Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 05:16 pm GMT

PDB ID	:	6SUF
EMDB ID	:	EMD-10313
Title	:	Structure of Photorhabdus luminescens Tc holotoxin pore
Authors	:	Roderer, D.; Raunser, S.
Deposited on	:	2019-09-13
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

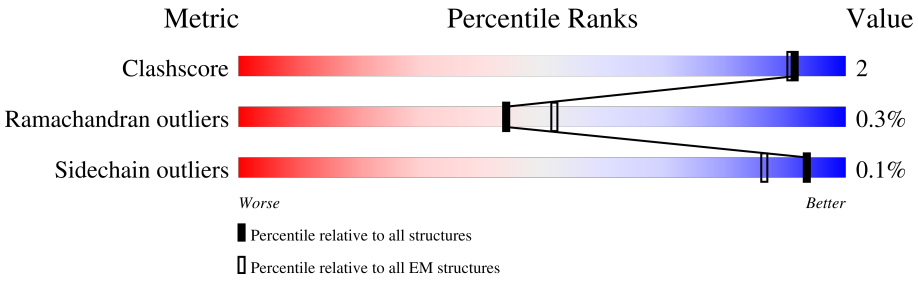
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.40 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	2516	22% 84% 7% 9%
1	B	2516	23% 84% 7% 9%
1	C	2516	22% 84% 6% 9%
1	D	2516	24% 84% 6% 9%
1	E	2516	19% 84% 7% 9%
2	F	2439	5% 81% 7% 12%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 108112 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 TcdA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2292	Total 18197	C 11530	N 3083	O 3525	S 59	0	0
1	B	2292	Total 18197	C 11530	N 3083	O 3525	S 59	0	0
1	C	2292	Total 18197	C 11530	N 3083	O 3525	S 59	0	0
1	D	2292	Total 18197	C 11530	N 3083	O 3525	S 59	0	0
1	E	2292	Total 18197	C 11530	N 3083	O 3525	S 59	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	904	GLU	GLN	conflict	UNP Q9RN43
B	904	GLU	GLN	conflict	UNP Q9RN43
C	904	GLU	GLN	conflict	UNP Q9RN43
D	904	GLU	GLN	conflict	UNP Q9RN43
E	904	GLU	GLN	conflict	UNP Q9RN43

- Molecule 2 is a protein called TcdB2,TccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2147	Total 17127	C 10729	N 3040	O 3323	S 35	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	543	GLU	ASP	conflict	UNP Q8GF99
F	1475	PRO	-	linker	UNP Q8GF99
F	1476	GLY	-	linker	UNP Q8GF99
F	1477	SER	-	linker	UNP Q8GF99

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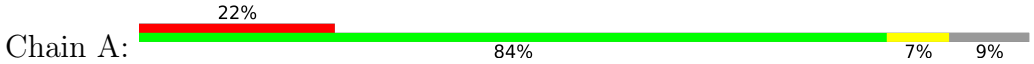
Chain	Residue	Modelled	Actual	Comment	Reference
F	1478	ARG	-	linker	UNP Q8GF99
F	1479	PRO	-	linker	UNP Q8GF99

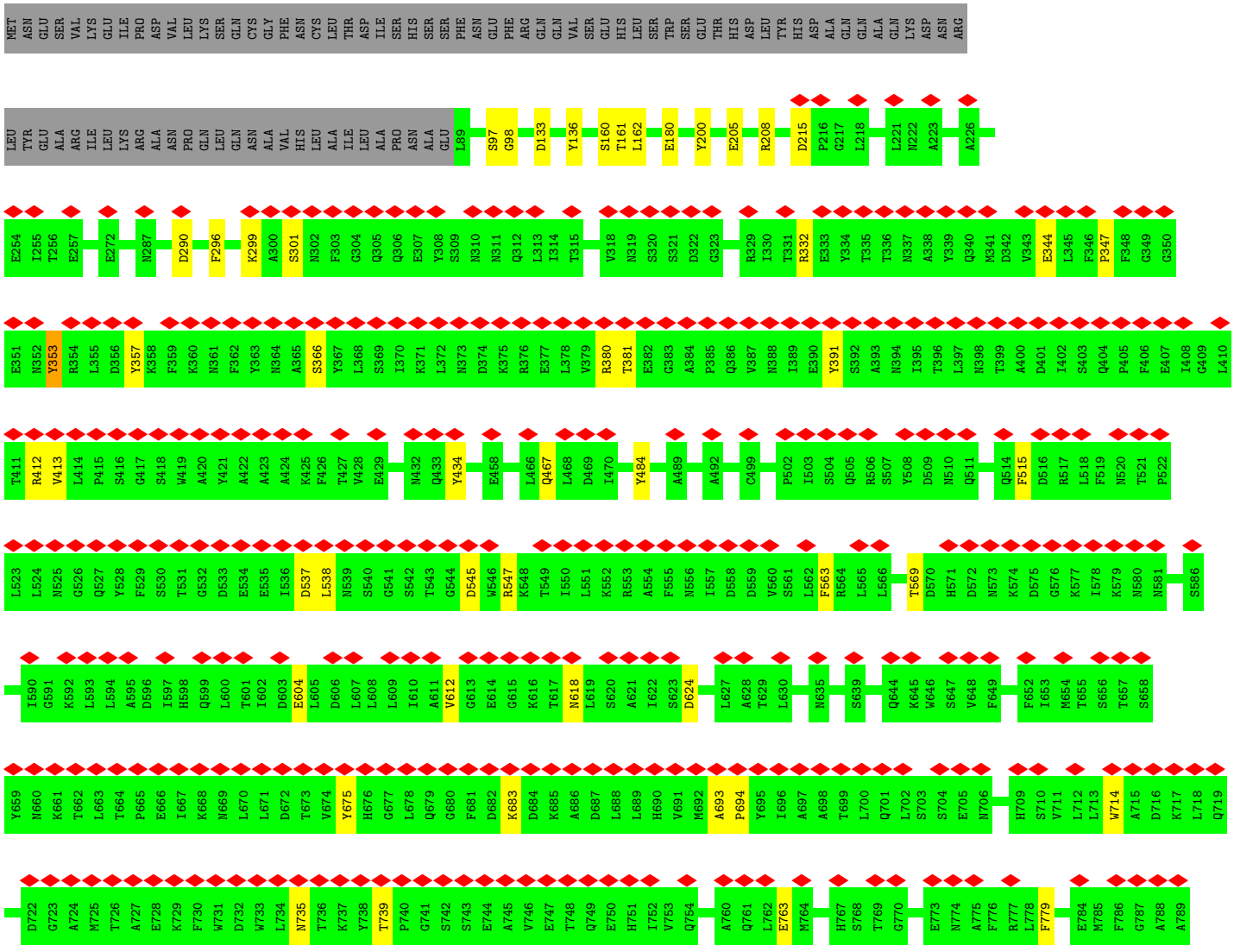
3 Residue-property plots (i)

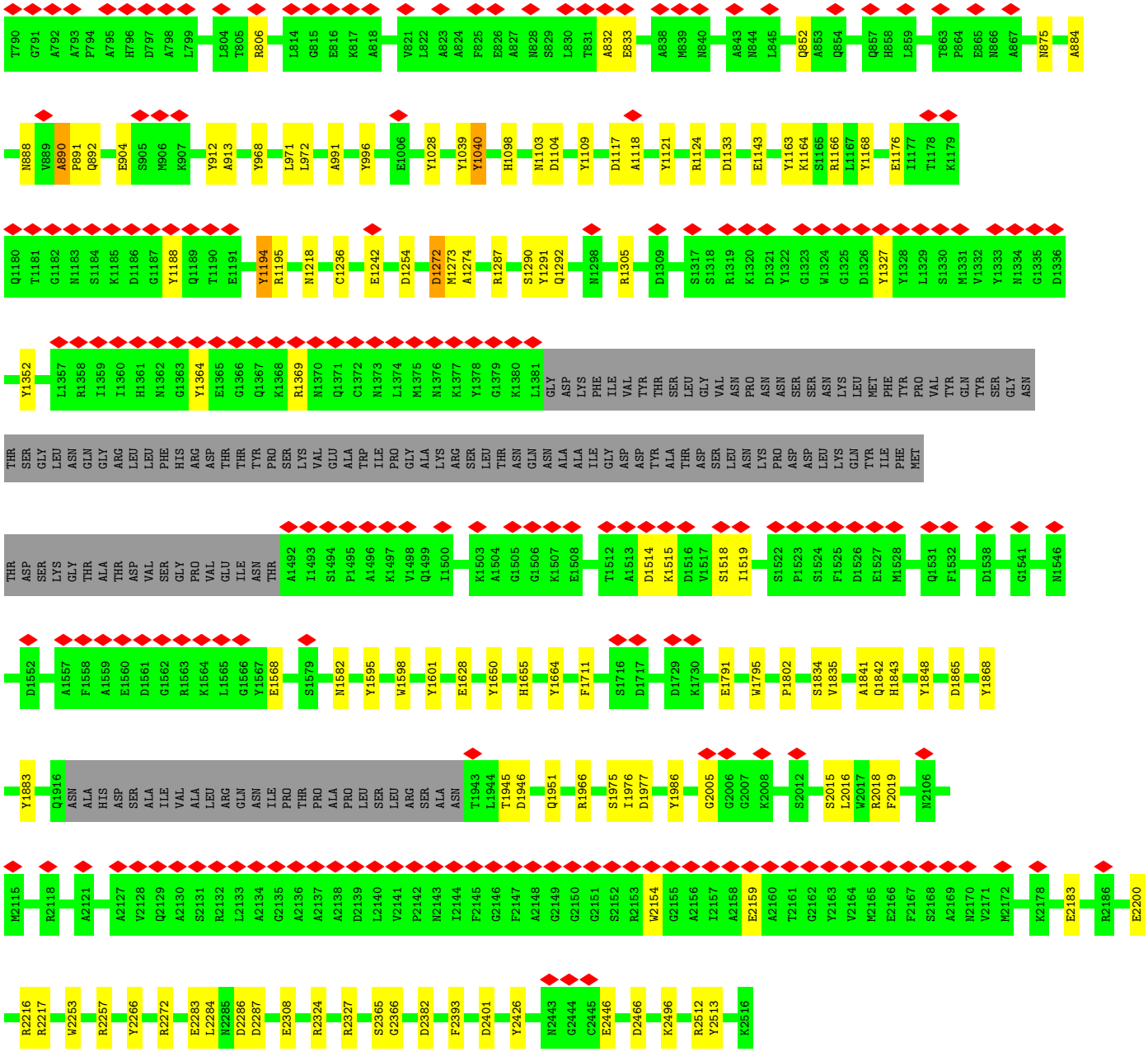
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: TcdA1

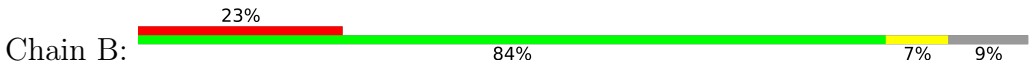
Chain A:

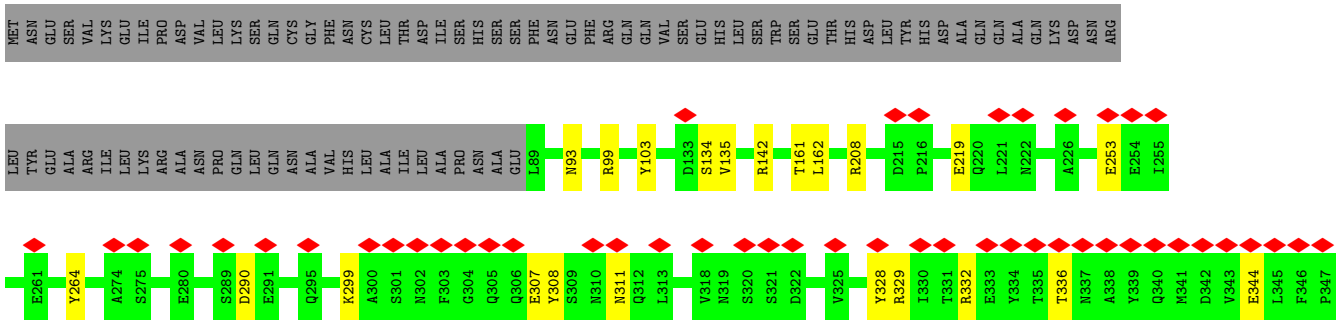


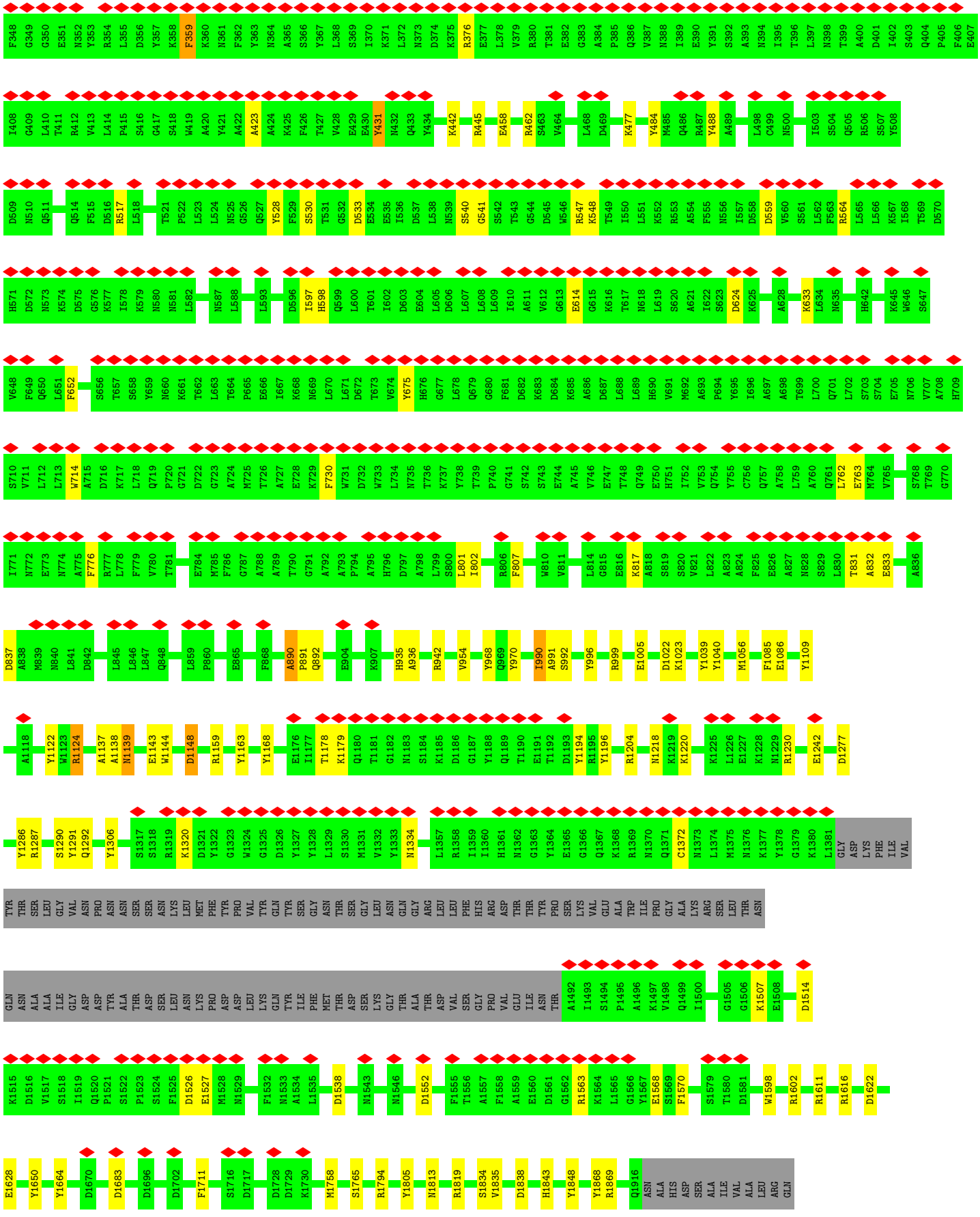




- Molecule 1: TcdA1



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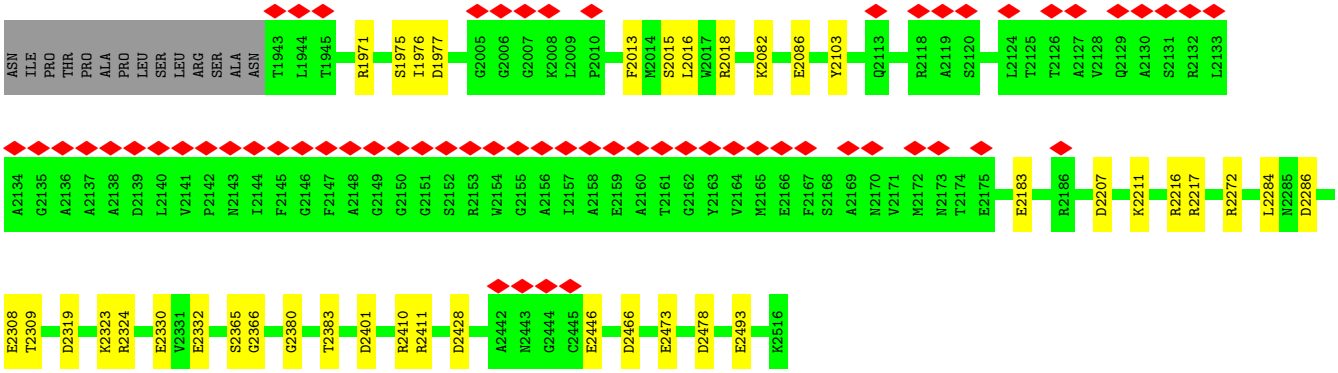
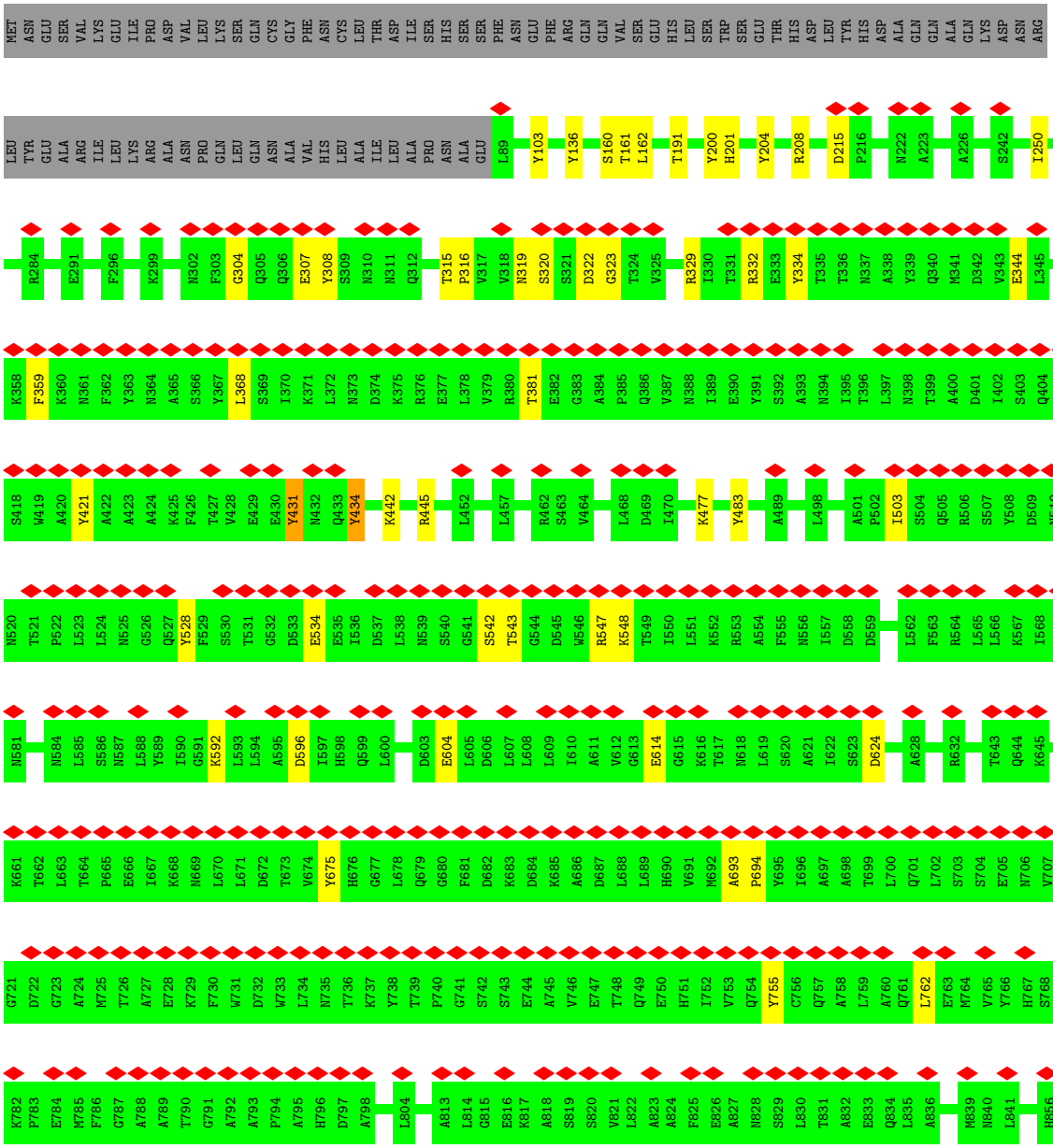
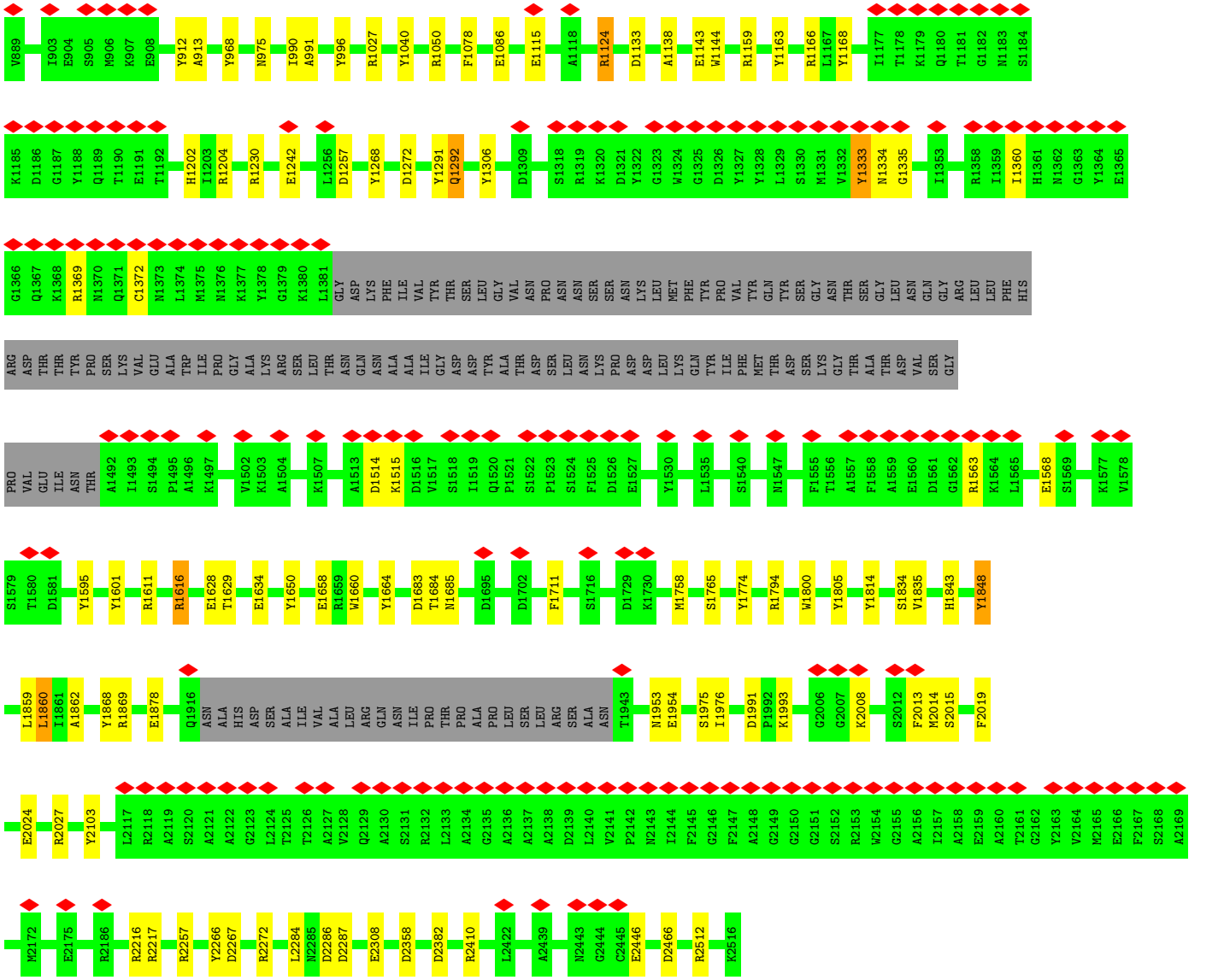
I408 G409 L410 T411 R412 Y413 L414 P415 S416 G417 S418 W419 A420 Y421 A422 A423 A424 K425 F426 T427 V428 E429 E430 Y431 N432 Q433 Y434 K442 R445 E458 R462 S463 V464 L468 D469 K477 Y484 N485 Q486 R487 Y488 A489 L498 C499 N500 I503 S504 Q505 R506 S507 Y508
D509 N510 Q511 Q514 F515 D516 R517 L518 T521 P522 L523 L524 N525 G526 Q527 Y528 F529 S530 T531 G532 D533 E534 E535 I536 D537 L538 N539 S540 G541 S542 T543 G544 D545 W546 R547 K548 T549 I550 L551 K552 R553 A554 F555 N556 I557 D558 D559 V560 S561 L562 F563 R564 L565 L566 K567 I568 T569 D570
H571 D572 N573 K574 D575 G576 K577 I578 K579 N580 N581 L582 N587 L588 L593 D596 I597 H598 Q599 L600 T601 I602 D603 E604 L605 D606 L607 L608 L609 I610 A611 V612 G613 E614 G615 K616 T617 N618 L619 S620 A621 I622 S623 D624 K625 A628 K633 L634 N635 H642 K645 W646 S647
V648 F649 Q650 L651 F652 S656 T657 S658 Y659 N660 K661 T662 L663 T664 P665 E666 I667 K668 N669 L670 L671 D672 T673 V674 Y675 H676 G677 L678 Q679 G680 F681 D682 K683 D684 K685 A686 D687 L688 L689 H690 V691 M692 A693 P694 Y695 I696 A697 A698 T699 L700 Q701 L702 S703 S704 E705 N706 V707 A708 H709
S710 V711 L712 L713 W714 A715 D716 K717 L718 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 F730 W731 D732 W733 L734 N735 T736 K737 Y738 T739 P740 G741 S742 S743 E744 A745 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 Y755 C756 Q757 A758 L759 A760 Q761 L762 E763 M764 V765 S768 T769 G770
I771 N772 E773 N774 A775 F776 R777 L778 F779 V780 T781 E784 M785 F786 G787 A788 A789 T790 G791 A792 A793 P794 A795 H796 D797 A798 L799 S800 L801 I802 R806 F807 W810 Y811 L814 G815 E816 K817 A818 S819 S820 V821 L822 A823 A824 F825 E826 A827 N828 S829 L830 T831 A832 E833 A836
D837 A838 M839 N840 L841 D842 L845 L846 L847 Q848 L859 P860 E865 F868 A890 P891 Q892 E904 K907 H935 A936 R942 Y954 Y968 Q969 Y970 I990 A991 S992 Y996 R999 E1005 D1022 K1023 Y1039 Y1040 M1056 F1085 E1086 Y1109
A1118 Y1122 W1123 R1124 A1137 A1138 N1139 E1143 W1144 D1148 R1159 Y1163 Y1168 E1176 I1177 T1178 K1179 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 T1192 D1193 Y1194 R1195 Y1196 R1204 N1218 K1219 K1220 K1225 L1226 E1227 K1228 N1229 R1230 E1242 D1277
Y1286 R1287 S1290 Y1291 Q1292 Y1306 S1317 S1318 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 L1357 R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 GLY ASP LYS PHE ILE VAL
TYR THR SER LEU GLY VAL ASN PRO ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL TYR GLN TYR SER GLY ASN THR SER GLY LEU ASN GLN GLY ARG LEU LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL GLU ALA TRP ILE PRO GLY ALA LYS ARG SER LEU THR ASN
GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LYS GLN TYR ILE PHE MET THR ASP SER LYS GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 I1500 G1505 G1506 K1507 E1508 D1514
K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522 P1523 S1524 F1525 D1526 E1527 M1528 N1529 F1532 N1533 A1534 L1535 D1538 N1543 N1546 D1552 F1555 T1556 A1557 F1558 A1559 E1560 D1561 G1562 R1563 K1564 L1565 G1566 Y1567 E1568 S1569 F1570 S1579 T1580 D1581 W1598 R1602 R1611 R1616 D1622
E1628 Y1650 Y1664 D1670 D1683 D1696 D1702 F1711 S1716 D1717 D1728 D1729 K1730 M1758 S1765 R1794 Y1805 N1813 R1819 S1834 V1835 D1838 H1843 Y1848 Y1868 R1869 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN



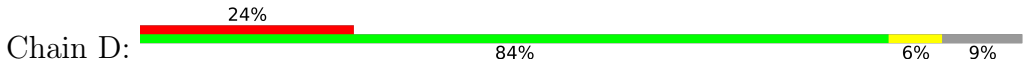
• Molecule 1: TcdA1

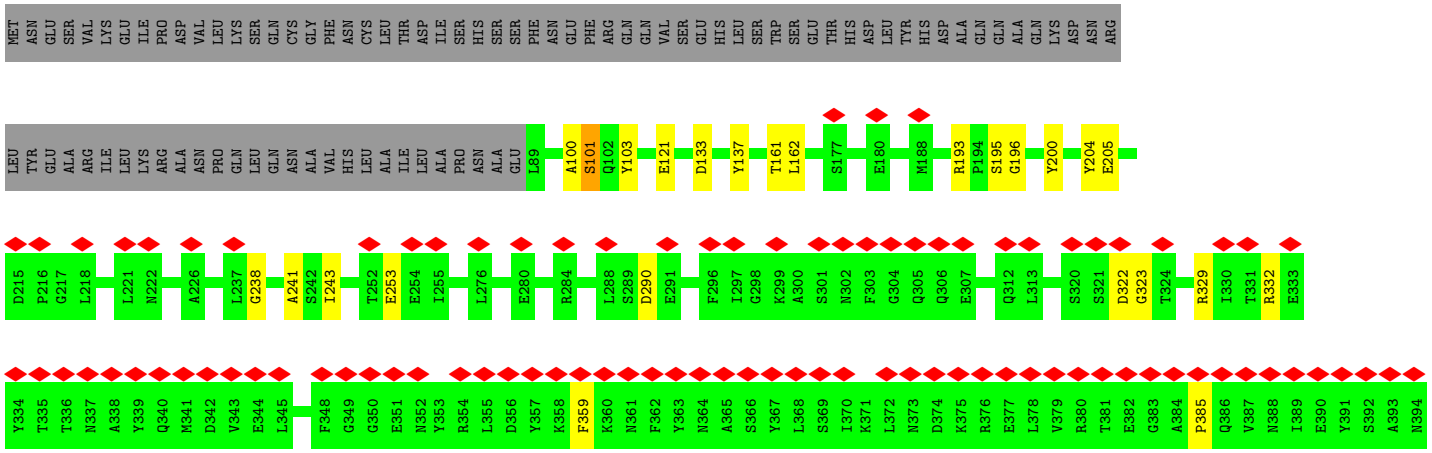
Chain C:

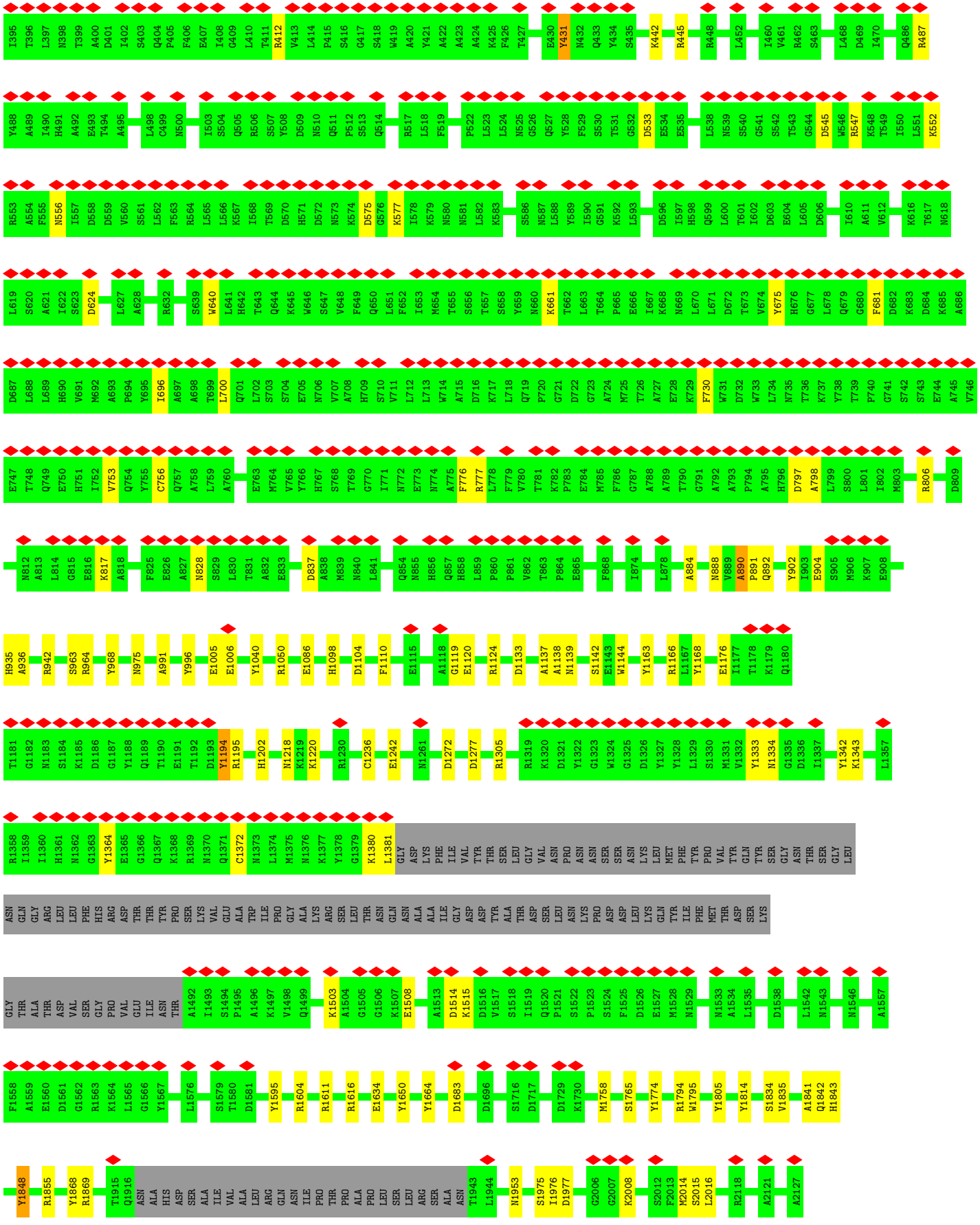




- Molecule 1: TcdA1



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H935 A936 R942 S963 R964 Y968 N975 A991 Y996 E1005 E1006 Y1040 R1050 E1086 H1098 D1104 F1110 E1115 A1118 G1119 E1120 R1124 D1133 A1137 A1138 N1139 S1142 E1143 W1144 Y1163 R1166 L1167 Y1168 E1176 I1177 T1178 K1179 Q1180
T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 T1192 D1193 Y1194 R1195 H1202 N1218 K1219 K1220 R1230 C1236 E1242 N1261 D1272 D1277 R1305 R1319 K1320 D1321 Y1322 G1323 W1324 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 D1336 I1337 Y1342 K1343 L1357
R1358 I1359 I1360 H1361 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 N1373 L1374 M1375 N1376 K1377 Y1378 G1379 K1380 L1381 GLY ASP LYS PHE ILE VAL TYR THR SER LEU GLY VAL ASN PRO ASN ASN SER SER ASN LYS LEU MET PHE TYR PRO VAL TYR GLN TYR SER GLY ASN THR SER GLY LEU
ASN GLN GLY ARG LEU LEU PHE HIS ARG ASP THR THR TYR PRO SER LYS VAL VAL GLU ALA TRP ILE PRO GLY ALA LYS ARG SER LEU THR ASN GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO ASP ASP LEU LYS GLN TYR ILE PHE MET THR ASP SER LYS
GLY THR ALA THR ASP VAL SER GLY PRO VAL GLU ILE ASN THR A1492 I1493 S1494 P1495 A1496 K1497 V1498 Q1499 K1503 A1504 G1505 G1506 K1507 E1508 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522 P1523 S1524 F1525 D1526 E1527 M1528 N1529 N1533 A1534 L1535 D1538 L1542 N1543 N1546 A1557
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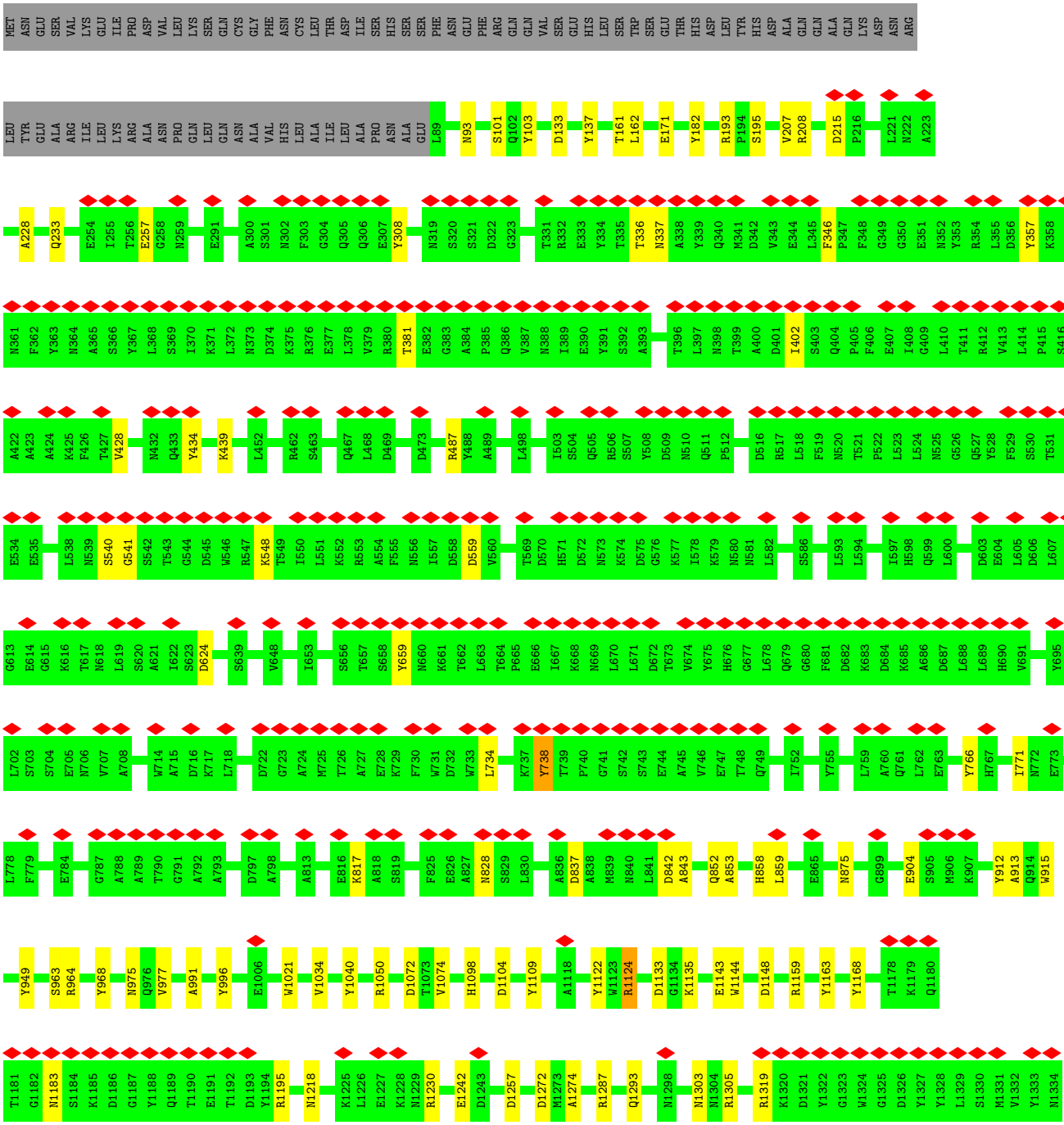
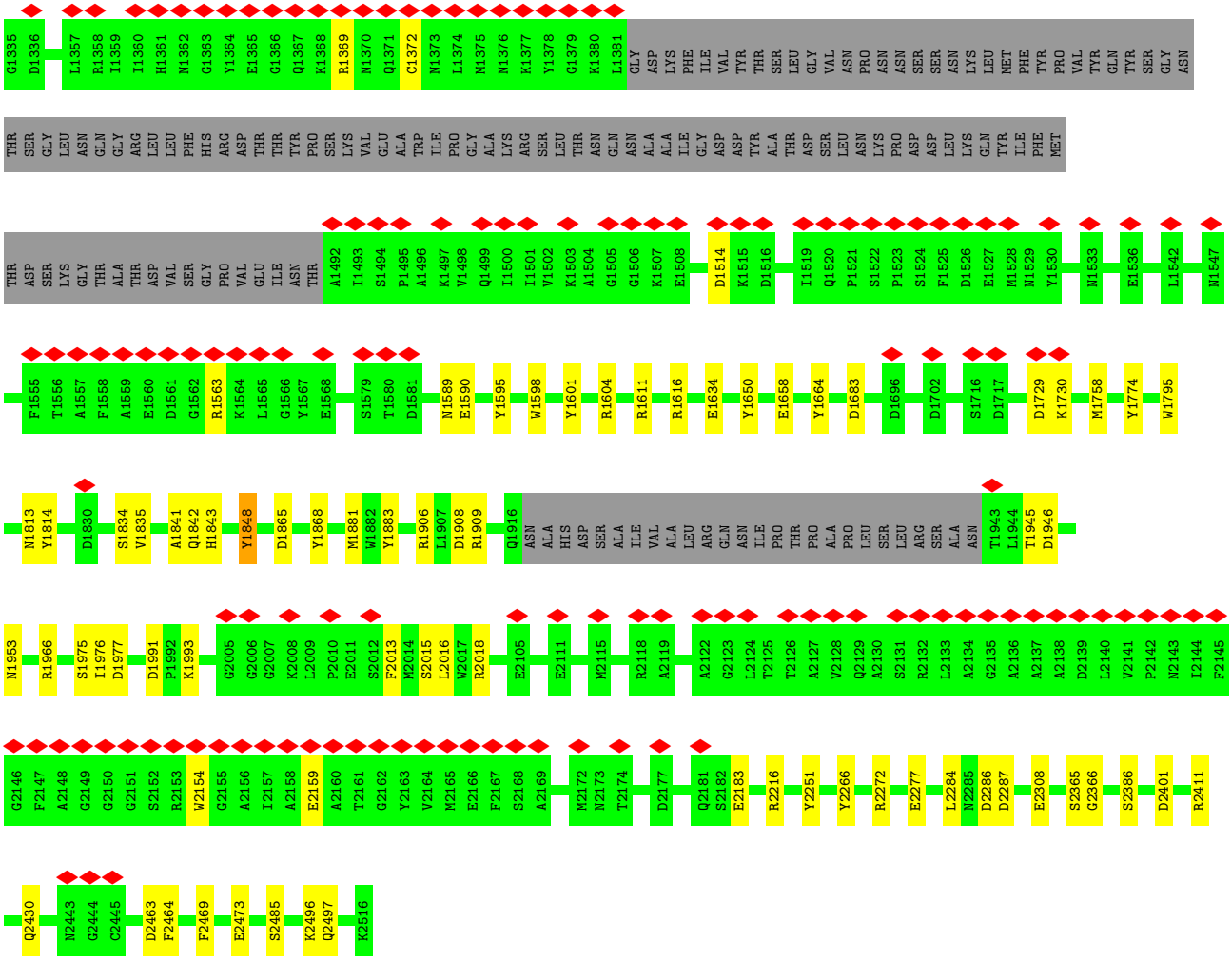
- Molecule 1: TcdA1

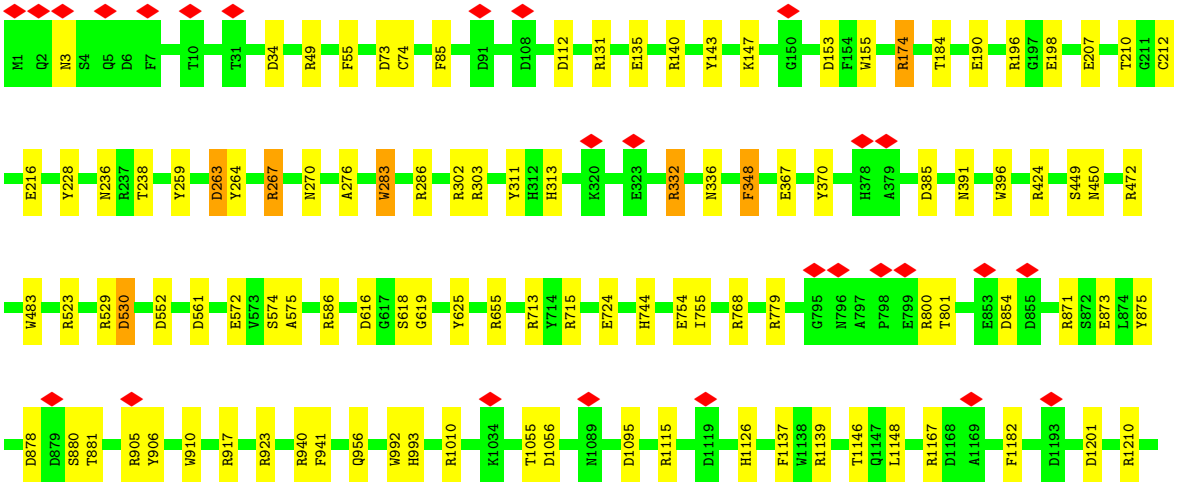
Chain E:

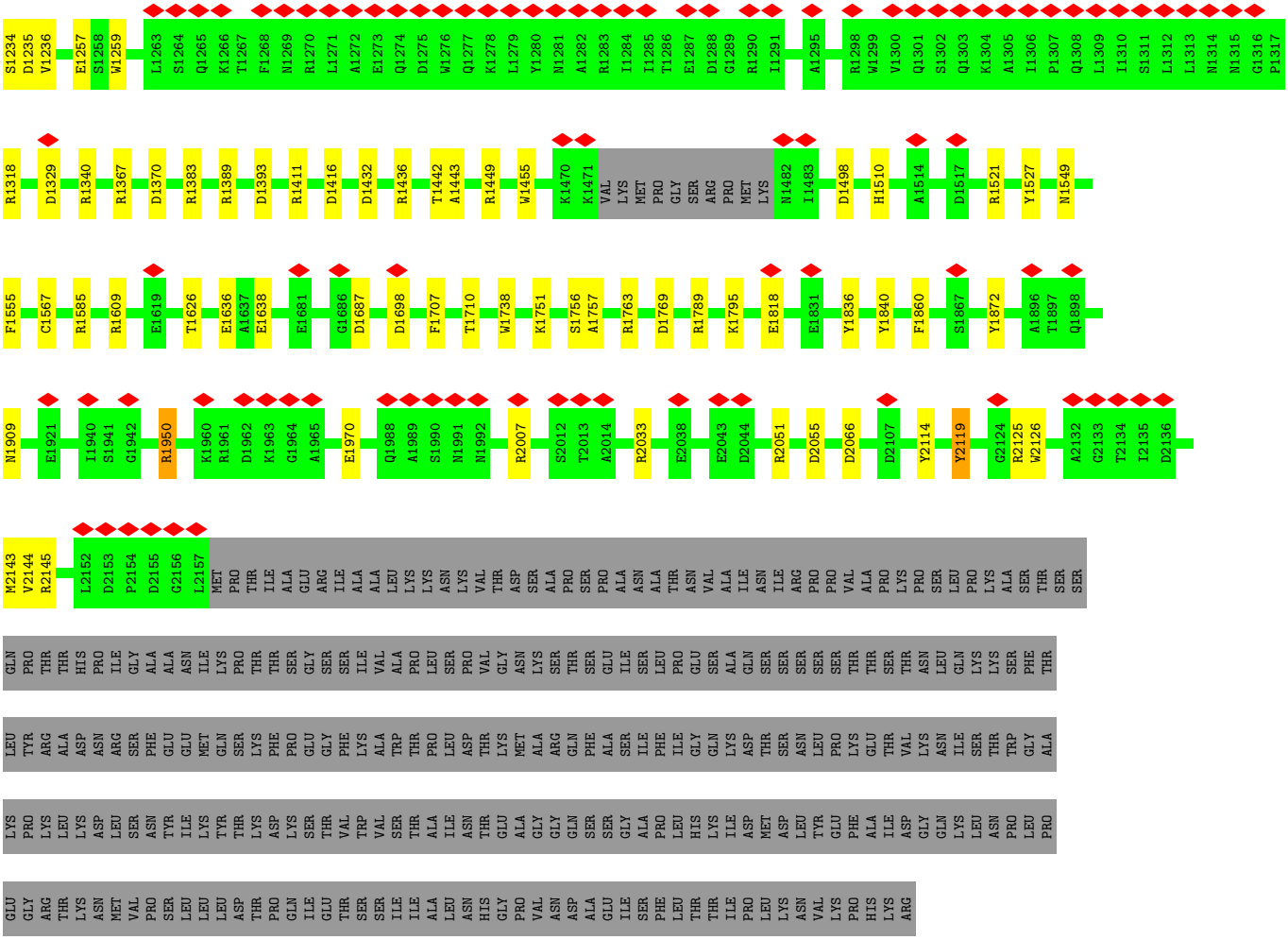




• Molecule 2: TcdB2,TccC3

Chain F:

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R1318 D1329 R1340 R1367 D1370 R1383 R1389 D1393 R1411 D1416 D1432 R1436 T1442 A1443 R1449 W1455 K1470 K1471 VAL LYS MET PRO GLY SER ARG PRO MET LYS N1482 I1483 D1498 H1510 A1514 D1517 R1521 Y1527 N1549
F1555 C1567 R1585 R1609 E1619 T1626 E1636 A1637 E1638 E1681 G1686 D1687 D1698 F1707 T1710 W1738 K1751 S1756 A1757 R1763 D1769 R1789 K1795 E1818 E1831 Y1836 Y1840 F1860 S1867 Y1872 A1896 T1897 Q1898
N1909 E1921 I1940 S1941 G1942 R1950 K1960 R1961 D1962 K1963 G1964 A1965 E1970 Q1988 A1989 S1990 N1991 N1992 R2007 S2012 T2013 A2014 R2033 E2038 E2043 D2044 R2051 D2055 D2066 D2107 Y2114 Y2119 G2124 R2125 W2126 A2132 G2133 T2134 I2135 D2136
M2143 V2144 R2145 L2152 D2153 P2154 D2155 G2156 L2157 MET PRO THR ILE ALA GLU ARG ILE ALA ALA LEU LYS LYS ASN LYS VAL THR ASP SER ALA PRO SER PRO ALA ASN ALA THR ASN VAL ALA ILE ASN ILE ARG PRO PRO VAL ALA PRO LYS PRO SER LEU PRO LYS ALA SER THR SER SER
GLN PRO THR THR HIS PRO ILE GLY ALA ALA ASN ILE LYS PRO THR THR SER GLY SER SER ILE VAL ALA PRO LEU SER PRO VAL GLY ASN LYS SER THR SER GLU ILE SER LEU PRO GLU SER ALA GLN SER SER SER SER SER THR THR SER THR ASN LEU GLN LYS LYS SER PHE THR
LEU TYR ARG ALA ASP ASN ARG SER PHE GLU GLU MET GLN SER LYS PHE PRO GLU GLY PHE LYS ALA TRP THR PRO LEU ASP THR LYS MET ALA ARG GLN PHE ALA SER ILE PHE ILE GLY GLN LYS ASP THR SER ASN LEU PRO LYS GLU THR VAL LYS ASN ILE SER THR TRP GLY ALA
LYS PRO LYS LEU LYS ASP LEU SER ASN TYR ILE LYS TYR THR LYS ASP LYS SER THR VAL TRP VAL SER THR ALA ILE ASN THR GLU ALA GLY GLY GLN SER SER GLY ALA PRO LEU HIS LYS ILE ASP MET ASP LEU TYR GLU PHE ALA ILE ASP GLY GLN LYS LEU ASN PRO LEU PRO
GLU GLY ARG THR LYS ASN MET VAL PRO SER LEU LEU LEU ASP THR PRO GLN ILE GLU THR SER SER ILE ILE ALA LEU ASN HIS GLY PRO VAL ASN ASP ALA GLU ILE SER PHE LEU THR THR ILE PRO LEU LYS ASN VAL LYS PRO HIS LYS ARG

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.113	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	440.99997, 440.99997, 440.99997	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	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	A	1.16	65/18587 (0.3%)	0.94	42/25239 (0.2%)
1	B	1.15	58/18587 (0.3%)	0.95	57/25239 (0.2%)
1	C	1.14	57/18587 (0.3%)	0.96	53/25239 (0.2%)
1	D	1.14	47/18587 (0.3%)	0.94	39/25239 (0.2%)
1	E	1.14	43/18587 (0.2%)	0.94	39/25239 (0.2%)
2	F	1.18	45/17548 (0.3%)	0.99	62/23921 (0.3%)
All	All	1.15	315/110483 (0.3%)	0.95	292/150116 (0.2%)

All (315) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1372	CYS	CB-SG	-12.62	1.60	1.82
1	A	675	TYR	CB-CG	-10.65	1.35	1.51
1	A	1242	GLU	CG-CD	-10.29	1.36	1.51
1	C	1242	GLU	CG-CD	-9.66	1.37	1.51
1	A	779	PHE	CB-CG	-9.56	1.35	1.51
1	D	1242	GLU	CG-CD	-8.88	1.38	1.51
1	E	1098	HIS	CB-CG	-8.77	1.34	1.50
1	C	1163	TYR	CB-CG	-8.76	1.38	1.51
1	A	675	TYR	CD2-CE2	-8.63	1.26	1.39
1	A	1568	GLU	CG-CD	-8.40	1.39	1.51
1	A	1242	GLU	CD-OE2	-8.28	1.16	1.25
2	F	2119	TYR	CB-CG	-8.20	1.39	1.51
1	B	1242	GLU	CG-CD	-8.19	1.39	1.51
1	C	614	GLU	CD-OE1	-7.97	1.16	1.25
2	F	259	TYR	CB-CG	-7.85	1.39	1.51
1	B	1848	TYR	CB-CG	-7.78	1.40	1.51
1	B	1163	TYR	CB-CG	-7.77	1.40	1.51
1	C	1242	GLU	CD-OE2	-7.63	1.17	1.25
1	B	359	PHE	CB-CG	-7.56	1.38	1.51
1	C	1634	GLU	CD-OE1	-7.53	1.17	1.25
1	D	1098	HIS	CB-CG	-7.49	1.36	1.50
1	B	431	TYR	CB-CG	-7.41	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1372	CYS	CB-SG	-7.39	1.69	1.82
1	D	1163	TYR	CB-CG	-7.29	1.40	1.51
1	A	344	GLU	CD-OE2	-7.29	1.17	1.25
1	B	1843	HIS	CB-CG	-7.26	1.36	1.50
1	C	1805	TYR	CB-CG	-7.25	1.40	1.51
1	A	1664	TYR	CB-CG	-7.24	1.40	1.51
1	E	1843	HIS	CB-CG	-7.20	1.37	1.50
1	B	1005	GLU	CD-OE1	-7.18	1.17	1.25
1	E	996	TYR	CB-CG	-7.17	1.40	1.51
1	D	681	PHE	CB-CG	-7.16	1.39	1.51
1	C	1143	GLU	CG-CD	-7.13	1.41	1.51
2	F	744	HIS	CB-CG	-7.13	1.37	1.50
1	A	1843	HIS	CB-CG	-7.10	1.37	1.50
1	E	1163	TYR	CB-CG	-7.08	1.41	1.51
1	A	1664	TYR	CD1-CE1	-7.04	1.28	1.39
2	F	1970	GLU	CG-CD	-7.01	1.41	1.51
1	A	968	TYR	CG-CD1	-6.98	1.30	1.39
1	B	996	TYR	CB-CG	-6.93	1.41	1.51
1	B	2330	GLU	CD-OE1	-6.92	1.18	1.25
1	B	1848	TYR	CE2-CZ	-6.91	1.29	1.38
1	B	1848	TYR	CG-CD1	-6.89	1.30	1.39
1	E	346	PHE	CB-CG	-6.82	1.39	1.51
1	D	756	CYS	CB-SG	-6.82	1.70	1.82
1	D	675	TYR	CG-CD1	-6.77	1.30	1.39
1	B	776	PHE	CB-CG	-6.74	1.39	1.51
1	E	1242	GLU	CD-OE2	-6.74	1.18	1.25
1	C	755	TYR	CB-CG	6.70	1.61	1.51
1	D	1843	HIS	CB-CG	-6.70	1.38	1.50
1	C	1658	GLU	CD-OE1	-6.68	1.18	1.25
1	C	675	TYR	CG-CD1	-6.66	1.30	1.39
2	F	198	GLU	CD-OE1	-6.62	1.18	1.25
2	F	174	ARG	CZ-NH2	-6.61	1.24	1.33
1	C	1202	HIS	CB-CG	-6.60	1.38	1.50
1	B	1805	TYR	CB-CG	-6.59	1.41	1.51
2	F	391	ASN	CB-CG	-6.59	1.35	1.51
2	F	367	GLU	CD-OE1	-6.58	1.18	1.25
1	A	1163	TYR	CB-CG	-6.54	1.41	1.51
1	A	763	GLU	CG-CD	-6.49	1.42	1.51
1	B	1124	ARG	CD-NE	-6.49	1.35	1.46
1	C	2272	ARG	CG-CD	-6.47	1.35	1.51
2	F	396	TRP	CB-CG	-6.47	1.38	1.50
1	C	1848	TYR	CB-CG	-6.44	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1143	GLU	CD-OE2	-6.43	1.18	1.25
1	A	344	GLU	CD-OE1	-6.42	1.18	1.25
1	C	1664	TYR	CB-CG	-6.42	1.42	1.51
1	E	1372	CYS	CB-SG	-6.40	1.71	1.82
1	B	1242	GLU	CD-OE1	-6.39	1.18	1.25
1	D	1218	ASN	CB-CG	-6.32	1.36	1.51
1	C	1848	TYR	CE2-CZ	-6.30	1.30	1.38
1	C	1843	HIS	CB-CG	-6.30	1.38	1.50
1	E	1595	TYR	CB-CG	-6.29	1.42	1.51
1	E	2272	ARG	CG-CD	-6.24	1.36	1.51
2	F	135	GLU	CD-OE1	-6.23	1.18	1.25
1	B	968	TYR	CG-CD1	-6.20	1.31	1.39
1	C	1878	GLU	CG-CD	-6.17	1.42	1.51
1	E	1664	TYR	CB-CG	-6.16	1.42	1.51
2	F	572	GLU	CD-OE1	-6.16	1.18	1.25
2	F	483	TRP	CB-CG	-6.10	1.39	1.50
1	D	1634	GLU	CD-OE1	-6.08	1.19	1.25
1	A	996	TYR	CB-CG	-6.08	1.42	1.51
1	D	1650	TYR	CG-CD1	-6.07	1.31	1.39
1	D	1202	HIS	CB-CG	-6.07	1.39	1.50
1	A	1121	TYR	CB-CG	-6.05	1.42	1.51
1	B	652	PHE	CB-CG	-6.05	1.41	1.51
1	B	954	VAL	CB-CG2	-6.05	1.40	1.52
2	F	228	TYR	CB-CG	-6.04	1.42	1.51
1	B	763	GLU	CD-OE1	-6.02	1.19	1.25
1	E	949	TYR	CG-CD1	-6.00	1.31	1.39
1	C	996	TYR	CB-CG	-6.00	1.42	1.51
1	A	1236	CYS	CB-SG	-5.98	1.72	1.81
1	C	1568	GLU	CG-CD	-5.98	1.43	1.51
1	A	763	GLU	CD-OE2	-5.97	1.19	1.25
1	B	1218	ASN	CB-CG	-5.97	1.37	1.51
2	F	1836	TYR	CB-CG	-5.96	1.42	1.51
1	E	738	TYR	CB-CG	-5.94	1.42	1.51
1	D	1595	TYR	CB-CG	-5.93	1.42	1.51
1	E	1848	TYR	CE2-CZ	-5.91	1.30	1.38
1	C	996	TYR	CG-CD1	-5.90	1.31	1.39
1	E	968	TYR	CG-CD1	-5.90	1.31	1.39
1	D	1805	TYR	CB-CG	-5.90	1.42	1.51
1	E	1021	TRP	CB-CG	-5.89	1.39	1.50
1	C	534	GLU	CD-OE2	-5.88	1.19	1.25
1	C	1124	ARG	CD-NE	-5.88	1.36	1.46
1	E	1143	GLU	CG-CD	-5.87	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	614	GLU	CG-CD	-5.87	1.43	1.51
2	F	941	PHE	CB-CG	-5.87	1.41	1.51
1	E	875	ASN	CB-CG	-5.86	1.37	1.51
1	C	1658	GLU	CD-OE2	-5.85	1.19	1.25
1	E	977	VAL	CB-CG1	-5.83	1.40	1.52
2	F	198	GLU	CG-CD	-5.83	1.43	1.51
1	E	2013	PHE	CB-CG	-5.82	1.41	1.51
1	A	434	TYR	CB-CG	-5.81	1.43	1.51
1	C	2308	GLU	CD-OE1	-5.81	1.19	1.25
1	C	431	TYR	CB-CG	-5.78	1.43	1.51
1	A	2272	ARG	CG-CD	-5.78	1.37	1.51
1	C	604	GLU	CG-CD	-5.77	1.43	1.51
1	D	1664	TYR	CB-CG	-5.76	1.43	1.51
1	D	996	TYR	CG-CD1	-5.76	1.31	1.39
1	A	1143	GLU	CG-CD	-5.74	1.43	1.51
1	D	1650	TYR	CD1-CE1	-5.74	1.30	1.39
1	B	530	SER	CB-OG	-5.74	1.34	1.42
1	E	1218	ASN	CB-CG	-5.74	1.37	1.51
1	C	2103	TYR	CB-CG	-5.73	1.43	1.51
1	D	1848	TYR	CE2-CZ	-5.72	1.31	1.38
2	F	283	TRP	CZ3-CH2	-5.72	1.30	1.40
2	F	992	TRP	CE2-CZ2	-5.71	1.30	1.39
1	A	2183	GLU	CD-OE1	-5.71	1.19	1.25
1	A	2308	GLU	CD-OE1	-5.70	1.19	1.25
1	D	1242	GLU	CD-OE2	-5.70	1.19	1.25
1	A	290	ASP	CB-CG	-5.68	1.39	1.51
1	A	515	PHE	CB-CG	-5.66	1.41	1.51
2	F	993	HIS	CB-CG	-5.66	1.39	1.50
1	A	904	GLU	CD-OE2	-5.65	1.19	1.25
1	A	1598	TRP	CB-CG	-5.65	1.40	1.50
1	E	2159	GLU	CD-OE1	-5.62	1.19	1.25
1	B	1664	TYR	CB-CG	-5.62	1.43	1.51
1	A	1595	TYR	CB-CG	-5.61	1.43	1.51
1	E	1242	GLU	CD-OE1	-5.61	1.19	1.25
1	D	1005	GLU	CG-CD	-5.60	1.43	1.51
2	F	1738	TRP	CB-CG	-5.59	1.40	1.50
1	C	1124	ARG	CB-CG	-5.58	1.37	1.52
1	C	1601	TYR	CB-CG	-5.58	1.43	1.51
1	A	1795	TRP	CB-CG	-5.55	1.40	1.50
1	B	1143	GLU	CD-OE1	-5.55	1.19	1.25
1	C	1765	SER	CA-CB	-5.55	1.44	1.52
1	D	2308	GLU	CD-OE1	-5.55	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2473	GLU	CG-CD	-5.54	1.43	1.51
1	C	1800	TRP	NE1-CE2	-5.54	1.30	1.37
1	B	328	TYR	CB-CG	-5.54	1.43	1.51
1	A	1568	GLU	CD-OE2	-5.54	1.19	1.25
1	C	1628	GLU	CD-OE2	-5.53	1.19	1.25
1	A	1242	GLU	CD-OE1	-5.52	1.19	1.25
1	A	675	TYR	CG-CD2	-5.51	1.31	1.39
1	D	1163	TYR	CE2-CZ	-5.51	1.31	1.38
1	A	1848	TYR	CB-CG	-5.51	1.43	1.51
1	A	1163	TYR	CG-CD1	-5.50	1.31	1.39
1	D	730	PHE	CB-CG	-5.50	1.42	1.51
2	F	207	GLU	CD-OE1	-5.49	1.19	1.25
1	D	1795	TRP	CB-CG	-5.49	1.40	1.50
1	C	1868	TYR	CB-CG	-5.49	1.43	1.51
1	C	968	TYR	CG-CD1	-5.49	1.32	1.39
1	A	904	GLU	CG-CD	-5.48	1.43	1.51
1	E	1634	GLU	CD-OE2	-5.48	1.19	1.25
1	B	1196	TYR	CB-CG	-5.48	1.43	1.51
1	A	1039	TYR	CG-CD2	-5.47	1.32	1.39
2	F	875	TYR	CB-CG	-5.47	1.43	1.51
1	A	996	TYR	CG-CD1	-5.47	1.32	1.39
1	C	779	PHE	CB-CG	-5.46	1.42	1.51
1	E	1122	TYR	CB-CG	-5.45	1.43	1.51
1	C	307	GLU	CD-OE2	-5.45	1.19	1.25
1	B	1848	TYR	CD1-CE1	-5.45	1.31	1.39
1	B	2272	ARG	CG-CD	-5.44	1.38	1.51
1	D	431	TYR	CB-CG	-5.44	1.43	1.51
1	A	604	GLU	CD-OE1	-5.43	1.19	1.25
1	C	1595	TYR	CB-CG	-5.43	1.43	1.51
2	F	348	PHE	CB-CG	-5.43	1.42	1.51
2	F	1455	TRP	CB-CG	-5.42	1.40	1.50
1	C	103	TYR	CB-CG	-5.42	1.43	1.51
1	E	996	TYR	CG-CD1	-5.42	1.32	1.39
1	D	1236	CYS	CB-SG	-5.41	1.73	1.81
2	F	212	CYS	CB-SG	-5.40	1.73	1.81
1	A	763	GLU	CD-OE1	-5.40	1.19	1.25
1	D	1005	GLU	CD-OE1	-5.39	1.19	1.25
1	B	1570	PHE	CB-CG	-5.39	1.42	1.51
1	B	359	PHE	CD1-CE1	-5.38	1.28	1.39
1	C	2019	PHE	CB-CG	-5.36	1.42	1.51
2	F	1970	GLU	CD-OE2	-5.36	1.19	1.25
1	B	344	GLU	CD-OE1	-5.35	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1110	PHE	CB-CG	-5.35	1.42	1.51
1	B	307	GLU	CD-OE2	-5.34	1.19	1.25
1	D	103	TYR	CB-CG	-5.34	1.43	1.51
2	F	370	TYR	CD1-CE1	-5.34	1.31	1.39
2	F	1840	TYR	CB-CG	-5.34	1.43	1.51
2	F	724	GLU	CD-OE2	-5.33	1.19	1.25
1	D	753	VAL	CB-CG2	-5.33	1.41	1.52
1	B	2332	GLU	CD-OE1	-5.33	1.19	1.25
1	E	1074	VAL	CB-CG2	-5.33	1.41	1.52
1	A	353	TYR	CB-CG	-5.33	1.43	1.51
1	A	1628	GLU	CD-OE2	-5.32	1.19	1.25
1	B	1163	TYR	CD1-CE1	-5.32	1.31	1.39
1	A	714	TRP	CD2-CE2	-5.31	1.34	1.41
2	F	992	TRP	NE1-CE2	-5.31	1.30	1.37
1	E	1143	GLU	CD-OE2	-5.30	1.19	1.25
2	F	910	TRP	CB-CG	-5.30	1.40	1.50
1	B	103	TYR	CB-CG	-5.30	1.43	1.51
1	E	1124	ARG	CD-NE	-5.29	1.37	1.46
1	B	2183	GLU	CD-OE1	-5.29	1.19	1.25
2	F	155	TRP	CB-CG	-5.29	1.40	1.50
1	B	1628	GLU	CD-OE2	-5.29	1.19	1.25
1	D	1242	GLU	CD-OE1	-5.28	1.19	1.25
2	F	1555	PHE	CB-CG	-5.28	1.42	1.51
1	D	904	GLU	CD-OE1	-5.28	1.19	1.25
1	D	996	TYR	CB-CG	-5.27	1.43	1.51
1	A	875	ASN	CB-CG	-5.27	1.39	1.51
1	A	1352	TYR	CB-CG	-5.27	1.43	1.51
1	E	2308	GLU	CD-OE1	-5.27	1.19	1.25
1	C	1143	GLU	CB-CG	-5.25	1.42	1.52
2	F	1836	TYR	CD2-CE2	-5.25	1.31	1.39
1	B	1122	TYR	CB-CG	-5.25	1.43	1.51
1	A	2019	PHE	CB-CG	-5.24	1.42	1.51
1	D	1848	TYR	CG-CD1	-5.24	1.32	1.39
1	B	1306	TYR	CG-CD2	-5.23	1.32	1.39
1	C	1660	TRP	CD2-CE2	-5.23	1.35	1.41
1	C	1333	TYR	CG-CD1	-5.23	1.32	1.39
1	B	2013	PHE	CB-CG	-5.23	1.42	1.51
1	C	2272	ARG	CD-NE	-5.23	1.37	1.46
1	D	205	GLU	CD-OE2	-5.22	1.20	1.25
1	B	528	TYR	CB-CG	-5.22	1.43	1.51
1	D	2318	GLU	CD-OE2	-5.22	1.20	1.25
2	F	1567	CYS	CB-SG	-5.22	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1638	GLU	CD-OE1	-5.22	1.20	1.25
1	A	612	VAL	CB-CG2	-5.21	1.41	1.52
1	A	1868	TYR	CG-CD1	-5.21	1.32	1.39
1	C	1954	GLU	CD-OE2	-5.21	1.20	1.25
1	A	1163	TYR	CE2-CZ	-5.21	1.31	1.38
1	A	1218	ASN	CB-CG	-5.21	1.39	1.51
2	F	873	GLU	CD-OE1	-5.21	1.20	1.25
1	A	1109	TYR	CD1-CE1	-5.20	1.31	1.39
1	B	1765	SER	CA-CB	-5.19	1.45	1.52
1	E	1658	GLU	CD-OE1	-5.19	1.20	1.25
1	A	1848	TYR	CE2-CZ	-5.17	1.31	1.38
1	E	103	TYR	CB-CG	-5.17	1.43	1.51
2	F	311	TYR	CB-CG	-5.17	1.43	1.51
1	C	1848	TYR	CG-CD1	-5.17	1.32	1.39
1	D	1372	CYS	CB-SG	-5.16	1.73	1.81
1	B	2308	GLU	CD-OE1	-5.16	1.20	1.25
1	E	2277	GLU	CB-CG	-5.15	1.42	1.52
1	A	1098	HIS	CB-CG	-5.15	1.40	1.50
1	C	2446	GLU	CD-OE2	-5.15	1.20	1.25
1	E	915	TRP	CB-CG	-5.15	1.41	1.50
1	B	1598	TRP	CB-CG	-5.14	1.41	1.50
1	A	2393	PHE	CB-CG	-5.14	1.42	1.51
1	E	1034	VAL	CB-CG2	-5.14	1.42	1.52
1	B	1039	TYR	CG-CD2	-5.14	1.32	1.39
1	D	1634	GLU	CD-OE2	-5.13	1.20	1.25
1	A	2253	TRP	CZ3-CH2	-5.12	1.31	1.40
1	C	1805	TYR	CD1-CE1	-5.12	1.31	1.39
2	F	1182	PHE	CB-CG	-5.12	1.42	1.51
1	A	205	GLU	CD-OE2	-5.12	1.20	1.25
1	C	1078	PHE	CB-CG	-5.12	1.42	1.51
1	E	2183	GLU	CD-OE1	-5.12	1.20	1.25
1	E	1881	MET	CG-SD	-5.12	1.67	1.81
1	B	264	TYR	CB-CG	-5.11	1.44	1.51
1	B	1163	TYR	CG-CD1	-5.11	1.32	1.39
2	F	190	GLU	CG-CD	-5.11	1.44	1.51
1	C	344	GLU	CD-OE2	-5.11	1.20	1.25
1	D	776	PHE	CG-CD2	-5.11	1.31	1.38
1	B	219	GLU	CD-OE2	-5.10	1.20	1.25
1	C	1163	TYR	CD1-CE1	-5.10	1.31	1.39
1	A	2159	GLU	CD-OE2	-5.10	1.20	1.25
1	E	1598	TRP	CB-CG	-5.09	1.41	1.50
1	B	1086	GLU	CD-OE1	-5.09	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	GLU	CD-OE2	-5.09	1.20	1.25
1	A	2283	GLU	CG-CD	-5.09	1.44	1.51
1	C	1115	GLU	CD-OE2	-5.09	1.20	1.25
1	B	2446	GLU	CD-OE1	-5.09	1.20	1.25
1	D	137	TYR	CB-CG	-5.08	1.44	1.51
1	B	1568	GLU	CG-CD	-5.08	1.44	1.51
1	D	1765	SER	CA-CB	-5.07	1.45	1.52
1	E	904	GLU	CD-OE1	-5.07	1.20	1.25
2	F	1636	GLU	CD-OE2	-5.07	1.20	1.25
2	F	779	ARG	CZ-NH1	-5.07	1.26	1.33
1	D	640	TRP	CB-CG	-5.06	1.41	1.50
1	E	2251	TYR	CB-CG	-5.06	1.44	1.51
1	A	2426	TYR	CB-CG	-5.05	1.44	1.51
1	B	1527	GLU	CD-OE2	-5.05	1.20	1.25
1	C	1650	TYR	CG-CD1	-5.05	1.32	1.39
1	A	1791	GLU	CD-OE1	-5.05	1.20	1.25
1	D	2487	PRO	N-CD	-5.05	1.40	1.47
1	C	1268	TYR	CB-CG	-5.05	1.44	1.51
1	D	121	GLU	CD-OE2	-5.05	1.20	1.25
1	E	1868	TYR	CB-CG	-5.04	1.44	1.51
2	F	216	GLU	CD-OE1	-5.04	1.20	1.25
1	C	1143	GLU	CD-OE2	-5.04	1.20	1.25
1	B	1527	GLU	CG-CD	-5.04	1.44	1.51
1	A	2446	GLU	CD-OE1	-5.04	1.20	1.25
1	E	996	TYR	CE2-CZ	-5.04	1.32	1.38
1	D	1342	TYR	CB-CG	-5.04	1.44	1.51
1	D	2446	GLU	CD-OE1	-5.04	1.20	1.25
2	F	1257	GLU	CD-OE2	-5.04	1.20	1.25
1	A	563	PHE	CB-CG	-5.03	1.42	1.51
1	B	730	PHE	CB-CG	-5.03	1.42	1.51
1	C	1086	GLU	CD-OE1	-5.03	1.20	1.25
2	F	1707	PHE	CB-CG	-5.03	1.42	1.51
1	A	2200	GLU	CD-OE1	-5.03	1.20	1.25
1	B	2103	TYR	CB-CG	-5.03	1.44	1.51
1	D	1086	GLU	CD-OE1	-5.02	1.20	1.25
1	A	1143	GLU	CD-OE1	-5.02	1.20	1.25
1	B	1139	ASN	CB-CG	-5.02	1.39	1.51
1	E	1795	TRP	CB-CG	-5.02	1.41	1.50
1	D	2202	GLU	CD-OE2	-5.01	1.20	1.25
1	E	2473	GLU	CG-CD	-5.01	1.44	1.51
1	B	2308	GLU	CD-OE2	-5.00	1.20	1.25

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1585	ARG	NE-CZ-NH2	-12.40	114.10	120.30
2	F	332	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	B	517	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	1124	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	A	2018	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	C	2410	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	C	547	ARG	NE-CZ-NH2	-9.35	115.62	120.30
2	F	1585	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	942	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	B	1869	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	E	1195	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	B	2018	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	C	1124	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	1664	TYR	CB-CG-CD1	-9.05	115.57	121.00
1	C	1563	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	B	547	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	B	462	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	E	1906	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	A	332	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	D	1869	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	E	2018	ARG	NE-CZ-NH2	-8.79	115.91	120.30
2	F	871	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	E	1563	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	C	1616	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	D	1195	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	D	1650	TYR	CB-CG-CD1	-8.27	116.03	121.00
1	E	1124	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	D	1611	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	B	1563	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	1601	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	D	487	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	E	1611	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	1611	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	1611	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	C	445	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	359	PHE	CB-CG-CD1	7.91	126.34	120.80
2	F	2125	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	D	806	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	C	208	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	C	2512	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	F	1411	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	E	1159	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	F	1383	ARG	NE-CZ-NH2	-7.75	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1287	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	D	1794	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	1305	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	1794	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	B	208	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	A	1868	TYR	CB-CG-CD1	-7.55	116.47	121.00
2	F	332	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	1124	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	C	1650	TYR	CB-CG-CD1	-7.50	116.50	121.00
1	A	1040	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	A	2324	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	484	TYR	CB-CG-CD1	-7.44	116.54	121.00
2	F	140	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	C	359	PHE	CB-CG-CD2	-7.39	115.63	120.80
1	D	1166	ARG	NE-CZ-NH1	7.37	123.99	120.30
2	F	1763	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	E	1369	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	1159	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	F	1367	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	C	1050	ARG	NE-CZ-NH2	7.24	123.92	120.30
2	F	302	ARG	NE-CZ-NH2	-7.23	116.68	120.30
2	F	800	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	F	1609	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	A	1194	TYR	CB-CG-CD2	-7.20	116.68	121.00
1	D	2216	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	1166	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	2216	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	1814	TYR	CB-CG-CD2	-7.11	116.74	121.00
2	F	529	ARG	NE-CZ-NH2	-7.09	116.76	120.30
2	F	196	ARG	NE-CZ-NH2	-6.99	116.81	120.30
2	F	131	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	E	1072	ASP	CB-CG-OD1	6.96	124.56	118.30
1	D	942	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	F	1449	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	C	334	TYR	CB-CG-CD1	-6.93	116.84	121.00
1	D	332	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	F	1436	ARG	NE-CZ-NH2	-6.91	116.84	120.30
2	F	2033	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	1868	TYR	CB-CG-CD1	-6.90	116.86	121.00
1	C	1794	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	E	137	TYR	CB-CG-CD1	-6.87	116.88	121.00
1	E	1287	ARG	NE-CZ-NH2	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1601	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	E	1168	TYR	CB-CG-CD2	-6.79	116.92	121.00
2	F	1010	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	B	2018	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	C	1868	TYR	CB-CG-CD1	-6.74	116.96	121.00
1	E	308	TYR	CB-CG-CD2	-6.74	116.96	121.00
2	F	1950	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	F	1167	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	2216	ARG	NE-CZ-NH2	-6.73	116.93	120.30
2	F	768	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	528	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	2324	ARG	NE-CZ-NH1	6.67	123.63	120.30
2	F	1389	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	1287	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	D	1364	TYR	CB-CG-CD1	-6.59	117.05	121.00
1	B	517	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	E	434	TYR	CB-CG-CD1	-6.56	117.06	121.00
2	F	906	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	C	1369	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	890	ALA	C-N-CD	-6.54	106.22	120.60
2	F	424	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	1168	TYR	CB-CG-CD2	-6.49	117.11	121.00
1	E	1050	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	1601	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	E	1072	ASP	CB-CG-OD2	-6.48	112.47	118.30
2	F	1836	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	380	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	1109	TYR	CB-CG-CD1	-6.46	117.13	121.00
1	D	1168	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	E	1868	TYR	CB-CG-CD1	-6.44	117.14	121.00
1	D	1794	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	B	2410	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	1650	TYR	CB-CG-CD1	-6.40	117.16	121.00
1	D	412	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	D	1050	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	2018	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	E	1604	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	A	412	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	D	777	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	1040	TYR	CB-CG-CD1	-6.33	117.20	121.00
2	F	2051	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	2512	ARG	NE-CZ-NH1	6.31	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2114	TYR	CB-CG-CD2	-6.31	117.22	121.00
2	F	424	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	675	TYR	CB-CG-CD1	-6.27	117.24	121.00
1	C	1168	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	E	1159	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	1286	TYR	CB-CG-CD2	-6.22	117.27	121.00
2	F	1115	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	D	902	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	A	136	TYR	CB-CG-CD1	-6.20	117.28	121.00
1	C	421	TYR	CB-CG-CD1	-6.17	117.30	121.00
2	F	2051	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	1650	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	C	2216	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	C	547	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	C	2266	TYR	CB-CG-CD2	-6.06	117.37	121.00
1	B	1109	TYR	CB-CG-CD1	-6.05	117.37	121.00
2	F	655	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	C	332	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	E	2266	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	B	1040	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	E	2018	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	F	2007	ARG	NE-CZ-NH2	-6.02	117.29	120.30
2	F	1201	ASP	CB-CG-OD1	6.02	123.72	118.30
2	F	940	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	2411	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	F	1789	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	2217	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	B	488	TYR	CB-CG-CD1	-5.96	117.43	121.00
1	E	1616	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	E	2216	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	F	263	ASP	CB-CG-OD2	5.94	123.65	118.30
1	E	1650	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	A	675	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	F	715	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	D	996	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	A	1195	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	1986	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	2217	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	564	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	990	ILE	N-CA-C	-5.77	95.43	111.00
1	E	1109	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	D	2428	ASP	CB-CG-OD1	5.76	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	55	PHE	CB-CG-CD2	-5.75	116.77	120.80
1	E	1563	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	376	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	F	713	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	2411	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	308	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	D	1604	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	E	103	TYR	CB-CG-CD2	-5.69	117.58	121.00
1	B	99	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	806	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	1194	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	B	208	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	547	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	970	TYR	CB-CG-CD1	-5.63	117.62	121.00
1	B	999	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	2217	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	1616	ARG	NE-CZ-NH2	-5.61	117.49	120.30
2	F	586	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	1124	ARG	CB-CA-C	-5.59	99.22	110.40
2	F	917	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	F	370	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	A	484	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	B	807	PHE	CB-CG-CD2	5.57	124.70	120.80
1	D	2014	MET	CG-SD-CE	-5.57	91.30	100.20
1	B	445	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	434	TYR	CB-CG-CD1	-5.55	117.67	121.00
2	F	1527	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	C	204	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	B	1616	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	2257	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	E	1230	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	F	286	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	1124	ARG	CB-CA-C	-5.51	99.38	110.40
1	B	1868	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	D	2411	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	208	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	1369	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	1027	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	1306	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	B	1230	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	1148	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	2005	GLY	N-CA-C	-5.47	99.41	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1794	ARG	NE-CZ-NH1	5.47	123.03	120.30
2	F	625	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	B	1794	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	1272	ASP	N-CA-C	-5.45	96.28	111.00
1	B	2428	ASP	CB-CG-OD1	5.45	123.20	118.30
2	F	905	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	2266	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	1028	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	B	359	PHE	CB-CG-CD1	-5.43	117.00	120.80
1	A	1327	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	F	303	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	332	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	F	2007	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	1655	HIS	CA-CB-CG	5.40	122.77	113.60
1	E	1883	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	C	1711	PHE	CB-CG-CD2	5.38	124.57	120.80
1	D	1272	ASP	N-CA-C	-5.37	96.50	111.00
1	E	1124	ARG	CB-CA-C	-5.35	99.71	110.40
2	F	1210	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	208	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	308	TYR	CB-CG-CD1	5.33	124.20	121.00
2	F	311	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	D	2267	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	1166	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	F	49	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	C	776	PHE	CB-CG-CD2	5.29	124.51	120.80
1	A	2512	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	B	890	ALA	C-N-CD	-5.26	109.02	120.60
1	E	1305	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	F	1860	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	D	2399	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	1814	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	E	1369	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	1194	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	D	487	ARG	NE-CZ-NH1	5.21	122.91	120.30
2	F	286	ARG	NE-CZ-NH2	5.21	122.90	120.30
2	F	523	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	1971	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	F	1860	PHE	CB-CG-CD2	5.20	124.44	120.80
1	C	1204	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	C	1230	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	1305	ARG	NE-CZ-NH2	-5.19	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2014	MET	CG-SD-CE	5.18	108.50	100.20
1	A	2513	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	1802	PRO	N-CA-C	-5.18	98.64	112.10
1	D	200	TYR	CB-CG-CD2	-5.17	117.89	121.00
1	B	142	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	E	1040	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	C	1272	ASP	N-CA-C	-5.17	97.05	111.00
1	C	1869	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	B	1159	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	1711	PHE	CB-CG-CD2	5.15	124.41	120.80
1	C	136	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	B	1168	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	E	2411	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	1602	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	1040	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	D	1616	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	E	487	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	1860	LEU	N-CA-C	-5.12	97.17	111.00
1	C	1159	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	F	131	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	1883	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	B	1204	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	F	143	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	1364	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	C	200	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	C	1369	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	1305	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	F	2055	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	1188	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	D	1855	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	C	1814	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	2217	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	332	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	1306	TYR	CB-CG-CD2	-5.04	117.97	121.00
1	C	2358	ASP	CB-CG-OD2	5.04	122.84	118.30
2	F	85	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	D	547	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	483	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	A	200	TYR	CB-CG-CD2	-5.00	118.00	121.00

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	A	18197	0	17794	53	0
1	B	18197	0	17794	58	0
1	C	18197	0	17794	48	0
1	D	18197	0	17794	55	0
1	E	18197	0	17794	60	0
2	F	17127	0	16494	54	0
All	All	108112	0	105464	322	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 2.

All (322) 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:D:290:ASP:N	1:D:290:ASP:OD1	2.35	0.59
2:F:153:ASP:O	2:F:174:ARG:NH2	2.37	0.58
1:B:624:ASP:OD1	1:B:624:ASP:N	2.37	0.58
1:C:575:ASP:OD2	1:C:577:LYS:NZ	2.35	0.57
1:B:2319:ASP:OD2	1:B:2323:LYS:NZ	2.37	0.57
1:E:1774:TYR:HH	1:E:1848:TYR:HH	1.53	0.57
1:C:624:ASP:N	1:C:624:ASP:OD1	2.37	0.57
1:E:624:ASP:OD1	1:E:624:ASP:N	2.37	0.57
1:A:624:ASP:N	1:A:624:ASP:OD1	2.35	0.57
1:C:250:ILE:O	1:C:442:LYS:NZ	2.38	0.57
1:E:817:LYS:NZ	1:E:837:ASP:OD2	2.38	0.57
2:F:1095:ASP:N	2:F:1095:ASP:OD1	2.37	0.56
1:D:817:LYS:NZ	1:D:837:ASP:OD2	2.38	0.56
1:C:1683:ASP:OD1	1:C:1683:ASP:N	2.38	0.56
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.33	0.56
1:E:207:VAL:O	1:E:208:ARG:CB	2.54	0.55
1:A:1164:LYS:NZ	1:B:1622:ASP:OD2	2.32	0.55
1:B:890:ALA:O	1:B:892:GLN:N	2.40	0.55
1:D:963:SER:OG	1:D:964:ARG:N	2.38	0.55
1:D:1124:ARG:NE	1:D:1142:SER:O	2.39	0.55
1:E:2015:SER:OG	1:E:2016:LEU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:624:ASP:OD1	1:D:624:ASP:N	2.36	0.55
1:D:2008:LYS:NZ	1:D:2267:ASP:OD2	2.40	0.55
1:A:1841:ALA:O	1:A:1842:GLN:HB2	2.06	0.55
1:B:336:THR:OG1	1:B:423:ALA:N	2.40	0.54
1:C:1514:ASP:OD2	1:C:1515:LYS:NZ	2.39	0.54
2:F:112:ASP:OD2	2:F:147:LYS:NZ	2.39	0.54
1:B:2207:ASP:OD2	1:B:2211:LYS:NZ	2.41	0.54
2:F:878:ASP:OD2	2:F:923:ARG:NH1	2.40	0.54
1:D:100:ALA:O	1:D:101:SER:C	2.47	0.54
1:D:533:ASP:OD1	1:D:533:ASP:N	2.37	0.54
2:F:263:ASP:OD1	2:F:264:TYR:N	2.41	0.53
1:D:322:ASP:OD1	1:D:323:GLY:N	2.42	0.53
1:E:193:ARG:NH1	1:E:195:SER:O	2.42	0.53
1:E:257:GLU:OE2	1:E:439:LYS:NZ	2.41	0.53
1:A:1291:TYR:O	1:A:1292:GLN:HB3	2.09	0.53
1:D:1104:ASP:OD1	1:D:1104:ASP:N	2.38	0.53
2:F:174:ARG:NH1	2:F:184:THR:OG1	2.42	0.53
2:F:1416:ASP:N	2:F:1416:ASP:OD1	2.37	0.53
1:D:890:ALA:O	1:D:892:GLN:N	2.42	0.53
1:D:1841:ALA:O	1:D:1842:GLN:HB2	2.09	0.53
1:E:1133:ASP:OD1	1:E:1133:ASP:N	2.41	0.53
1:A:1133:ASP:OD1	1:A:1133:ASP:N	2.39	0.53
1:D:253:GLU:O	1:D:442:LYS:NZ	2.42	0.53
1:B:253:GLU:O	1:B:442:LYS:NZ	2.41	0.53
1:C:1616:ARG:NE	1:C:1629:THR:OG1	2.42	0.53
2:F:263:ASP:OD2	2:F:267:ARG:HD2	2.10	0.52
1:A:2257:ARG:NH2	1:B:2309:THR:OG1	2.43	0.52
1:B:1758:MET:O	1:B:1819:ARG:NH2	2.43	0.52
1:E:1841:ALA:O	1:E:1842:GLN:HB2	2.10	0.52
1:C:592:LYS:NZ	1:C:596:ASP:OD2	2.43	0.52
1:A:2327:ARG:NH2	1:E:2469:PHE:O	2.42	0.52
2:F:449:SER:OG	2:F:450:ASN:N	2.41	0.52
1:A:1977:ASP:N	1:A:1977:ASP:OD1	2.41	0.51
1:B:990:ILE:O	1:B:991:ALA:HB3	2.10	0.51
1:B:817:LYS:NZ	1:B:837:ASP:OD2	2.44	0.51
1:D:575:ASP:OD2	1:D:577:LYS:NZ	2.40	0.51
1:D:1514:ASP:OD2	1:D:1515:LYS:NZ	2.39	0.51
1:D:1975:SER:OG	1:D:1976:ILE:N	2.43	0.51
1:E:1257:ASP:OD1	1:E:1257:ASP:N	2.41	0.51
1:A:1254:ASP:OD1	1:A:1254:ASP:N	2.42	0.51
2:F:2143:MET:O	2:F:2145:ARG:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:385:ASP:N	2:F:385:ASP:OD1	2.42	0.51
1:B:1290:SER:C	1:B:1291:TYR:O	2.45	0.50
1:A:1103:ASN:ND2	1:A:1582:ASN:O	2.44	0.50
1:B:1291:TYR:O	1:B:1292:GLN:HB2	2.12	0.50
1:E:540:SER:OG	1:E:541:GLY:N	2.44	0.50
1:A:735:ASN:N	1:A:735:ASN:OD1	2.34	0.50
1:A:1272:ASP:O	1:A:1274:ALA:N	2.44	0.50
2:F:754:GLU:O	2:F:755:ILE:HB	2.11	0.50
1:D:1683:ASP:N	1:D:1683:ASP:OD1	2.41	0.50
1:B:299:LYS:NZ	1:B:458:GLU:OE2	2.44	0.49
1:E:842:ASP:OD1	1:E:843:ALA:N	2.45	0.49
1:A:1290:SER:C	1:A:1291:TYR:O	2.50	0.49
1:B:134:SER:OG	1:B:135:VAL:N	2.45	0.49
2:F:880:SER:OG	2:F:881:THR:N	2.44	0.49
2:F:1340:ARG:NH2	2:F:1710:THR:OG1	2.45	0.49
2:F:3:ASN:HA	2:F:1126:HIS:CG	2.46	0.49
2:F:270:ASN:O	2:F:332:ARG:NH2	2.45	0.49
2:F:1234:SER:OG	2:F:1235:ASP:N	2.44	0.49
1:C:1291:TYR:O	1:C:1292:GLN:CB	2.60	0.49
1:C:1975:SER:OG	1:C:1976:ILE:N	2.44	0.49
1:C:2284:LEU:O	1:C:2286:ASP:N	2.45	0.49
1:B:1975:SER:OG	1:B:1976:ILE:N	2.46	0.49
1:E:1865:ASP:OD1	1:E:1966:ARG:NH1	2.46	0.49
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.45	0.48
1:C:322:ASP:OD1	1:C:323:GLY:N	2.46	0.48
1:A:1518:SER:OG	1:A:1519:ILE:N	2.46	0.48
1:B:548:LYS:NZ	1:B:559:ASP:OD2	2.45	0.48
2:F:1756:SER:OG	2:F:1757:ALA:N	2.47	0.48
1:B:329:ARG:HB3	1:B:431:TYR:CE1	2.49	0.48
1:E:2463:ASP:OD1	1:E:2464:PHE:N	2.47	0.48
1:D:1119:GLY:O	1:D:1120:GLU:HB2	2.13	0.48
1:D:1006:GLU:OE1	1:D:1343:LYS:NZ	2.46	0.48
2:F:616:ASP:OD1	2:F:616:ASP:N	2.45	0.48
1:B:1526:ASP:N	1:B:1526:ASP:OD1	2.45	0.48
2:F:1146:THR:HG23	2:F:1148:LEU:H	1.79	0.48
1:A:160:SER:C	1:A:161:THR:O	2.50	0.48
1:B:1320:LYS:NZ	1:B:1552:ASP:OD1	2.38	0.48
1:D:1133:ASP:OD1	1:D:1133:ASP:N	2.46	0.48
2:F:561:ASP:C	2:F:561:ASP:OD1	2.51	0.48
1:A:161:THR:O	1:A:162:LEU:HB3	2.14	0.47
1:A:2401:ASP:OD1	1:E:2496:LYS:NZ	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2287:ASP:N	1:E:2287:ASP:OD1	2.44	0.47
1:C:329:ARG:HB3	1:C:431:TYR:CE1	2.49	0.47
1:C:571:HIS:O	1:C:574:LYS:NZ	2.46	0.47
1:C:161:THR:O	1:C:162:LEU:HB2	2.14	0.47
1:D:1220:LYS:NZ	1:D:1277:ASP:OD1	2.44	0.47
1:E:2365:SER:OG	1:E:2366:GLY:N	2.48	0.47
1:A:912:TYR:CG	1:A:913:ALA:N	2.82	0.47
1:B:2380:GLY:N	1:B:2383:THR:OG1	2.46	0.47
1:E:1975:SER:OG	1:E:1976:ILE:N	2.47	0.47
2:F:1329:ASP:OD1	2:F:1329:ASP:N	2.46	0.47
1:E:171:GLU:OE1	1:E:182:TYR:OH	2.32	0.47
1:B:359:PHE:CD1	1:B:359:PHE:N	2.83	0.47
1:C:1834:SER:OG	1:C:1835:VAL:N	2.48	0.47
1:C:2466:ASP:OD1	1:C:2466:ASP:N	2.47	0.47
1:D:797:ASP:OD1	1:D:798:ALA:N	2.48	0.47
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.38	0.47
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.48	0.47
1:C:477:LYS:NZ	1:C:624:ASP:OD2	2.37	0.47
1:C:1124:ARG:HD3	1:C:1144:TRP:CD2	2.49	0.47
1:E:1834:SER:OG	1:E:1835:VAL:N	2.48	0.47
1:C:304:GLY:O	1:C:354:ARG:NH2	2.47	0.47
1:D:359:PHE:CE1	1:D:385:PRO:HB2	2.50	0.47
1:E:1991:ASP:OD2	1:E:1993:LYS:NZ	2.48	0.47
2:F:1370:ASP:OD1	2:F:1370:ASP:N	2.46	0.47
1:A:296:PHE:O	1:A:299:LYS:NZ	2.46	0.47
1:A:1841:ALA:O	1:A:1842:GLN:CB	2.63	0.47
1:A:537:ASP:OD1	1:A:538:LEU:N	2.48	0.47
1:B:540:SER:OG	1:B:541:GLY:N	2.48	0.47
1:E:1683:ASP:OD1	1:E:1683:ASP:N	2.43	0.47
1:B:1514:ASP:OD1	1:B:1514:ASP:N	2.47	0.46
1:D:359:PHE:N	1:D:359:PHE:CD1	2.83	0.46
1:E:1293:GLN:O	1:E:1303:ASN:ND2	2.48	0.46
1:D:1834:SER:OG	1:D:1835:VAL:N	2.48	0.46
2:F:1795:LYS:NZ	2:F:1818:GLU:OE1	2.47	0.46
1:A:1865:ASP:OD1	1:A:1966:ARG:NH1	2.48	0.46
1:A:2496:LYS:NZ	1:B:2401:ASP:OD1	2.35	0.46
1:A:832:ALA:O	1:A:833:GLU:HB2	2.15	0.46
1:E:357:TYR:OH	1:E:381:THR:OG1	2.28	0.46
1:E:1945:THR:OG1	1:E:1946:ASP:N	2.49	0.46
1:A:1834:SER:OG	1:A:1835:VAL:N	2.48	0.46
1:B:290:ASP:OD1	1:B:290:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:263:ASP:OD1	2:F:263:ASP:C	2.51	0.46
1:A:890:ALA:O	1:A:892:GLN:N	2.49	0.46
1:D:133:ASP:OD1	1:D:133:ASP:N	2.43	0.46
1:E:1183:ASN:OD1	1:E:1183:ASN:N	2.48	0.46
1:E:1908:ASP:OD1	1:E:1909:ARG:N	2.48	0.46
2:F:1235:ASP:OD1	2:F:1236:VAL:N	2.49	0.46
2:F:1626:THR:OG1	2:F:1950:ARG:NH2	2.49	0.46
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.47	0.46
1:D:2284:LEU:O	1:D:2286:ASP:N	2.49	0.46
1:B:1220:LYS:NZ	1:B:1277:ASP:OD1	2.45	0.46
1:C:329:ARG:NH1	1:C:434:TYR:OH	2.49	0.46
1:E:852:GLN:O	1:E:853:ALA:C	2.53	0.46
1:A:2365:SER:OG	1:A:2366:GLY:N	2.48	0.46
1:D:161:THR:O	1:D:162:LEU:HB2	2.16	0.46
1:D:2365:SER:OG	1:D:2366:GLY:N	2.49	0.46
1:B:2082:LYS:NZ	1:B:2086:GLU:OE2	2.44	0.46
1:A:1514:ASP:OD2	1:A:1515:LYS:NZ	2.43	0.45
2:F:1510:HIS:ND1	2:F:1521:ARG:NH2	2.64	0.45
1:B:714:TRP:CG	1:B:762:LEU:HD22	2.51	0.45
1:C:578:ILE:HG12	1:C:580:ASN:H	1.80	0.45
1:A:2284:LEU:O	1:A:2286:ASP:N	2.49	0.45
1:B:1507:LYS:NZ	1:B:1538:ASP:OD2	2.40	0.45
1:C:1133:ASP:OD1	1:C:1133:ASP:N	2.43	0.45
1:E:2284:LEU:O	1:E:2286:ASP:N	2.50	0.45
2:F:34:ASP:OD1	2:F:34:ASP:N	2.49	0.45
1:B:1977:ASP:N	1:B:1977:ASP:OD1	2.42	0.45
1:E:1124:ARG:HD3	1:E:1144:TRP:CD2	2.50	0.45
1:B:1022:ASP:OD2	1:B:1023:LYS:NZ	2.49	0.45
1:A:133:ASP:N	1:A:133:ASP:OD1	2.45	0.45
1:A:1291:TYR:O	1:A:1292:GLN:CB	2.64	0.45
1:D:975:ASN:N	1:D:975:ASN:OD1	2.43	0.45
1:E:1514:ASP:OD1	1:E:1514:ASP:N	2.50	0.45
1:E:2430:GLN:OE1	1:E:2497:GLN:NE2	2.50	0.45
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.50	0.45
1:C:693:ALA:HB3	1:C:694:PRO:HD3	1.99	0.45
1:C:2024:GLU:OE2	1:C:2027:ARG:NH1	2.50	0.45
1:A:1176:GLU:HG2	1:A:1194:TYR:CE2	2.52	0.45
1:B:161:THR:O	1:B:162:LEU:HB2	2.17	0.45
1:D:1124:ARG:HG2	1:D:1144:TRP:CE3	2.52	0.45
1:E:1841:ALA:O	1:E:1842:GLN:CB	2.65	0.45
1:E:161:THR:O	1:E:162:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:975:ASN:OD1	1:E:975:ASN:N	2.40	0.45
1:A:569:THR:O	1:A:618:ASN:HB2	2.17	0.45
1:A:1975:SER:OG	1:A:1976:ILE:N	2.49	0.44
1:A:2015:SER:OG	1:A:2016:LEU:N	2.50	0.44
1:C:912:TYR:CG	1:C:913:ALA:N	2.83	0.44
1:E:207:VAL:O	1:E:208:ARG:HB3	2.15	0.44
1:B:1056:MET:HE1	1:B:1085:PHE:HB2	1.98	0.44
1:C:1774:TYR:OH	1:C:1848:TYR:OH	2.29	0.44
1:A:301:SER:HB2	1:A:467:GLN:HB2	2.00	0.44
1:A:366:SER:N	1:A:413:VAL:O	2.50	0.44
1:C:191:THR:HG22	1:C:201:HIS:HA	2.00	0.44
1:D:1380:LYS:O	1:D:1381:LEU:C	2.56	0.44
1:D:204:TYR:OH	1:D:238:GLY:O	2.34	0.44
1:D:2496:LYS:NZ	1:E:2401:ASP:OD1	2.43	0.44
1:A:97:SER:OG	1:A:98:GLY:N	2.50	0.44
1:C:160:SER:C	1:C:161:THR:O	2.53	0.44
1:B:1139:ASN:ND2	1:B:1838:ASP:O	2.50	0.44
1:D:1774:TYR:OH	1:D:1848:TYR:OH	2.25	0.44
2:F:530:ASP:OD1	2:F:530:ASP:N	2.50	0.44
2:F:854:ASP:C	2:F:854:ASP:OD1	2.54	0.44
1:B:801:LEU:O	1:B:802:ILE:HB	2.17	0.44
1:E:963:SER:OG	1:E:964:ARG:N	2.49	0.44
2:F:236:ASN:ND2	2:F:238:THR:O	2.50	0.44
2:F:267:ARG:NH1	2:F:276:ALA:O	2.51	0.44
1:A:347:PRO:HB3	1:A:353:TYR:CE2	2.53	0.44
1:A:545:ASP:OD2	1:A:547:ARG:NH1	2.50	0.44
1:A:1040:TYR:OH	1:A:1951:GLN:O	2.35	0.44
1:B:2466:ASP:N	1:B:2466:ASP:OD1	2.47	0.44
1:D:329:ARG:HB3	1:D:431:TYR:CE1	2.53	0.44
1:D:1176:GLU:HG2	1:D:1194:TYR:CE2	2.53	0.44
1:D:545:ASP:OD1	1:D:545:ASP:C	2.57	0.43
1:E:336:THR:OG1	1:E:337:ASN:N	2.50	0.43
2:F:1393:ASP:N	2:F:1393:ASP:OD1	2.50	0.43
2:F:2119:TYR:HB2	2:F:2126:TRP:CZ3	2.53	0.43
1:A:2287:ASP:N	1:A:2287:ASP:OD1	2.40	0.43
1:B:2284:LEU:O	1:B:2286:ASP:N	2.51	0.43
1:C:975:ASN:OD1	1:C:975:ASN:N	2.48	0.43
2:F:210:THR:OG1	2:F:283:TRP:NE1	2.52	0.43
1:A:357:TYR:CZ	1:A:391:TYR:HB2	2.54	0.43
1:B:1178:THR:OG1	1:B:1179:LYS:N	2.51	0.43
1:B:2365:SER:OG	1:B:2366:GLY:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:73:ASP:OD1	2:F:74:CYS:N	2.50	0.43
1:B:2478:ASP:OD1	1:B:2478:ASP:N	2.51	0.43
1:B:1834:SER:OG	1:B:1835:VAL:N	2.51	0.43
1:E:1813:ASN:OD1	1:E:1813:ASN:N	2.45	0.43
1:A:852:GLN:NE2	1:A:892:GLN:OE1	2.52	0.43
1:E:228:ALA:O	1:E:233:GLN:NE2	2.51	0.43
1:B:1137:ALA:O	1:B:1138:ALA:HB3	2.19	0.43
1:D:193:ARG:NH1	1:D:195:SER:O	2.52	0.43
1:A:357:TYR:OH	1:A:381:THR:OG1	2.37	0.43
1:D:884:ALA:O	1:D:888:ASN:N	2.51	0.43
1:E:2386:SER:HG	1:E:2485:SER:HG	1.67	0.43
1:B:831:THR:OG1	1:B:832:ALA:N	2.52	0.42
1:A:1945:THR:OG1	1:A:1946:ASP:N	2.49	0.42
1:D:552:LYS:O	1:D:556:ASN:N	2.52	0.42
1:E:133:ASP:OD1	1:E:133:ASP:N	2.44	0.42
1:E:734:LEU:O	1:E:738:TYR:HB3	2.19	0.42
1:C:1684:THR:OG1	1:C:1685:ASN:N	2.52	0.42
1:E:93:ASN:OD1	1:E:93:ASN:N	2.48	0.42
1:D:828:ASN:N	1:D:828:ASN:OD1	2.47	0.42
1:D:1137:ALA:O	1:D:1139:ASN:N	2.52	0.42
1:E:1977:ASP:N	1:E:1977:ASP:OD1	2.43	0.42
2:F:336:ASN:HB2	2:F:348:PHE:HB3	2.02	0.42
2:F:1751:LYS:NZ	2:F:1769:ASP:OD1	2.47	0.42
1:E:533:ASP:OD1	1:E:533:ASP:N	2.47	0.42
2:F:1137:PHE:O	2:F:1139:ARG:N	2.52	0.42
1:B:1813:ASN:OD1	1:B:1813:ASN:N	2.48	0.42
1:D:2015:SER:OG	1:D:2016:LEU:N	2.49	0.42
1:E:1272:ASP:O	1:E:1274:ALA:N	2.52	0.42
2:F:1432:ASP:OD1	2:F:1432:ASP:C	2.58	0.42
1:A:884:ALA:O	1:A:888:ASN:N	2.52	0.42
1:B:935:HIS:O	1:B:936:ALA:C	2.57	0.42
1:C:1991:ASP:OD2	1:C:1993:LYS:NZ	2.47	0.42
1:D:1333:TYR:CG	1:D:1334:ASN:N	2.87	0.42
1:E:402:ILE:HG23	1:E:428:VAL:HB	2.02	0.42
1:E:1589:ASN:OD1	1:E:1590:GLU:N	2.52	0.42
2:F:1698:ASP:N	2:F:1698:ASP:OD1	2.43	0.42
1:A:1104:ASP:N	1:A:1104:ASP:OD1	2.40	0.42
1:C:1257:ASP:N	1:C:1257:ASP:OD1	2.45	0.42
1:B:477:LYS:NZ	1:B:624:ASP:OD2	2.41	0.41
1:C:503:ILE:HB	1:C:515:PHE:CZ	2.54	0.41
1:D:196:GLY:O	1:D:445:ARG:NH2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1841:ALA:O	1:D:1842:GLN:CB	2.69	0.41
1:E:1148:ASP:N	1:E:1148:ASP:OD1	2.45	0.41
1:A:2466:ASP:OD1	1:A:2466:ASP:N	2.51	0.41
1:B:2015:SER:OG	1:B:2016:LEU:N	2.52	0.41
1:C:2008:LYS:NZ	1:C:2267:ASP:OD2	2.49	0.41
1:E:548:LYS:NZ	1:E:559:ASP:OD1	2.50	0.41
1:E:1133:ASP:OD2	1:E:1135:LYS:NZ	2.53	0.41
1:B:533:ASP:OD1	1:B:533:ASP:N	2.44	0.41
1:C:319:ASN:OD1	1:C:320:SER:N	2.53	0.41
1:D:241:ALA:O	1:D:243:ILE:N	2.54	0.41
1:E:858:HIS:O	1:E:859:LEU:C	2.58	0.41
1:B:614:GLU:OE2	1:B:633:LYS:NZ	2.42	0.41
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.42	0.41
1:D:2491:MET:HB3	1:D:2492:PRO:HD3	2.03	0.41
1:B:1683:ASP:N	1:B:1683:ASP:OD1	2.43	0.41
1:E:1729:ASP:OD1	1:E:1730:LYS:N	2.53	0.41
1:C:1333:TYR:O	1:C:1335:GLY:N	2.53	0.41
2:F:574:SER:OG	2:F:575:ALA:N	2.53	0.41
2:F:1259:TRP:O	2:F:1318:ARG:HG2	2.21	0.41
1:C:714:TRP:CD2	1:C:762:LEU:HD22	2.55	0.41
1:D:1977:ASP:OD1	1:D:1977:ASP:N	2.50	0.41
1:E:828:ASN:OD1	1:E:828:ASN:N	2.51	0.41
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.54	0.41
2:F:1549:ASN:OD1	2:F:1549:ASN:N	2.50	0.41
1:C:542:SER:OG	1:C:543:THR:N	2.50	0.41
1:B:308:TYR:CZ	1:B:311:ASN:HA	2.56	0.41
1:B:832:ALA:O	1:B:833:GLU:HB2	2.21	0.41
1:C:315:THR:HA	1:C:316:PRO:HD2	1.93	0.41
1:C:1333:TYR:CD1	1:C:1360:ILE:HB	2.56	0.41
1:D:696:ILE:O	1:D:700:LEU:HG	2.21	0.41
1:D:1503:LYS:NZ	1:D:1508:GLU:OE2	2.48	0.41
1:E:766:TYR:CD2	1:E:771:ILE:HD11	2.56	0.41
1:E:912:TYR:CG	1:E:913:ALA:N	2.89	0.41
2:F:1909:ASN:OD1	2:F:1909:ASN:N	2.53	0.41
1:B:597:ILE:HG13	1:B:598:HIS:CD2	2.55	0.40
1:B:1124:ARG:HD3	1:B:1144:TRP:CD2	2.56	0.40
1:D:2430:GLN:O	1:D:2487:PRO:HD2	2.20	0.40
1:A:971:LEU:O	1:A:972:LEU:HB2	2.21	0.40
1:B:990:ILE:O	1:B:992:SER:N	2.54	0.40
1:C:2013:PHE:O	1:C:2015:SER:N	2.54	0.40
1:D:935:HIS:O	1:D:936:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1104:ASP:N	1:E:1104:ASP:OD1	2.43	0.40
2:F:552:ASP:OD1	2:F:552:ASP:C	2.60	0.40
2:F:618:SER:OG	2:F:619:GLY:N	2.51	0.40
2:F:1498:ASP:C	2:F:1498:ASP:OD1	2.60	0.40
2:F:1872:TYR:CD1	2:F:1872:TYR:N	2.90	0.40
1:C:1860:LEU:O	1:C:1862:ALA:N	2.55	0.40
2:F:2066:ASP:C	2:F:2066:ASP:OD1	2.60	0.40
1:B:93:ASN:N	1:B:93:ASN:OD1	2.50	0.40
1:C:368:LEU:HB3	1:C:381:THR:HB	2.04	0.40
1:C:872:THR:O	1:C:873:SER:HB2	2.21	0.40
1:C:990:ILE:O	1:C:990:ILE:HG22	2.20	0.40
1:C:1859:LEU:C	1:C:1860:LEU:O	2.54	0.40
1:A:693:ALA:HB3	1:A:694:PRO:HD3	2.04	0.40
1:C:2382:ASP:OD1	1:C:2382:ASP:N	2.46	0.40

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	A	2286/2516 (91%)	2220 (97%)	58 (2%)	8 (0%)	41	72
1	B	2286/2516 (91%)	2222 (97%)	61 (3%)	3 (0%)	51	82
1	C	2286/2516 (91%)	2228 (98%)	51 (2%)	7 (0%)	41	72
1	D	2286/2516 (91%)	2223 (97%)	57 (2%)	6 (0%)	41	72
1	E	2286/2516 (91%)	2230 (98%)	49 (2%)	7 (0%)	41	72
2	F	2143/2439 (88%)	2089 (98%)	50 (2%)	4 (0%)	47	78
All	All	13573/15019 (90%)	13212 (97%)	326 (2%)	35 (0%)	44	72

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	891	PRO
1	B	891	PRO
1	D	101	SER
1	D	891	PRO
1	D	1138	ALA
2	F	956	GLN
2	F	2144	VAL
1	A	991	ALA
1	A	1711	PHE
1	B	2493	GLU
1	C	991	ALA
1	C	1292	GLN
1	C	1334	ASN
1	D	991	ALA
1	E	991	ALA
1	E	2154	TRP
1	C	1138	ALA
1	A	1273	MET
1	C	1758	MET
1	C	1953	ASN
1	D	1953	ASN
1	E	1953	ASN
1	A	2154	TRP
1	B	1334	ASN
1	D	1758	MET
1	E	101	SER
1	E	659	TYR
1	E	1758	MET
2	F	530	ASP
1	A	739	THR
1	A	890	ALA
1	A	215	ASP
1	C	215	ASP
1	E	215	ASP
2	F	801	THR

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	A	1960/2157 (91%)	1959 (100%)	1 (0%)	93 98
1	B	1960/2157 (91%)	1960 (100%)	0	100 100
1	C	1960/2157 (91%)	1959 (100%)	1 (0%)	93 98
1	D	1960/2157 (91%)	1958 (100%)	2 (0%)	93 98
1	E	1960/2157 (91%)	1959 (100%)	1 (0%)	93 98
2	F	1854/2109 (88%)	1851 (100%)	3 (0%)	93 98
All	All	11654/12894 (90%)	11646 (100%)	8 (0%)	93 98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	683	LYS
1	C	548	LYS
1	D	661	LYS
1	D	968	TYR
1	E	1319	ARG
2	F	267	ARG
2	F	313	HIS
2	F	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1671	ASN
1	A	1951	GLN
1	B	201	HIS
1	B	679	GLN
1	B	1671	ASN
1	B	1951	GLN
1	C	361	ASN
1	C	735	ASN
1	C	1520	GLN
1	C	1655	HIS
1	C	1951	GLN
1	E	735	ASN
2	F	183	GLN
2	F	1650	HIS
2	F	1825	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

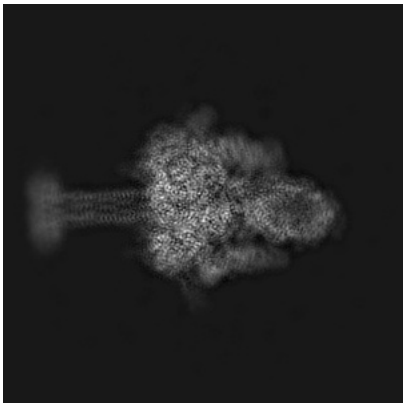
This section contains visualisations of the EMDB entry EMD-10313. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

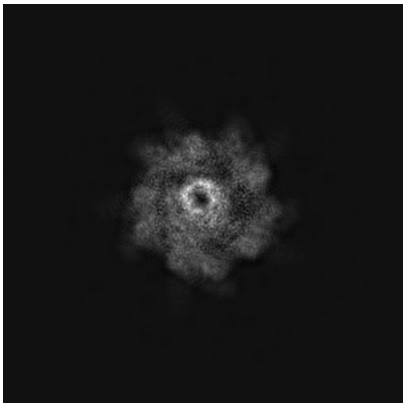
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

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

6.2 Central slices

6.2.1 Primary map

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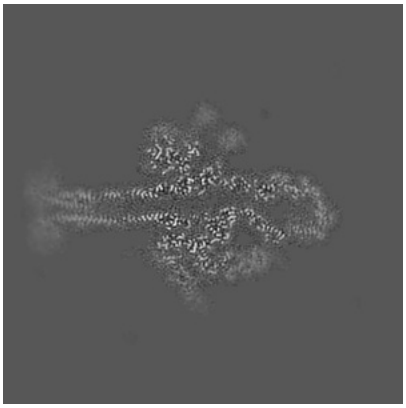
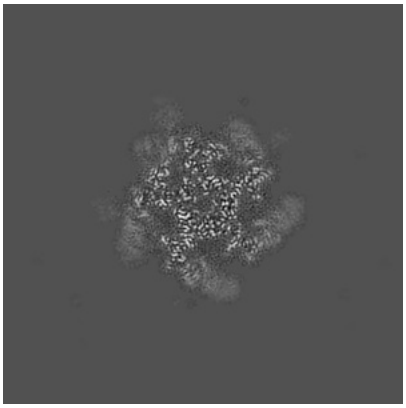


Y Index: 210



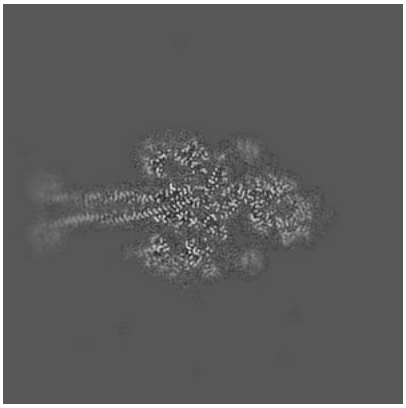
Z Index: 210

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

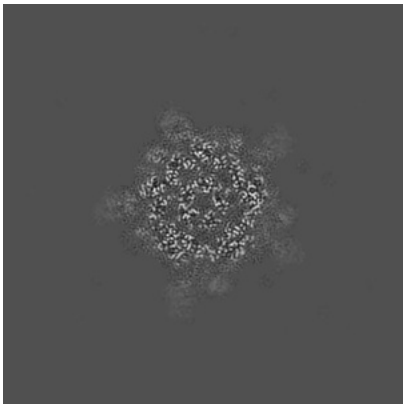
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 197



Y Index: 225



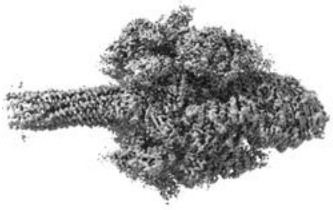
Z Index: 196

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

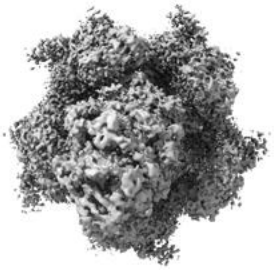
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

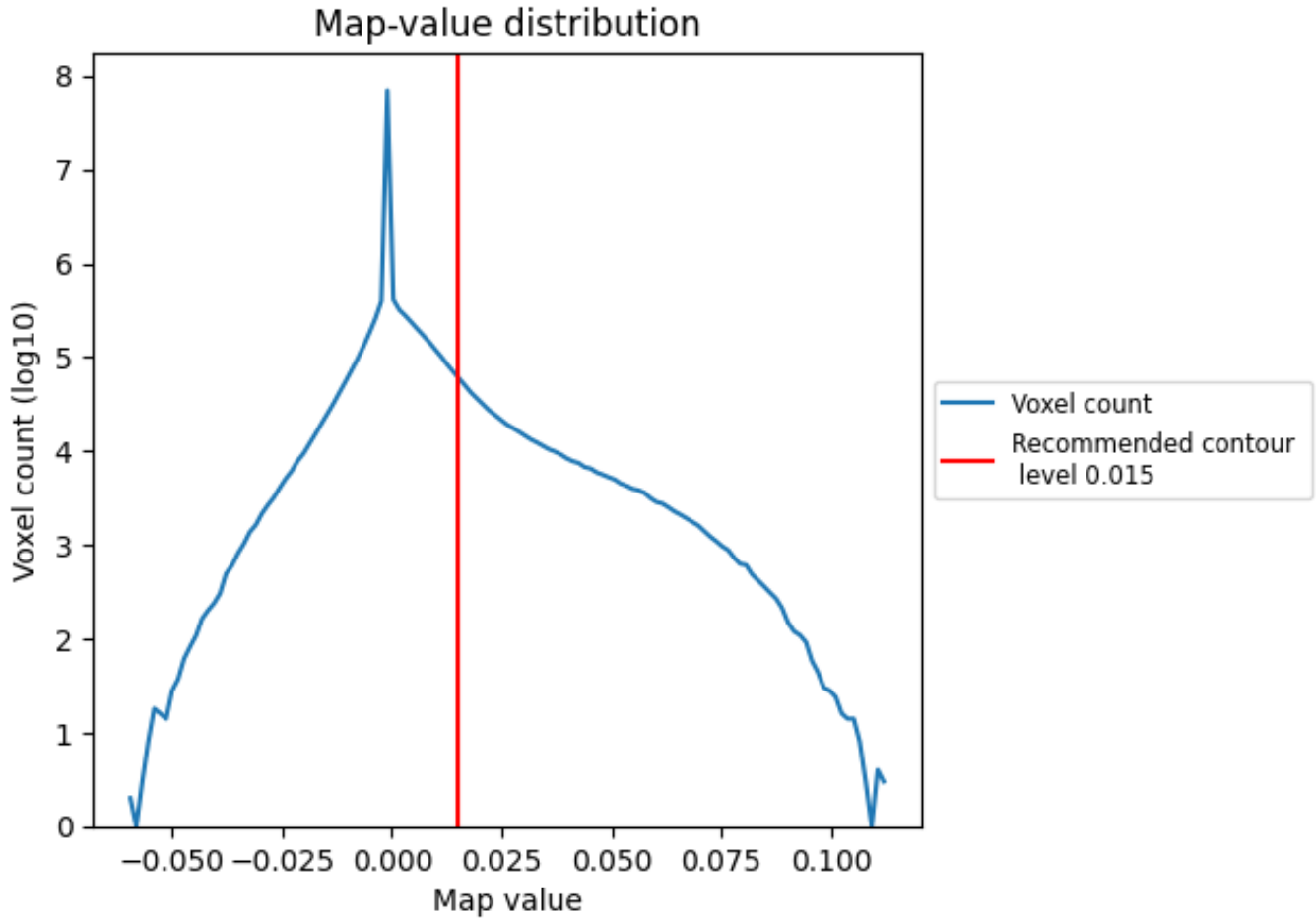
6.5 Mask visualisation (i)

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

7 Map analysis

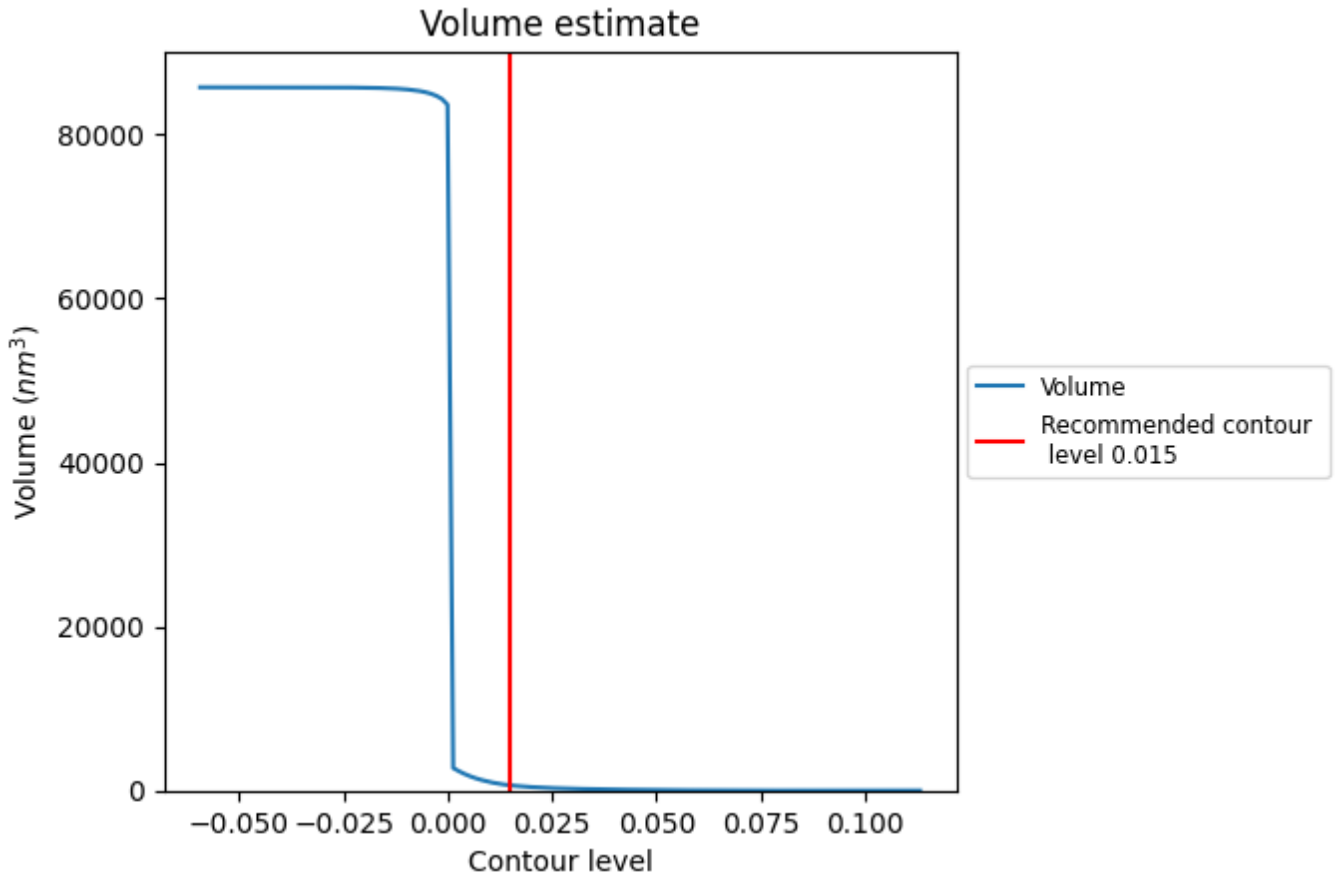
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

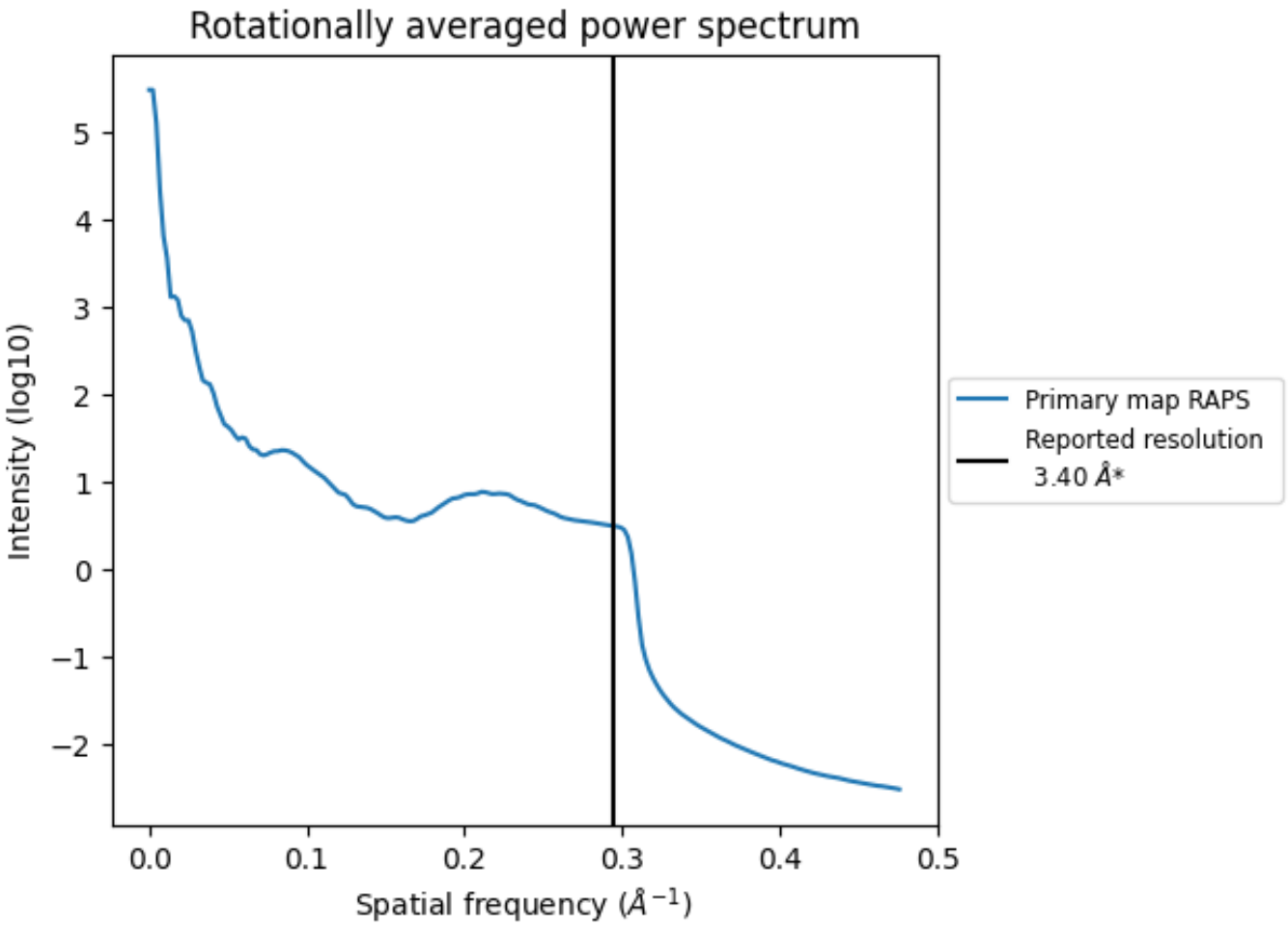
7.2 Volume estimate



The volume at the recommended contour level is 639 nm^3; this corresponds to an approximate mass of 577 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 0.294 Å^{-1}

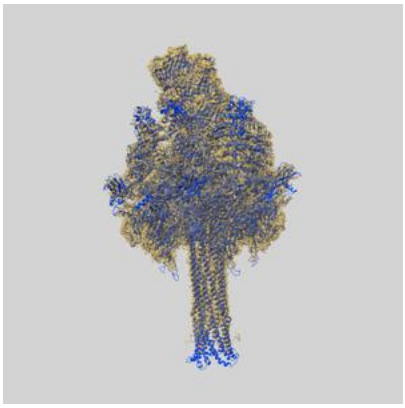
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

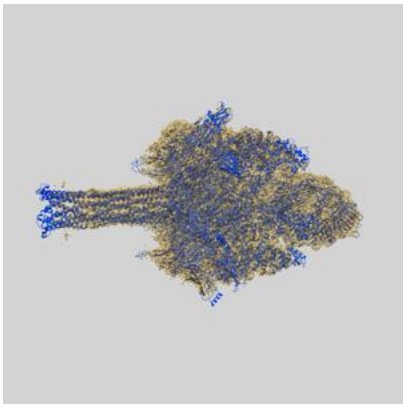
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10313 and PDB model 6SUF. Per-residue inclusion information can be found in section 3 on page 5.

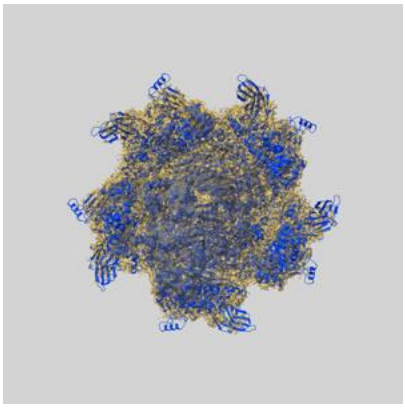
9.1 Map-model overlay



X



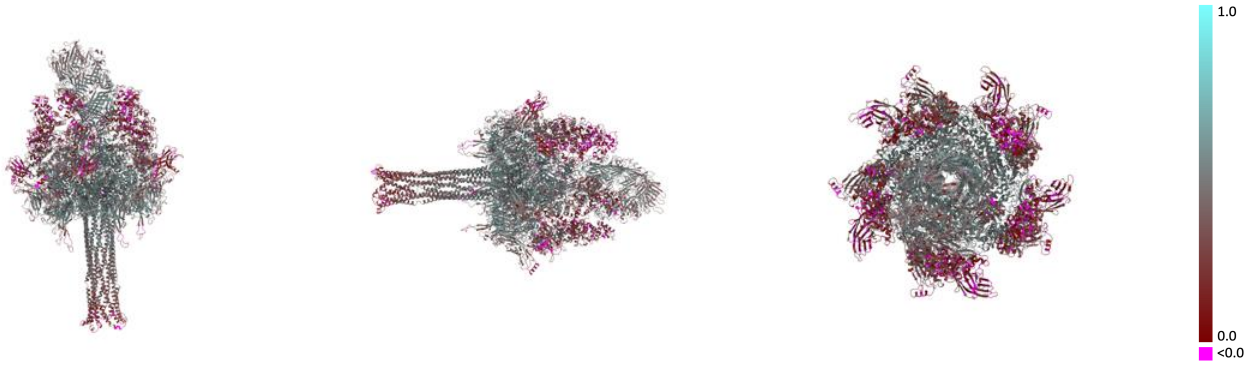
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

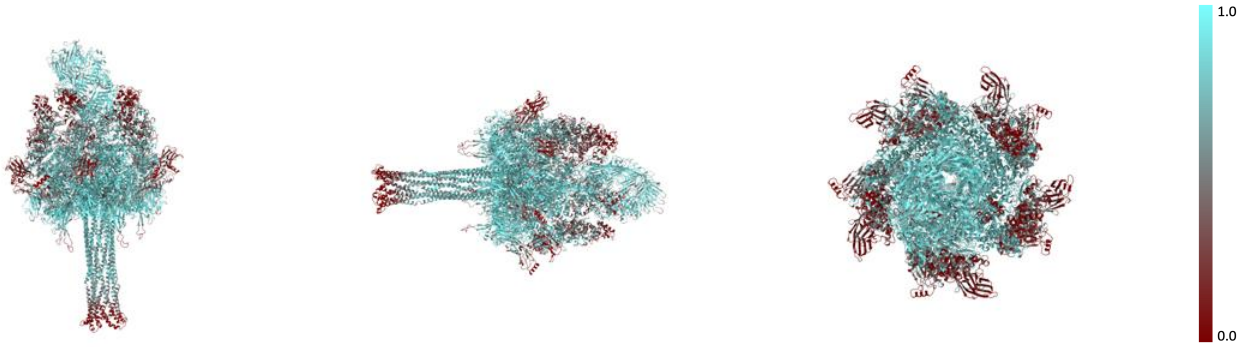
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

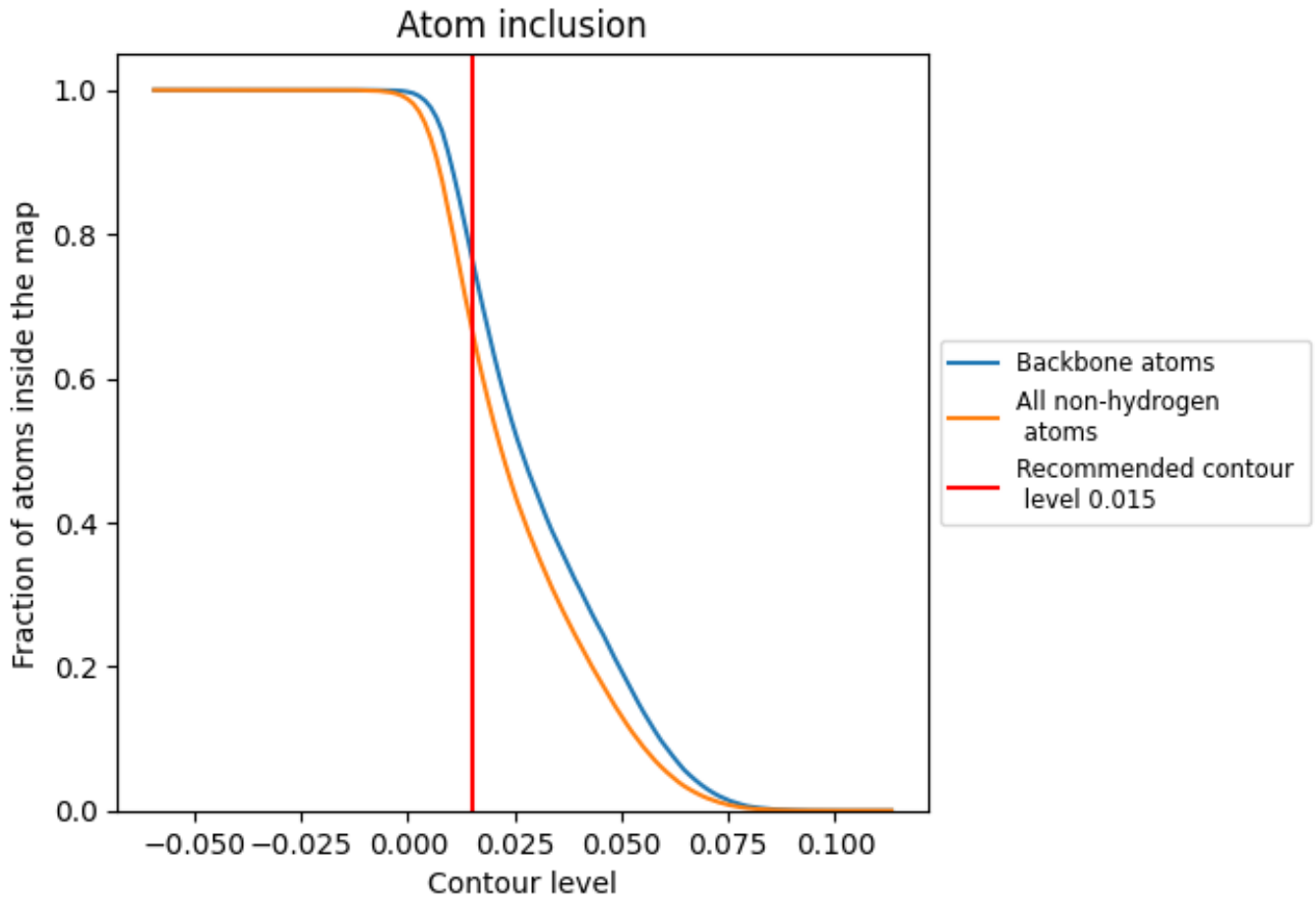
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6675	0.3960
A	0.6463	0.3870
B	0.6358	0.3810
C	0.6387	0.3850
D	0.6306	0.3760
E	0.6649	0.3940
F	0.7970	0.4590