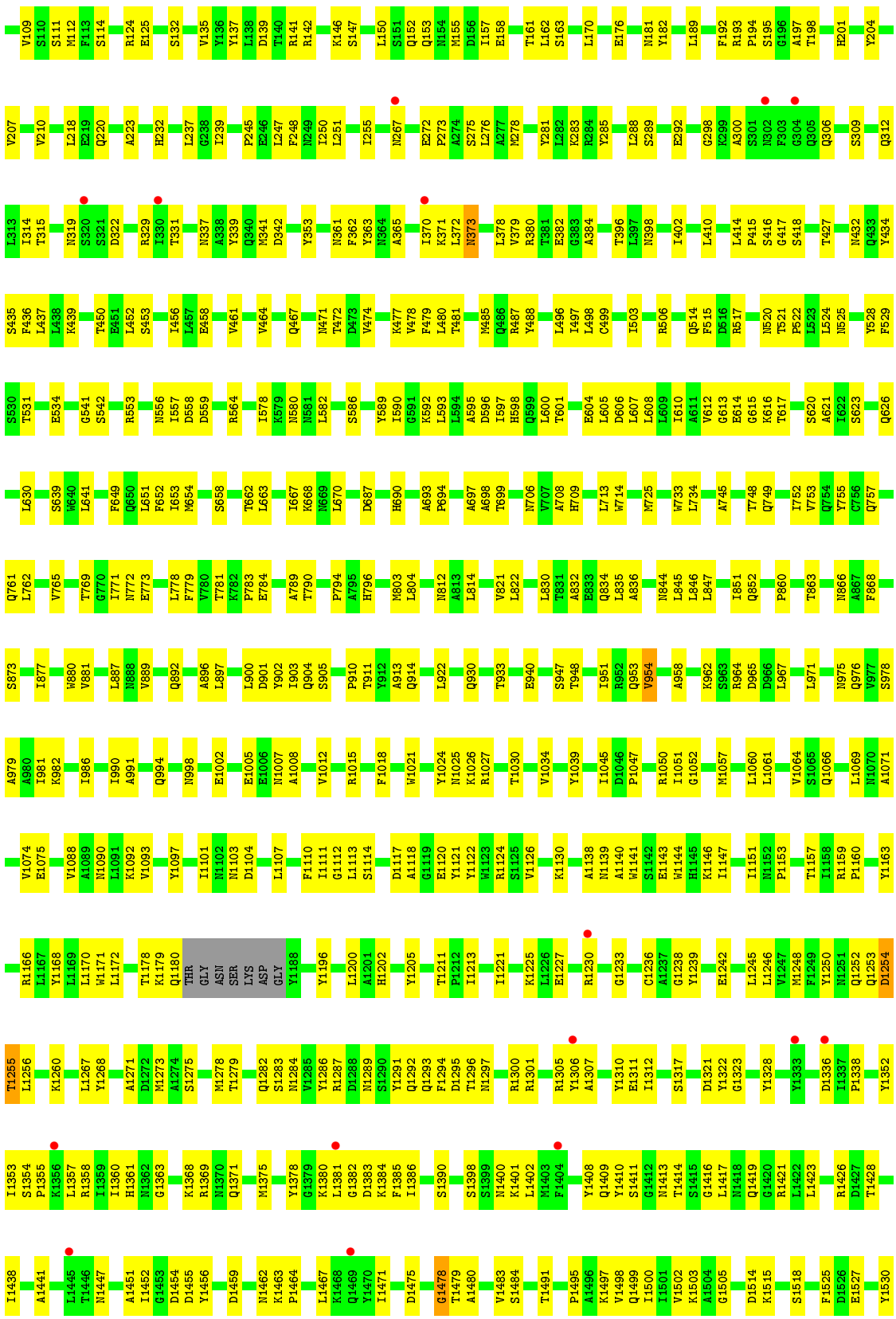
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- Molecule 1: TcdA1

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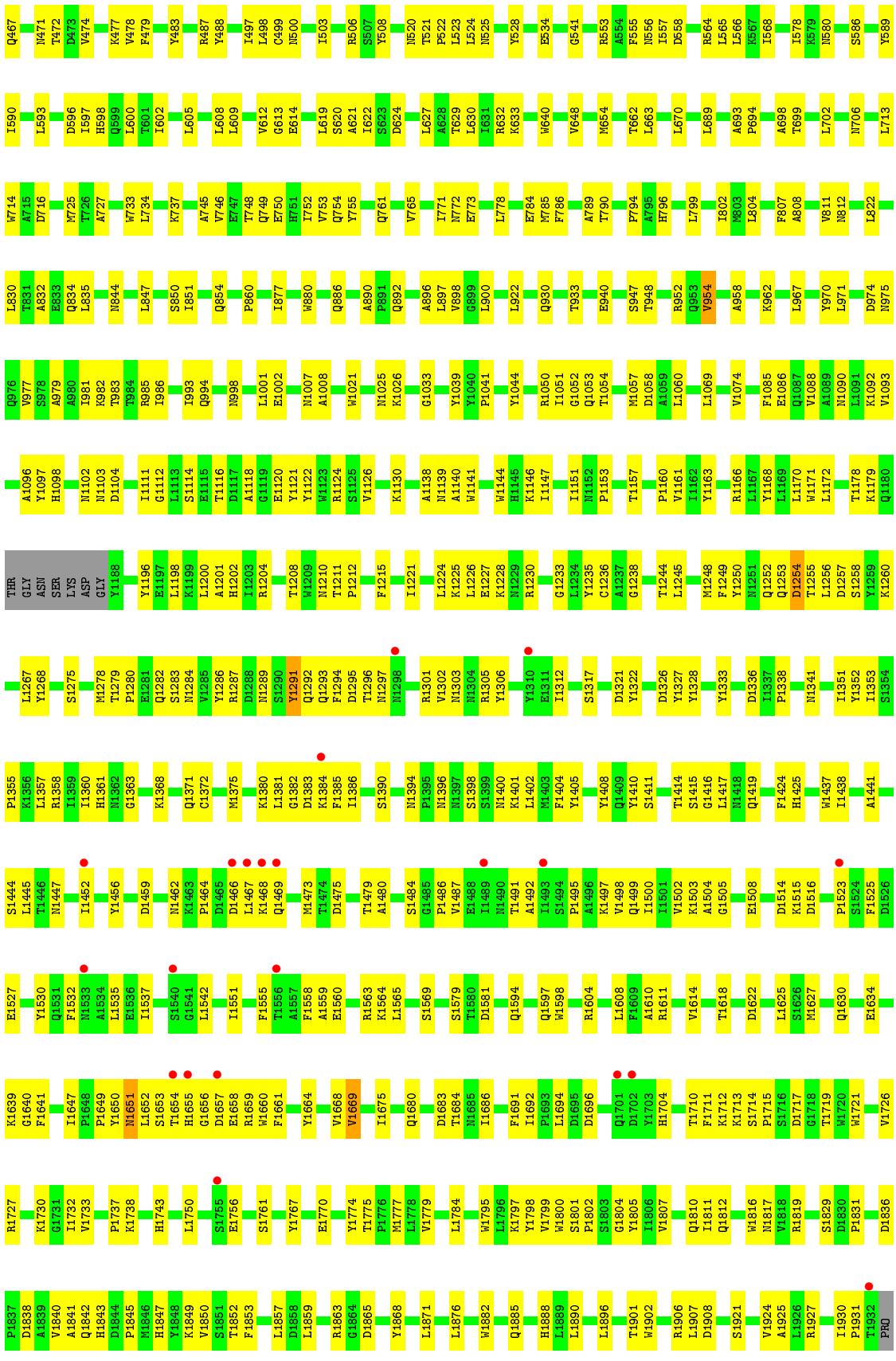
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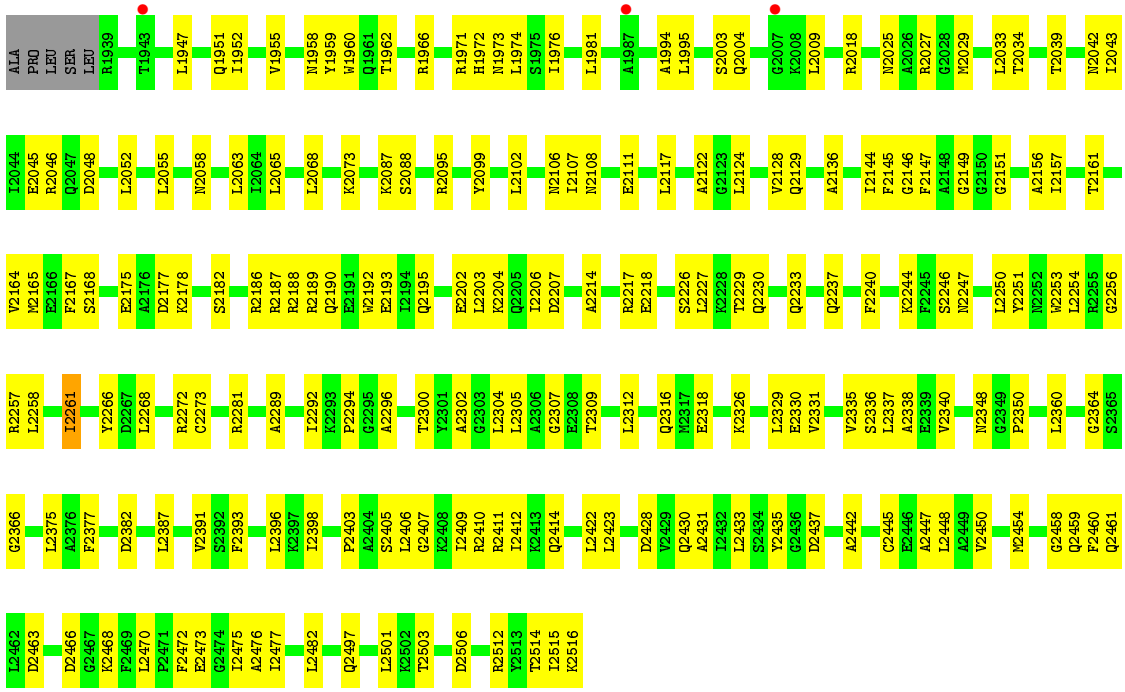
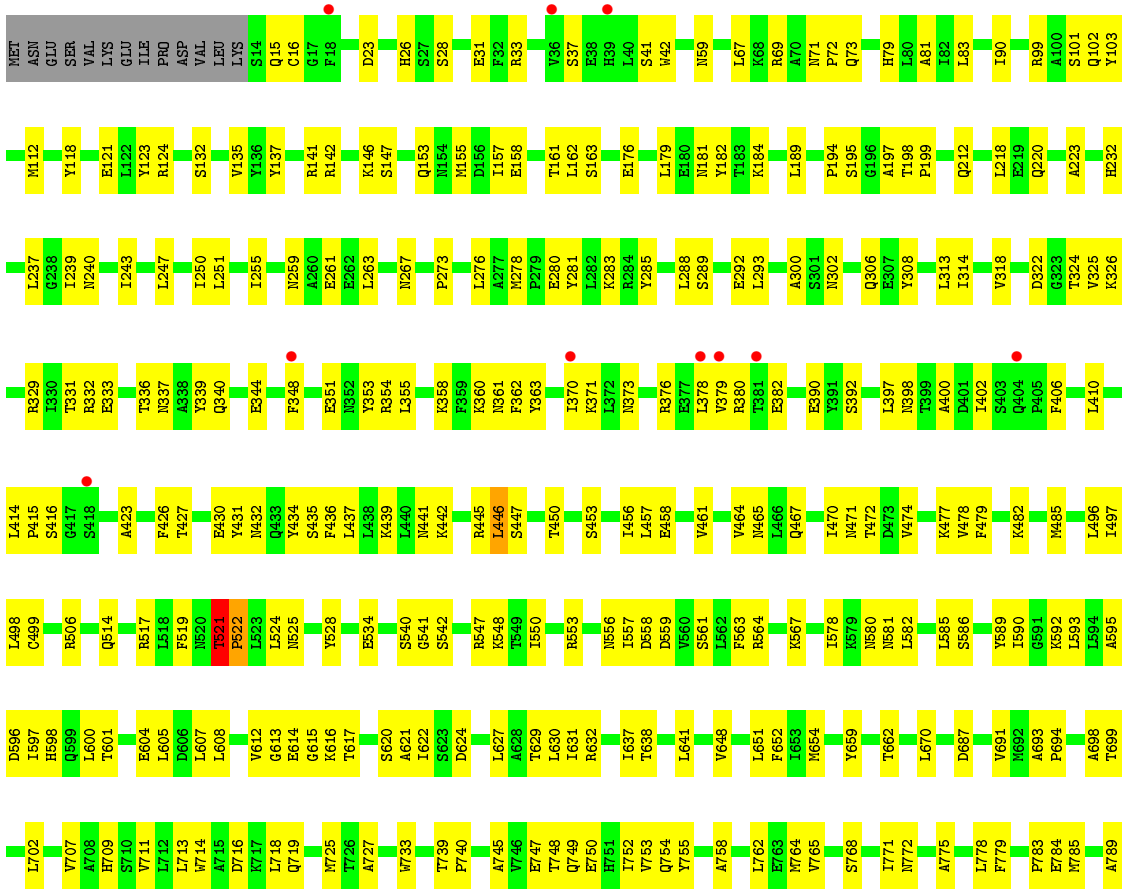
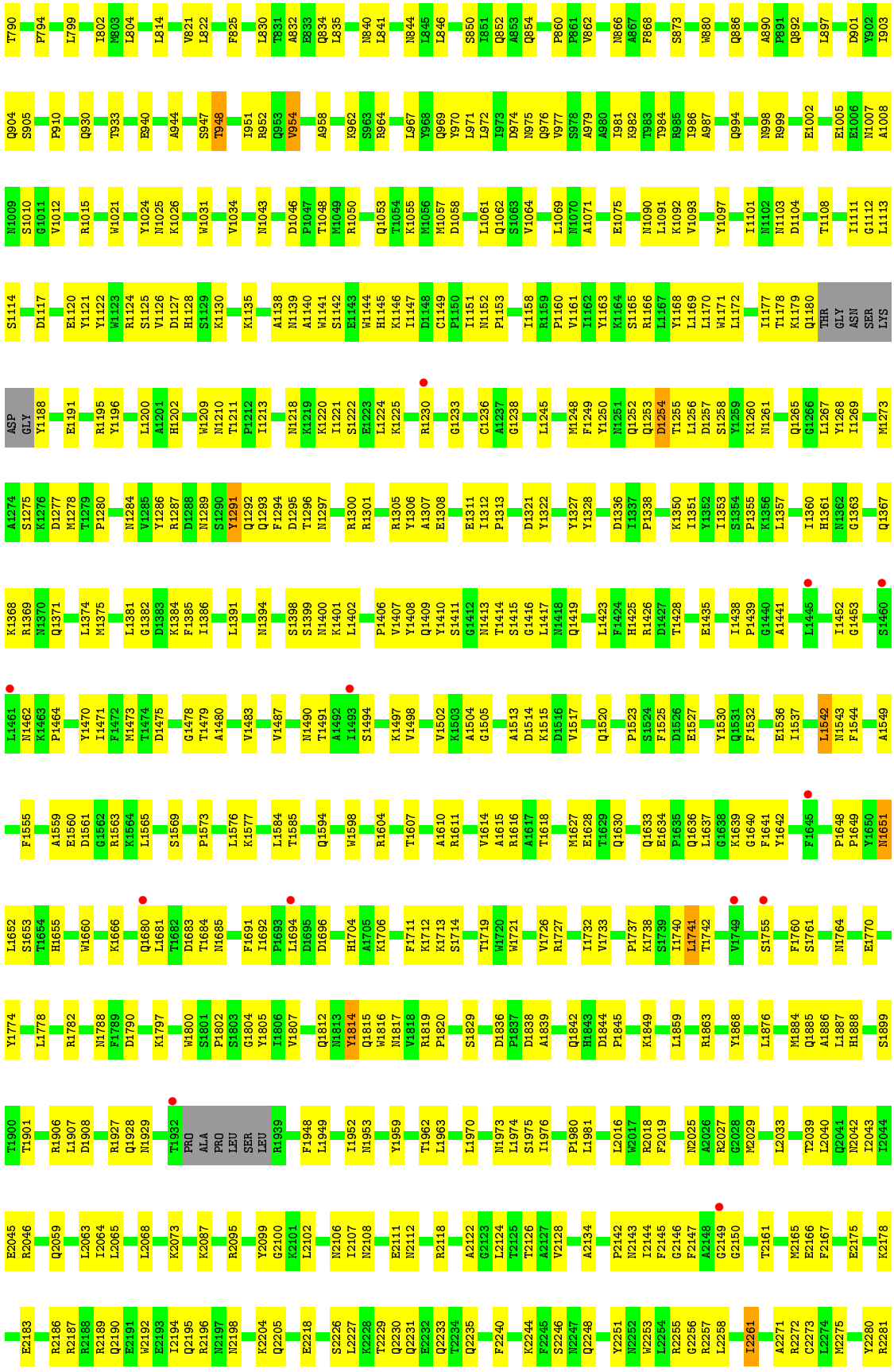


- Molecule 1: TcdA1

Chain I:

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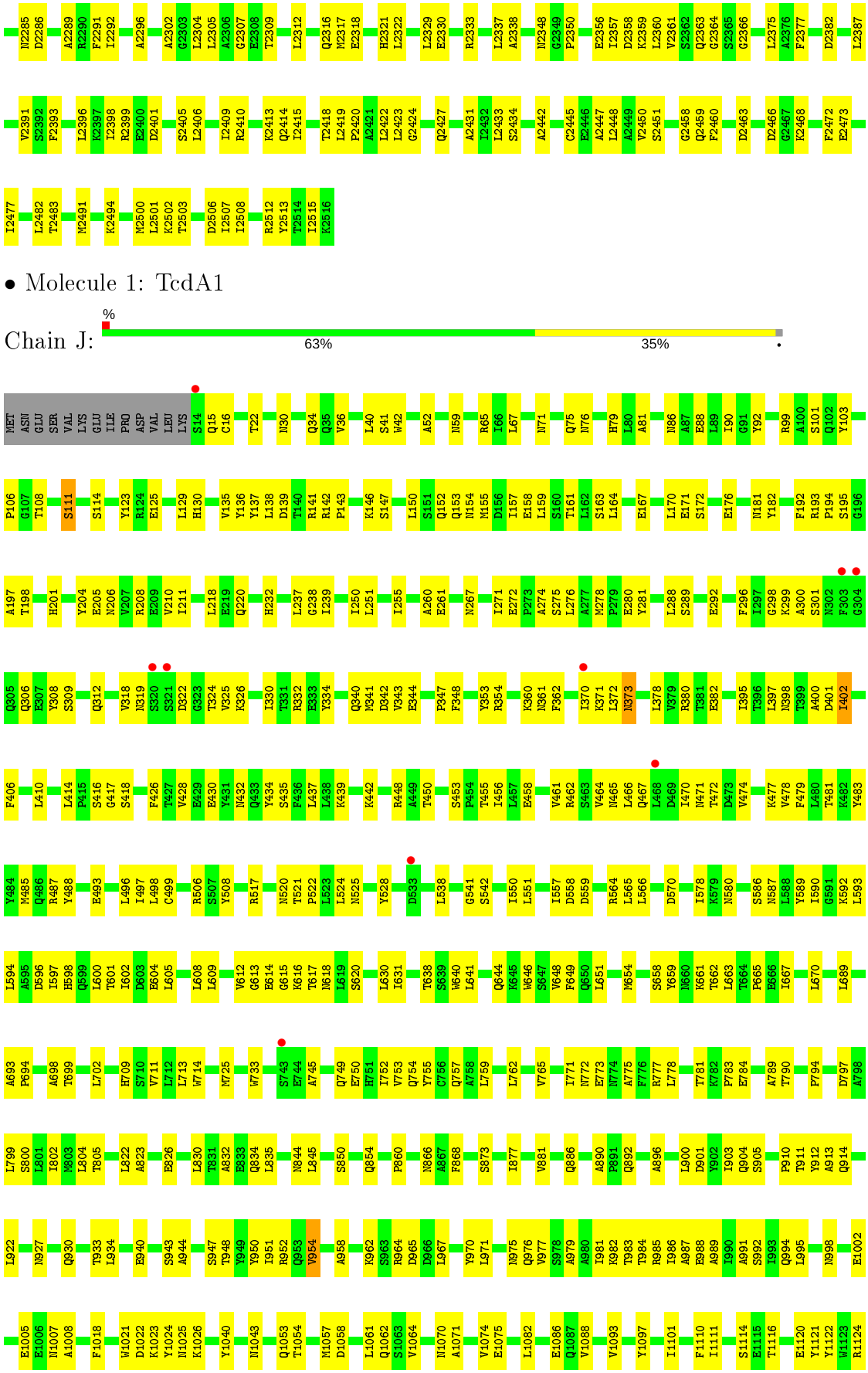
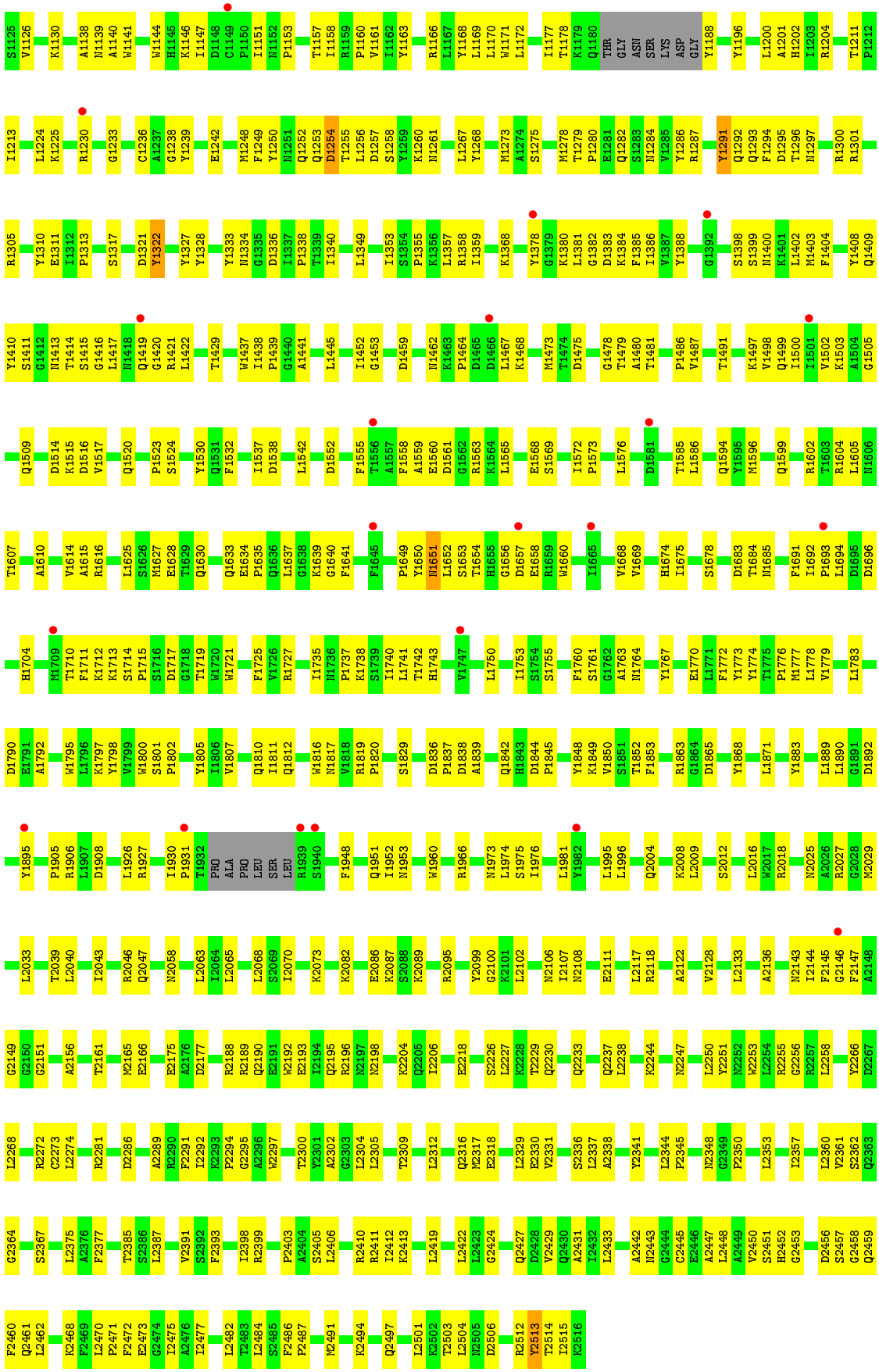


• Molecule 1: TcdA1

Chain J: % 63% 35%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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	303.25Å 320.73Å 667.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 73.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	78.3 (20.00-3.50) 78.4 (73.11-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 3.49Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.243 , 0.295 0.245 , 0.297	Depositor DCC
R_{free} test set	19006 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 14.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	197663	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.41	0/20194	0.66	4/27427 (0.0%)
1	B	0.41	0/20194	0.66	5/27427 (0.0%)
1	C	0.40	0/20194	0.65	7/27427 (0.0%)
1	D	0.41	0/20194	0.66	3/27427 (0.0%)
1	E	0.41	0/20194	0.67	5/27427 (0.0%)
1	F	0.38	0/20194	0.63	4/27427 (0.0%)
1	G	0.39	0/20177	0.64	2/27405 (0.0%)
1	H	0.38	0/20194	0.64	3/27427 (0.0%)
1	I	0.39	0/20194	0.64	3/27427 (0.0%)
1	J	0.39	0/20194	0.64	3/27427 (0.0%)
All	All	0.40	0/201923	0.65	39/274248 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	521	THR	C-N-CD	-7.83	103.37	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1461	LEU	CA-CB-CG	7.83	133.30	115.30
1	I	1291	TYR	N-CA-C	-7.48	90.79	111.00
1	F	1291	TYR	N-CA-C	-6.93	92.28	111.00
1	H	1291	TYR	N-CA-C	-6.20	94.25	111.00

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1730	LYS	Peptide
1	C	1730	LYS	Peptide
1	C	521	THR	Peptide
1	D	1730	LYS	Peptide
1	F	1730	LYS	Peptide

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	A	19768	0	19307	696	0
1	B	19768	0	19307	693	0
1	C	19768	0	19307	705	0
1	D	19768	0	19307	704	0
1	E	19768	0	19307	705	0
1	F	19768	0	19307	694	0
1	G	19751	0	19289	663	0
1	H	19768	0	19307	654	0
1	I	19768	0	19307	706	0
1	J	19768	0	19307	702	0
All	All	197663	0	193052	6448	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 16.

The worst 5 of 6448 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)
1:A:1653:SER:H	1:A:1713:LYS:HE3	1.13	1.09
1:J:1653:SER:H	1:J:1713:LYS:HE3	1.22	1.04
1:C:1117:ASP:H	1:D:1211:THR:HG21	1.21	1.03
1:J:1250:TYR:HE2	1:J:1294:PHE:HB3	1.20	1.03
1:E:1250:TYR:HE2	1:E:1294:PHE:HB3	1.26	1.01

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	A	2484/2516 (99%)	2384 (96%)	94 (4%)	6 (0%)	47	81
1	B	2484/2516 (99%)	2397 (96%)	82 (3%)	5 (0%)	47	81
1	C	2484/2516 (99%)	2394 (96%)	85 (3%)	5 (0%)	47	81
1	D	2484/2516 (99%)	2390 (96%)	90 (4%)	4 (0%)	47	81
1	E	2484/2516 (99%)	2387 (96%)	92 (4%)	5 (0%)	47	81
1	F	2484/2516 (99%)	2389 (96%)	90 (4%)	5 (0%)	47	81
1	G	2482/2516 (99%)	2393 (96%)	84 (3%)	5 (0%)	47	81
1	H	2484/2516 (99%)	2393 (96%)	86 (4%)	5 (0%)	47	81
1	I	2484/2516 (99%)	2393 (96%)	86 (4%)	5 (0%)	47	81
1	J	2484/2516 (99%)	2395 (96%)	84 (3%)	5 (0%)	47	81
All	All	24838/25160 (99%)	23915 (96%)	873 (4%)	50 (0%)	47	81

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1651	ASN
1	C	522	PRO
1	D	954	VAL

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Mol	Chain	Res	Type
1	F	954	VAL
1	F	1651	ASN

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 X-ray entries followed by that with respect to entries of similar resolution.

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	A	2134/2157 (99%)	2131 (100%)	3 (0%)	93	98
1	B	2134/2157 (99%)	2129 (100%)	5 (0%)	93	98
1	C	2134/2157 (99%)	2130 (100%)	4 (0%)	93	98
1	D	2134/2157 (99%)	2128 (100%)	6 (0%)	92	97
1	E	2134/2157 (99%)	2126 (100%)	8 (0%)	91	96
1	F	2134/2157 (99%)	2131 (100%)	3 (0%)	93	98
1	G	2132/2157 (99%)	2129 (100%)	3 (0%)	93	98
1	H	2134/2157 (99%)	2130 (100%)	4 (0%)	93	98
1	I	2134/2157 (99%)	2123 (100%)	11 (0%)	88	94
1	J	2134/2157 (99%)	2128 (100%)	6 (0%)	92	97
All	All	21338/21570 (99%)	21285 (100%)	53 (0%)	93	98

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2112	ASN
1	G	658	SER
1	J	402	ILE
1	E	2261	ILE
1	F	1685	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1105	GLN

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Mol	Chain	Res	Type
1	F	1367	GLN
1	J	398	ASN
1	E	1419	GLN
1	E	2047	GLN

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 carbohydrates 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 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	2490/2516 (98%)	-0.12	8 (0%)	94	91	11, 61, 112, 209	0
1	B	2490/2516 (98%)	-0.11	9 (0%)	92	90	19, 63, 114, 190	0
1	C	2490/2516 (98%)	-0.09	13 (0%)	91	88	14, 67, 116, 184	0
1	D	2490/2516 (98%)	-0.10	12 (0%)	91	88	10, 64, 115, 186	0
1	E	2490/2516 (98%)	-0.13	13 (0%)	91	88	11, 58, 112, 187	0
1	F	2490/2516 (98%)	-0.04	25 (1%)	82	77	8, 71, 134, 210	0
1	G	2488/2516 (98%)	-0.06	24 (0%)	82	77	6, 67, 128, 210	0
1	H	2490/2516 (98%)	-0.04	29 (1%)	79	73	13, 68, 128, 194	0
1	I	2490/2516 (98%)	-0.05	22 (0%)	84	79	10, 68, 127, 195	0
1	J	2490/2516 (98%)	-0.04	30 (1%)	79	73	8, 69, 130, 197	0
All	All	24898/25160 (98%)	-0.08	185 (0%)	87	83	6, 65, 123, 210	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1932	THR	7.2
1	F	1718	GLY	7.1
1	C	1932	THR	6.8
1	H	1932	THR	6.1
1	J	320	SER	5.5

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.