Full wwPDB EM Validation Report (i)

May 18, 2024 – 04:19 pm BST

PDB ID	:	6SUE
EMDB ID	:	EMD-10312
Title	:	Structure of Photorhabdus luminescens Tc holotoxin pore, Mutation TccC3-D651A
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 (i) symbol.

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

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

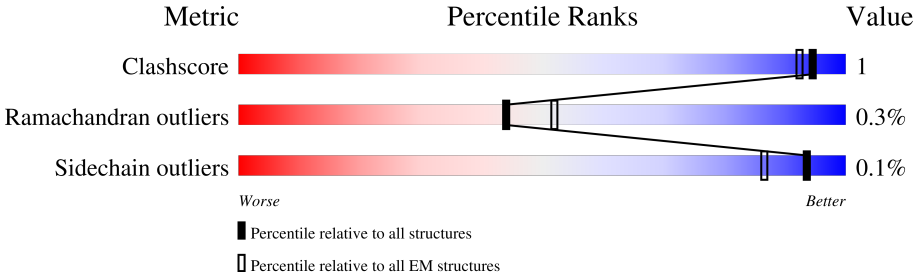
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	5% 86% 5% 9%
1	B	2516	6% 85% 6% 9%
1	C	2516	5% 85% 6% 9%
1	D	2516	8% 86% 5% 9%
1	E	2516	5% 86% 5% 9%
2	F	2439	• 83% 6% 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 108270 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
			Total	C	N	O	S		
1	A	2292	18197	11530	3083	3525	59	0	0
1	B	2292	18197	11530	3083	3525	59	0	0
1	C	2292	18197	11530	3083	3525	59	0	0
1	D	2292	18197	11530	3083	3525	59	0	0
1	E	2292	18197	11530	3083	3525	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
			Total	C	N	O	S		
2	F	2168	17285	10833	3064	3351	37	0	0

There are 7 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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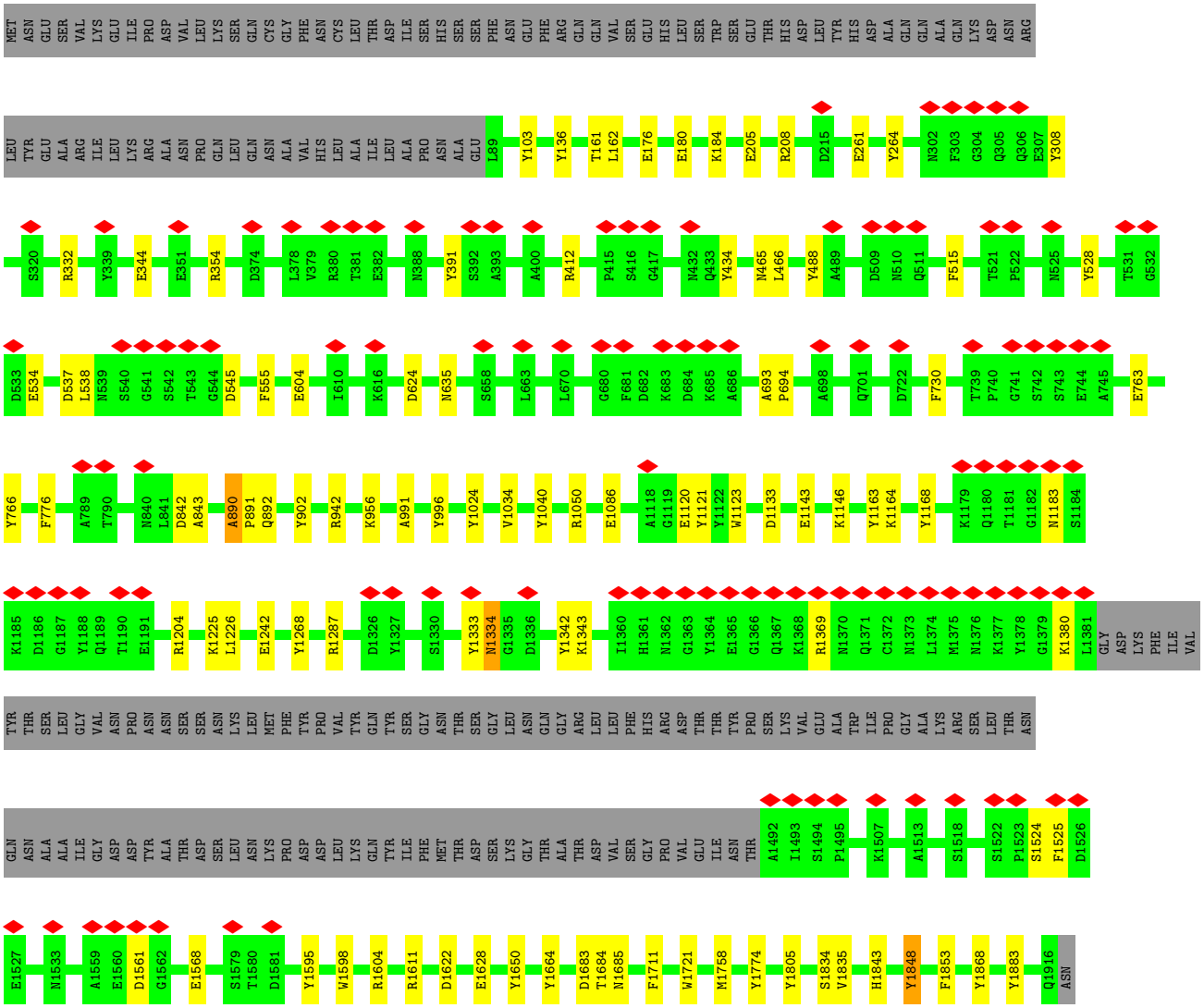
Chain	Residue	Modelled	Actual	Comment	Reference
F	1478	ARG	-	linker	UNP Q8GF99
F	1479	PRO	-	linker	UNP Q8GF99
F	2130	ALA	ASP	engineered mutation	UNP Q8GF97

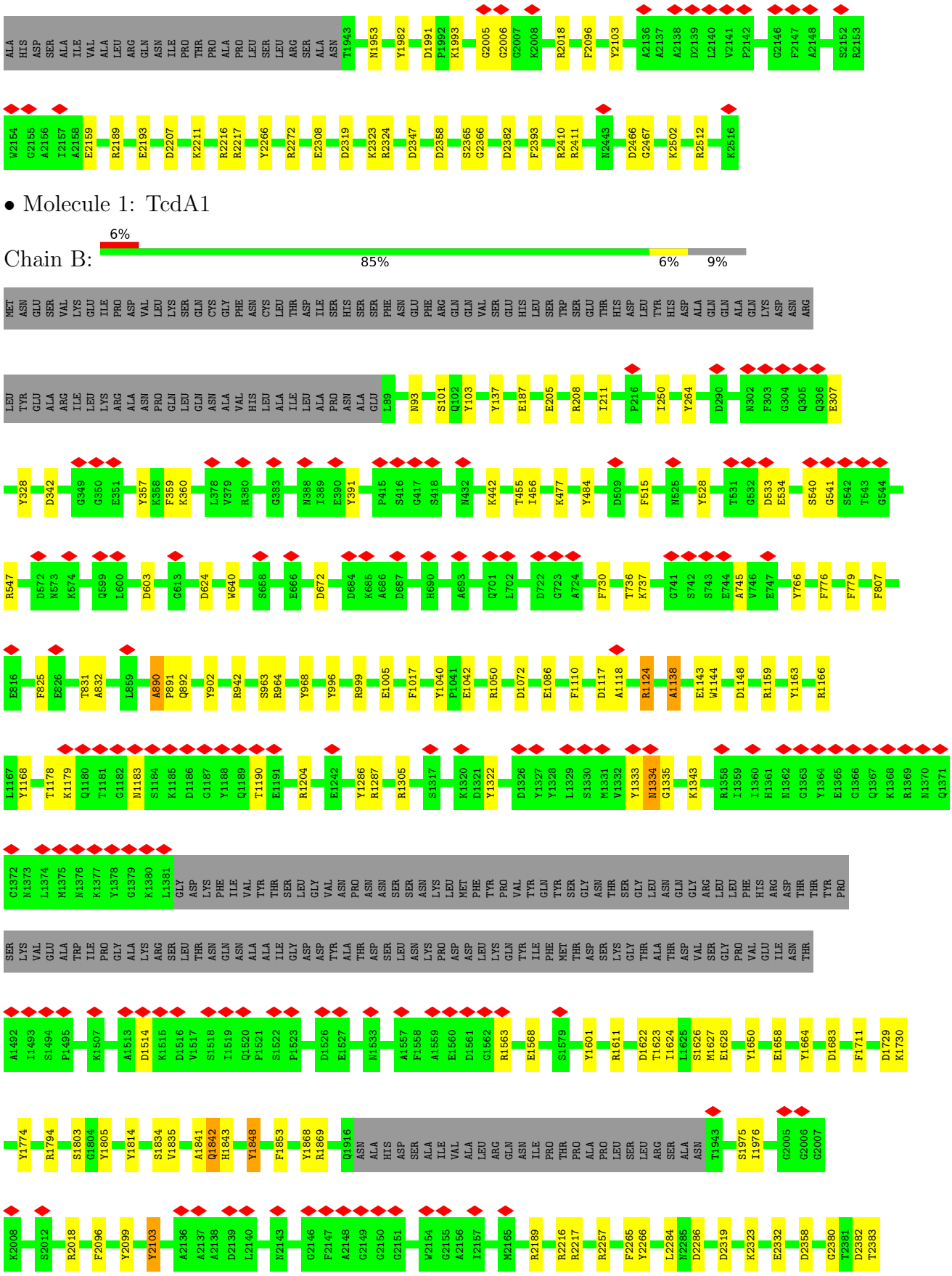
3 Residue-property plots (i)

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:

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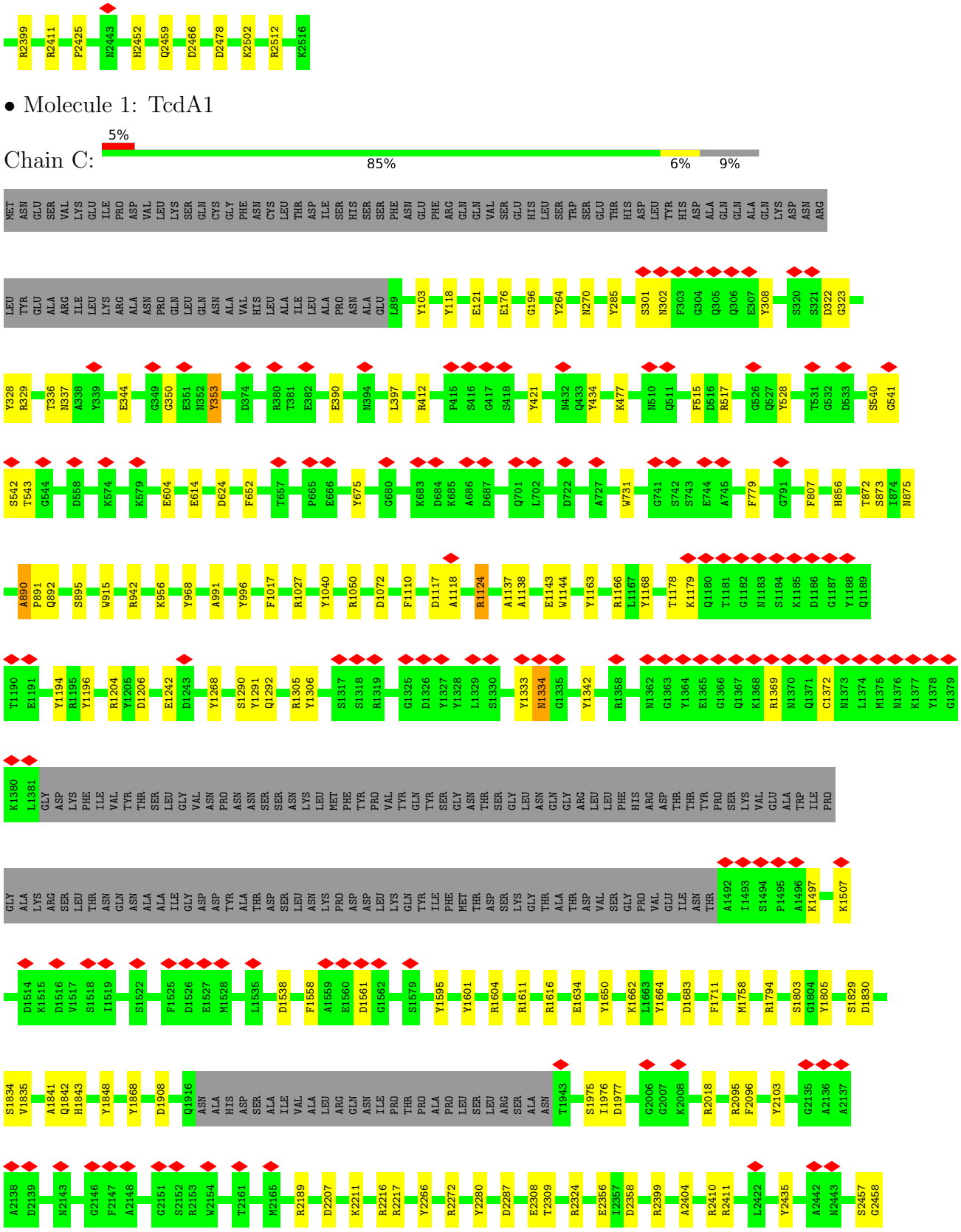
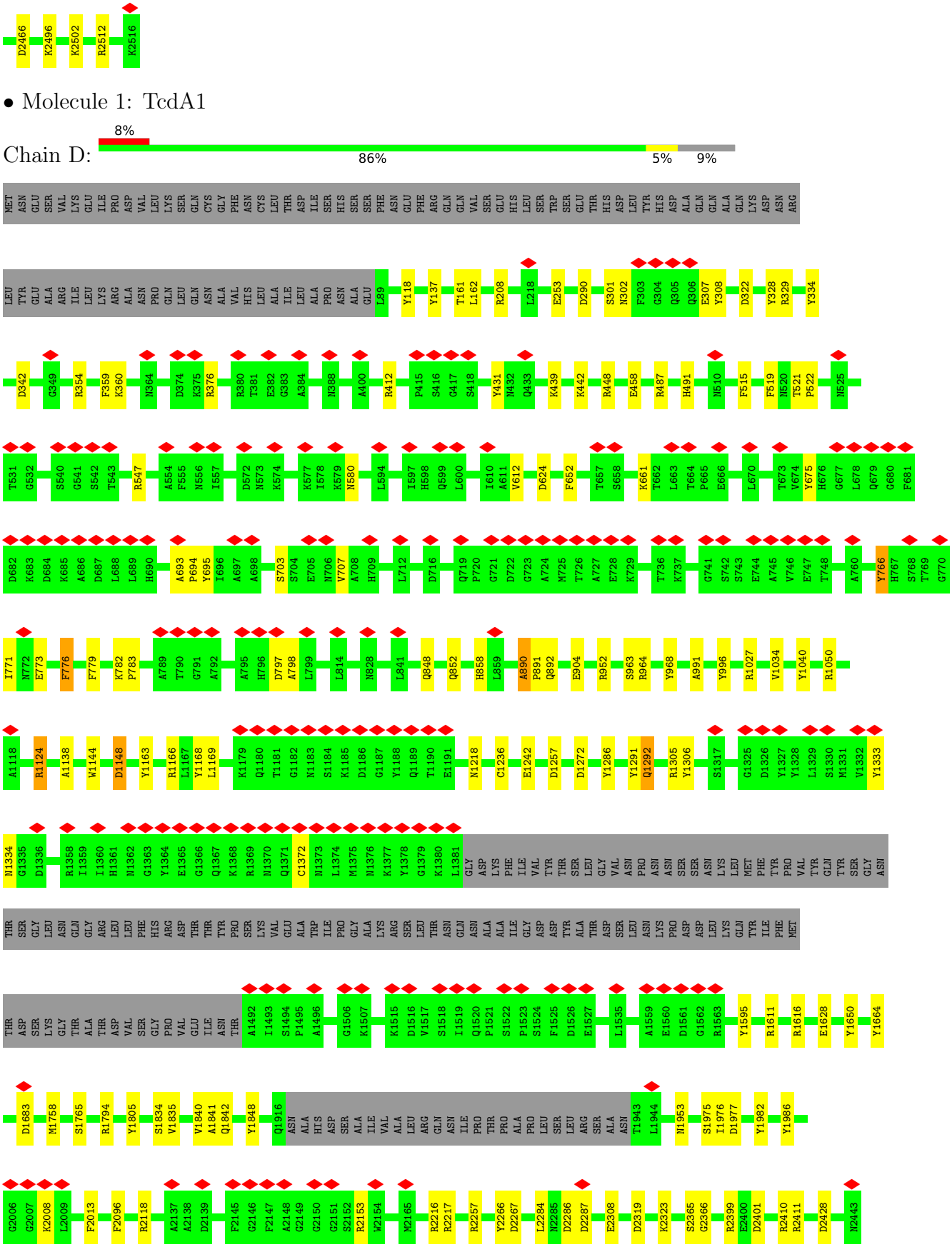
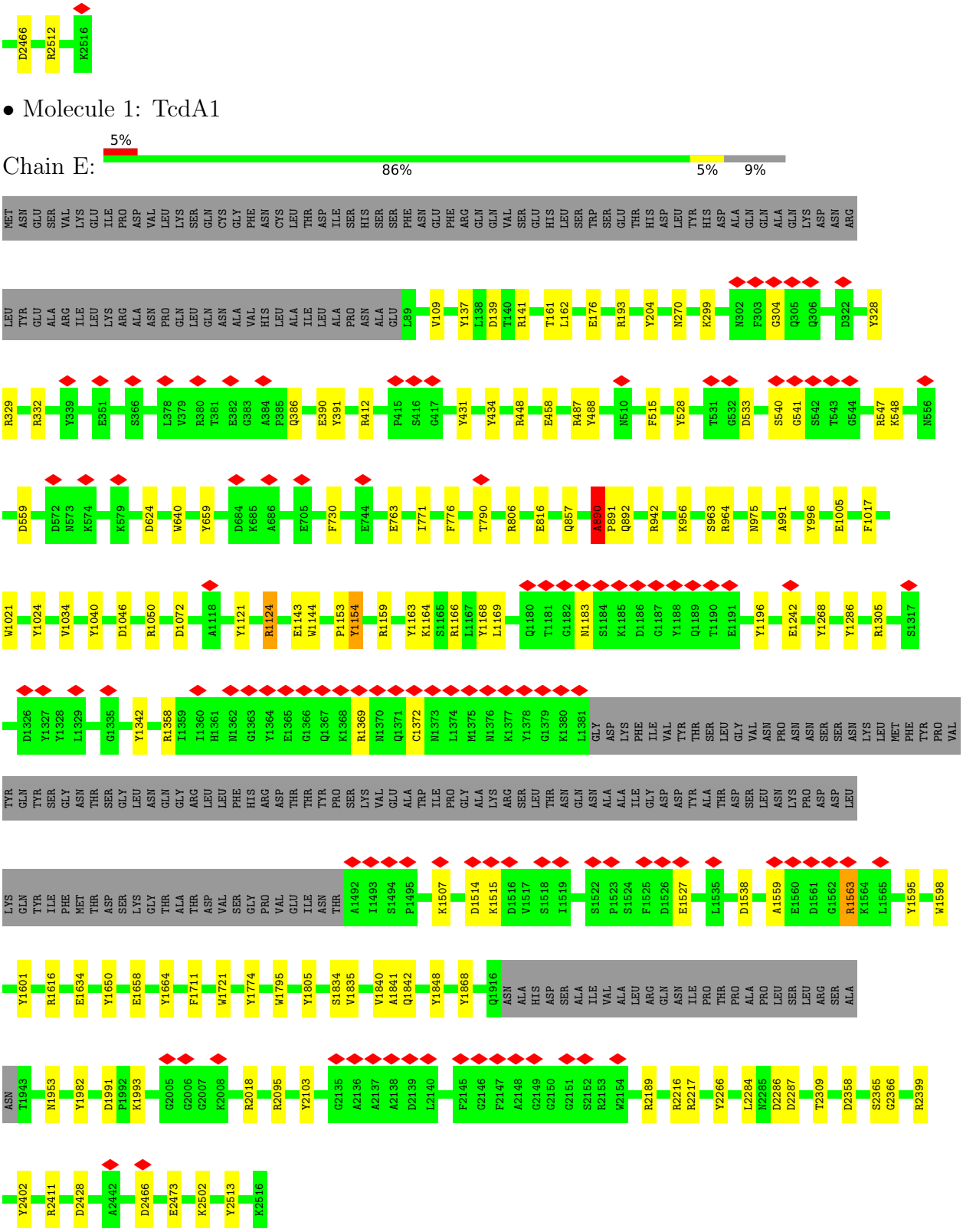
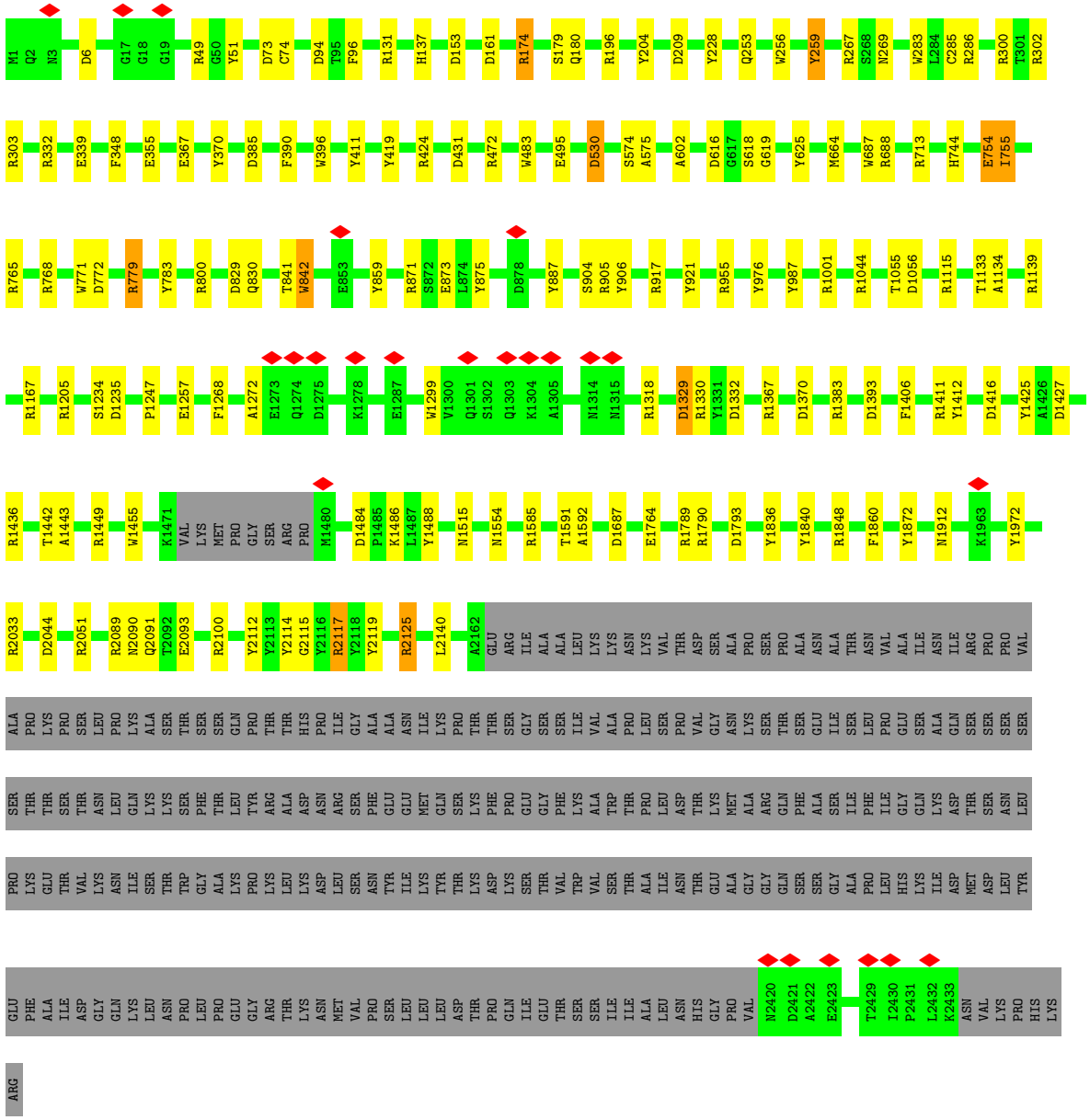
W2154 G2155 A2156 I2157 A2158 E2159 R2189 E2193 D2207 K2211 R2216 R2217 Y2266 R2272 E2308 D2319 K2323 R2324 D2347 D2358 S2365 G2366 D2382 F2393 R2410 R2411 N2443 D2466 G2467 K2502 R2512 K2516
• Molecule 1: TcdA1
Chain B:
6%
85%
6%
9%
MET ASN GLU SER VAL LYS GLU ILE PRO ASP VAL LEU LYS SER GLN CYS GLY PHE ASN CYS LEU THR ASP ILE SER HIS SER SER PHE ASN GLU PHE ARG GLN GLN VAL SER GLU HIS LEU SER TRP SER GLU THR HIS ASP LEU TYR HIS ASP ALA GLN GLN ALA GLN LYS ASP ASN ARG
LEU TYR GLU ALA ARG ILE LEU LYS ARG ALA ASN PRO GLN LEU GLN ASN ALA VAL HIS LEU ALA ILE LEU ALA PRO ASN ALA GLU L89 N93 S101 Q102 Y103 Y137 E187 E205 R208 I211 P216 I250 Y264 D290 M302 F303 G304 Q305 Q306 E307
Y328 D342 G349 G350 E351 Y357 K358 F359 K360 L378 V379 R380 G383 N388 I389 E390 Y391 P415 S416 G417 S418 N432 K442 T455 I456 K477 Y484 D509 F515 N525 Y528 T531 G532 D533 E534 S540 G541 S542 T543 G544
R547 D572 N573 K574 Q599 L600 D603 G613 D624 W640 S658 E666 D672 D684 K685 A686 D687 H690 A693 Q701 L702 D722 G723 A724 F730 T736 K737 G741 S742 S743 E744 A745 V746 E747 Y766 F776 F779 F807
E816 F825 E826 T831 A832 L859 A890 P891 Q892 Y902 R942 S963 R964 Y968 Y996 R999 E1005 F1017 Y1040 P1041 E1042 R1050 D1072 E1086 F1110 D1117 A1118 R1124 A1138 E1143 W1144 D1148 R1159 Y1163 R1166
L1167 Y1168 T1178 K1179 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 R1204 E1242 Y1286 R1287 R1305 S1317 K1320 D1321 Y1322 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333 N1334 G1335 K1343 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 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 K1507 A1513 D1514 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522 P1523 D1526 E1527 M1533 A1557 F1558 A1559 E1560 D1561 G1562 R1563 E1568 S1579 Y1601 R1611 D1622 T1623 I1624 L1625 S1626 M1627 E1628 Y1650 E1658 Y1664 D1683 F1711 D1729 K1730
Y1774 R1794 S1803 G1804 Y1805 Y1814 S1834 V1835 A1841 Q1842 H1843 Y1848 F1853 Y1868 R1869 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN T1943 S1975 I1976 G2005 G2006 G2007
K2008 S2012 R2018 F2096 Y2099 Y2103 A2136 A2137 A2138 D2139 L2140 N2143 G2146 F2147 A2148 G2149 G2150 G2151 W2154 G2155 A2156 I2157 M2165 R2189 R2216 R2217 R2257 F2265 Y2266 L2284 N2285 D2286 D2319 K2323 E2332 D2358 G2380 T2381 D2382 T2383


R2399 R2411 P2425 N2443 H2452 Q2459 D2466 D2478 K2502 R2512 K2516
• Molecule 1: TcdA1
Chain C:
5%
85%
6%
9%
MET ASN GLU SER VAL LYS GLU ILE PRO ASP VAL LEU LYS SER GLN CYS GLY PHE ASN CYS LEU THR ASP ILE SER HIS SER SER PHE ASN GLU PHE ARG GLN GLN VAL SER GLU HIS LEU SER TRP SER GLU THR HIS ASP LEU TYR HIS ASP ALA GLN GLN ALA GLN LYS ASP ASN ARG
LEU TYR GLU ALA ARG ILE LEU LYS ARG ALA ASN PRO GLN LEU GLN ASN ALA VAL HIS LEU ALA ILE LEU ALA PRO ASN ALA GLU L89 Y103 Y118 E121 E176 G196 Y264 N270 Y285 S301 N302 F303 G304 Q305 Q306 E307 Y308 S320 S321 D322 G323
Y328 R329 T336 N337 A338 Y339 E344 G349 G350 E351 N352 Y353 D374 R380 T381 E382 E390 N394 L397 R412 P415 S416 G417 S418 Y421 M432 Q433 Y434 K477 N510 Q511 F515 D516 R517 G526 Q527 Y528 T531 G532 D533 S540 G541
S542 T543 G544 D558 K574 K579 E604 E614 D624 F652 T657 P665 E666 Y675 G680 K683 D684 K685 A686 D687 Q701 L702 D722 A727 W731 G741 S742 S743 E744 A745 F779 G791 F807 H856 T872 S873 I874 N875
A890 P891 Q892 S895 W915 R942 K956 Y968 A991 Y996 F1017 R1027 Y1040 R1050 D1072 F1110 D1117 A1118 R1124 A1137 A1138 E1143 W1144 Y1163 R1166 L1167 Y1168 T1178 K1179 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189
T1190 E1191 Y1194 R1195 Y1196 R1204 Y1205 D1206 E1242 D1243 Y1268 S1290 Y1291 Q1292 R1305 Y1306 S1317 S1318 R1319 G1325 D1326 Y1327 Y1328 L1329 S1330 Y1333 N1334 G1335 Y1342 R1358 N1362 G1363 Y1364 E1365 G1366 Q1367 K1368 R1369 N1370 Q1371 C1372 M1373 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 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 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 K1507
D1514 K1515 D1516 V1517 S1518 I1519 S1522 F1525 D1526 E1527 M1528 L1535 D1538 F1558 A1559 E1560 D1561 G1562 S1579 Y1595 Y1601 R1604 R1611 R1616 E1634 Y1650 K1662 L1663 Y1664 D1683 F1711 M1758 R1794 S1803 G1804 Y1805 S1829 D1830
S1834 V1835 A1841 Q1842 H1843 Y1848 Y1868 D1908 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN T1943 S1975 I1976 D1977 G2006 G2007 K2008 R2018 R2095 F2096 Y2103 G2135 A2136 A2137
A2138 D2139 N2143 G2146 F2147 A2148 G2151 S2152 R2153 W2154 T2161 M2165 R2189 D2207 K2211 R2216 R2217 Y2266 R2272 Y2280 D2287 E2308 T2309 R2324 E2356 I2357 D2358 R2399 A2404 R2410 R2411 L2422 Y2435 A2442 N2443 S2457 G2458


D2466 K2496 K2502 R2512 K2516
• Molecule 1: TcdA1
Chain D:
8%
86%
5%
9%
MET ASN GLU SER VAL LYS GLU ILE PRO ASP VAL LEU LYS SER GLN CYS GLY PHE ASN CYS LEU THR ASP ILE SER HIS SER SER PHE ASN GLU PHE ARG GLN GLN VAL SER GLU HIS LEU SER TRP SER GLU THR HIS ASP LEU TYR HIS ASP ALA GLN GLN ALA GLN LYS ASP ASN ARG
LEU TYR GLU ALA ARG ILE LEU LYS ARG ALA ASN PRO GLN LEU GLN ASN ALA VAL HIS LEU ALA ILE LEU ALA PRO ASN ALA GLU L89 Y118 Y137 T161 L162 R208 L218 E253 D290 S301 N302 F303 G304 Q305 Q306 E307 Y308 D322 Y328 R329 Y334
D342 G349 R354 F359 K360 N364 D374 K375 R376 R380 T381 E382 G383 A384 N388 A400 R412 P415 S416 G417 S418 Y431 N432 Q433 K439 K442 R448 E458 R487 H491 N510 F515 F519 N520 T521 P522 N525
T531 G532 S540 G541 S542 T543 R547 A554 F555 N556 I557 D572 N573 K574 K577 I578 K579 N580 L594 I597 H598 Q599 L600 I610 A611 V612 D624 F652 T657 S658 K661 T662 L663 T664 P665 E666 L670 T673 V674 Y675 H676 G677 L678 Q679 G680 F681
D682 K683 D684 K685 A686 D687 L688 L689 H690 A693 P694 Y695 I696 A697 A698 S703 S704 E705 N706 V707 A708 H709 L712 D716 Q719 P720 G721 D722 G723 A724 M725 T726 A727 E728 K729 T736 K737 G741 S742 S743 E744 A745 V746 E747 T748 A760 Y766 H767 S768 T769 G770
I771 N772 E773 F776 F779 K782 P783 A789 T790 G791 A792 A795 H796 D797 A798 L799 L814 N828 L841 Q848 Q852 H858 L859 A890 P891 Q892 E904 R952 S963 R964 Y968 A991 Y996 R1027 V1034 Y1040 R1050
A1118 R1124 A1138 W1144 D1148 Y1163 R1166 L1167 Y1168 L1169 K1179 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 N1218 C1236 E1242 D1257 D1272 Y1286 Y1291 Q1292 R1305 Y1306 S1317 G1325 D1326 Y1327 Y1328 L1329 S1330 M1331 V1332 Y1333
N1334 G1335 D1336 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 GLU ALA TRP ILE PRO GLY ALA LYS ARG SER LEU THR ASN GLN ASN 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 G1506 K1507 K1515 D1516 V1517 S1518 I1519 Q1520 P1521 S1522 P1523 S1524 F1525 D1526 E1527 L1535 A1559 E1560 D1561 G1562 R1563 Y1595 R1611 R1616 E1628 Y1650 Y1664
D1683 M1758 S1765 R1794 Y1805 S1834 V1835 V1840 A1841 Q1842 Y1848 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA ASN T1943 L1944 N1953 S1975 I1976 D1977 Y1982 Y1986
G2006 G2007 K2008 L2009 F2013 F2096 R2118 A2137 A2138 D2139 F2145 G2146 F2147 A2148 G2149 G2150 G2151 S2152 R2153 W2154 M2165 R2216 R2217 R2257 Y2266 D2267 L2284 W2285 D2286 D2287 E2308 D2319 K2323 S2365 G2366 R2399 E2400 D2401 R2410 R2411 D2428 N2443


D2466 R2512 K2516
• Molecule 1: TcdA1
Chain E:
5%
86%
5%
9%
MET ASN GLU SER VAL LYS GLU ILE PRO ASP VAL LEU LYS SER GLN CYS GLY PHE ASN CYS LEU THR ASP ILE SER HIS SER SER PHE ASN GLU PHE ARG GLN GLN VAL SER GLU HIS LEU SER TRP SER GLU THR HIS ASP LEU TYR HIS ASP ALA GLN GLN ALA GLN LYS ASP ASN ARG
LEU TYR GLU ALA ARG ILE LEU LYS ARG ALA ASN PRO GLN LEU GLN ASN ALA VAL HIS LEU ALA ILE LEU ALA PRO ASN ALA GLU L89 V109 Y137 L138 D139 T140 R141 T161 L162 E176 R193 Y204 N270 K299 N302 F303 G304 Q305 Q306 D322 Y328
R329 R332 Y339 E351 S366 L378 V379 R380 T381 E382 G383 A384 P385 Q386 E390 Y391 R412 P415 S416 G417 Y431 Y434 R448 E458 R487 Y488 N510 F515 Y528 T531 G532 D533 S540 G541 S542 T543 G544 R547 K548 N556
D559 D572 N573 K574 K579 D624 W640 Y659 D684 K685 A686 E705 F730 E744 E763 I771 F776 T790 R806 E816 Q857 A890 P891 Q892 R942 K956 S963 R964 N975 A991 Y996 E1005 F1017
W1021 Y1024 V1034 Y1040 D1046 R1050 D1072 A1118 Y1121 R1124 E1143 W1144 P1153 Y1154 R1159 Y1163 K1164 S1165 R1166 L1167 Y1168 L1169 Q1180 T1181 G1182 N1183 S1184 K1185 D1186 G1187 Y1188 Q1189 T1190 E1191 Y1196 E1242 Y1268 Y1286 R1305 S1317
D1326 Y1327 Y1328 L1329 G1335 Y1342 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 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 K1507 D1514 K1515 D1516 V1517 S1518 I1519 S1522 P1523 S1524 F1525 D1526 E1527 L1535 D1538 A1559 E1560 D1561 G1562 R1563 K1564 L1565 Y1595 W1598
Y1601 R1616 E1634 Y1650 E1658 Y1664 F1711 W1721 Y1774 W1795 Y1805 S1834 V1835 V1840 A1841 Q1842 Y1848 Y1868 Q1916 ASN ALA HIS ASP SER ALA ILE VAL ALA LEU ARG GLN ASN ILE PRO THR PRO ALA PRO LEU SER LEU ARG SER ALA
ASN T1943 N1953 Y1982 D1991 P1992 K1993 G2005 G2006 G2007 K2008 R2018 R2095 Y2103 G2135 A2136 A2137 A2138 D2139 L2140 F2145 G2146 F2147 A2148 G2149 G2150 G2151 S2152 R2153 W2154 R2189 R2216 R2217 Y2266 L2284 M2285 D2286 D2287 T2309 D2358 S2365 G2366 R2399
Y2402 R2411 D2428 A2442 D2466 E2473 K2502 Y2513 K2516
• Molecule 2: TcdB2,TccC3
Chain F:
83%
6%
11%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R303 R332 E339 F348 E355 E367 Y370 D385 F390 W396 Y411 Y419 R424 D431 R472 W483 E495 D530 S574 A575 A602 D616 G617 S618 G619 Y625 M664 W687 R688 R713 H744 E754 I755
R765 R768 W771 D772 R779 Y783 R800 D829 Q830 T841 W842 E853 Y859 R871 S872 E873 L874 Y875 D878 Y887 S904 R905 Y906 R917 Y921 R955 Y976 Y987 R1001 R1044 T1055 D1056 R1115 T1133 A1134 R1139
R1167 R1205 S1234 D1235 P1247 E1257 F1268 A1272 E1273 Q1274 D1275 K1278 E1287 W1299 V1300 Q1301 S1302 Q1303 K1304 A1305 N1314 M1315 R1318 D1329 R1330 Y1331 D1332 R1367 D1370 R1383 D1393 F1406 R1411 Y1412 D1416 Y1425 A1426 D1427
R1436 T1442 A1443 R1449 W1455 K1471 VAL LYS MET PRO GLY SER ARG PRO M1480 D1484 P1485 K1486 L1487 Y1488 N1515 N1554 R1585 T1591 A1592 D1687 E1764 R1789 R1790 D1793 Y1836 Y1840 R1848 F1860 Y1872 N1912 K1963 Y1972
R2033 D2044 R2051 R2089 N2090 Q2091 T2092 E2093 R2100 Y2112 Y2113 Y2114 G2115 Y2116 R2117 Y2118 Y2119 R2125 L2140 A2162 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 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 N2420 D2421 A2422 E2423 T2429 I2430 P2431 L2432 K2433 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	337823	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 ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.165	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	426.24, 426.24, 426.24	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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	1.12	46/18587 (0.2%)	0.93	40/25239 (0.2%)
1	B	1.12	47/18587 (0.3%)	0.93	48/25239 (0.2%)
1	C	1.13	54/18587 (0.3%)	0.94	52/25239 (0.2%)
1	D	1.12	38/18587 (0.2%)	0.93	43/25239 (0.2%)
1	E	1.12	43/18587 (0.2%)	0.94	50/25239 (0.2%)
2	F	1.18	46/17708 (0.3%)	0.98	70/24137 (0.3%)
All	All	1.13	274/110643 (0.2%)	0.94	303/150332 (0.2%)

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	D	0	1

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1242	GLU	CG-CD	-10.17	1.36	1.51
1	A	1242	GLU	CG-CD	-10.04	1.36	1.51
1	A	308	TYR	CB-CG	-9.65	1.37	1.51
1	C	1242	GLU	CG-CD	-9.22	1.38	1.51
2	F	1860	PHE	CB-CG	-9.12	1.35	1.51
1	E	996	TYR	CB-CG	-8.73	1.38	1.51
1	B	1124	ARG	CD-NE	-8.33	1.32	1.46
1	D	1163	TYR	CB-CG	-8.26	1.39	1.51
1	E	1163	TYR	CB-CG	-8.07	1.39	1.51
1	A	902	TYR	CB-CG	-8.06	1.39	1.51
1	E	1664	TYR	CB-CG	-8.02	1.39	1.51
1	B	1163	TYR	CB-CG	-7.99	1.39	1.51
1	A	1242	GLU	CD-OE2	-7.85	1.17	1.25
1	E	1242	GLU	CG-CD	-7.83	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	996	TYR	CB-CG	-7.69	1.40	1.51
1	B	1843	HIS	CB-CG	-7.66	1.36	1.50
1	A	1163	TYR	CB-CG	-7.51	1.40	1.51
1	B	1848	TYR	CG-CD1	-7.46	1.29	1.39
1	E	515	PHE	CB-CG	-7.46	1.38	1.51
1	C	1242	GLU	CD-OE2	-7.45	1.17	1.25
1	C	1163	TYR	CB-CG	-7.44	1.40	1.51
1	E	1372	CYS	CB-SG	-7.44	1.69	1.82
2	F	1872	TYR	CE1-CZ	-7.39	1.28	1.38
1	A	1843	HIS	CB-CG	-7.31	1.36	1.50
2	F	744	HIS	CB-CG	-7.28	1.36	1.50
1	C	1601	TYR	CB-CG	-7.27	1.40	1.51
1	D	1664	TYR	CB-CG	-7.27	1.40	1.51
1	D	1242	GLU	CD-OE2	-7.25	1.17	1.25
1	D	996	TYR	CB-CG	-7.17	1.40	1.51
1	D	1124	ARG	CD-NE	-7.15	1.34	1.46
1	D	776	PHE	CG-CD2	-7.14	1.28	1.38
1	B	640	TRP	CB-CG	-7.12	1.37	1.50
2	F	875	TYR	CB-CG	-7.09	1.41	1.51
1	D	580	ASN	CB-CG	-6.94	1.35	1.51
1	B	1842	GLN	CG-CD	-6.87	1.35	1.51
1	B	776	PHE	CB-CG	-6.86	1.39	1.51
1	C	1843	HIS	CB-CG	-6.85	1.37	1.50
1	B	1664	TYR	CB-CG	-6.84	1.41	1.51
2	F	483	TRP	CB-CG	-6.81	1.38	1.50
1	C	807	PHE	CG-CD1	-6.75	1.28	1.38
1	B	1805	TYR	CB-CG	-6.71	1.41	1.51
1	E	1634	GLU	CD-OE1	-6.68	1.18	1.25
1	D	491	HIS	CB-CG	-6.67	1.38	1.50
1	A	1848	TYR	CE2-CZ	-6.57	1.30	1.38
2	F	348	PHE	CB-CG	-6.55	1.40	1.51
1	A	1268	TYR	CB-CG	-6.54	1.41	1.51
1	B	902	TYR	CB-CG	-6.51	1.41	1.51
1	A	1664	TYR	CB-CG	-6.49	1.42	1.51
2	F	2119	TYR	CB-CG	-6.49	1.42	1.51
1	C	1848	TYR	CE2-CZ	-6.48	1.30	1.38
1	A	776	PHE	CB-CG	-6.45	1.40	1.51
1	E	1595	TYR	CB-CG	-6.43	1.42	1.51
1	A	996	TYR	CB-CG	-6.42	1.42	1.51
2	F	174	ARG	CD-NE	-6.41	1.35	1.46
1	D	515	PHE	CB-CG	-6.35	1.40	1.51
1	A	1721	TRP	CB-CG	-6.33	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1848	TYR	CB-CG	-6.30	1.42	1.51
1	D	1124	ARG	CB-CG	-6.29	1.35	1.52
1	A	1143	GLU	CG-CD	-6.28	1.42	1.51
2	F	285	CYS	CB-SG	-6.25	1.71	1.82
1	D	776	PHE	CG-CD1	-6.21	1.29	1.38
1	D	2013	PHE	CB-CG	-6.20	1.40	1.51
1	A	763	GLU	CG-CD	-6.20	1.42	1.51
1	B	1124	ARG	CB-CG	-6.19	1.35	1.52
1	A	1121	TYR	CB-CG	-6.18	1.42	1.51
1	E	1805	TYR	CB-CG	-6.18	1.42	1.51
1	C	1634	GLU	CD-OE1	-6.17	1.18	1.25
1	A	2272	ARG	CG-CD	-6.16	1.36	1.51
1	E	1005	GLU	CD-OE1	-6.16	1.18	1.25
1	C	779	PHE	CB-CG	-6.16	1.40	1.51
1	D	359	PHE	CB-CG	-6.14	1.41	1.51
2	F	339	GLU	CG-CD	-6.13	1.42	1.51
2	F	259	TYR	CB-CG	-6.12	1.42	1.51
1	C	515	PHE	CB-CG	-6.11	1.41	1.51
2	F	779	ARG	CZ-NH1	-6.11	1.25	1.33
1	B	1848	TYR	CE2-CZ	-6.09	1.30	1.38
1	A	1568	GLU	CG-CD	-6.09	1.42	1.51
1	C	1306	TYR	CB-CG	-6.08	1.42	1.51
1	E	1268	TYR	CB-CG	-6.03	1.42	1.51
1	A	515	PHE	CB-CG	-5.99	1.41	1.51
1	A	344	GLU	CD-OE1	-5.97	1.19	1.25
1	B	515	PHE	CB-CG	-5.97	1.41	1.51
1	C	1664	TYR	CB-CG	-5.97	1.42	1.51
1	A	1595	TYR	CB-CG	-5.95	1.42	1.51
1	E	1658	GLU	CD-OE1	-5.94	1.19	1.25
1	E	1242	GLU	CD-OE1	-5.93	1.19	1.25
1	C	2272	ARG	CG-CD	-5.93	1.37	1.51
1	B	807	PHE	CG-CD1	-5.93	1.29	1.38
1	A	103	TYR	CB-CG	-5.91	1.42	1.51
1	A	1650	TYR	CG-CD1	-5.90	1.31	1.39
1	A	1342	TYR	CB-CG	-5.90	1.42	1.51
2	F	339	GLU	CD-OE2	-5.88	1.19	1.25
1	D	308	TYR	CB-CG	-5.88	1.42	1.51
1	C	968	TYR	CG-CD1	-5.88	1.31	1.39
1	A	1805	TYR	CB-CG	-5.88	1.42	1.51
1	C	1650	TYR	CG-CD1	-5.87	1.31	1.39
1	E	1795	TRP	CB-CG	-5.87	1.39	1.50
2	F	783	TYR	CB-CG	-5.86	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	996	TYR	CG-CD1	-5.82	1.31	1.39
1	E	528	TYR	CB-CG	-5.82	1.43	1.51
2	F	1406	PHE	CB-CG	-5.81	1.41	1.51
1	C	264	TYR	CB-CG	-5.81	1.43	1.51
1	D	307	GLU	CD-OE2	-5.81	1.19	1.25
1	E	1650	TYR	CD1-CE1	-5.80	1.30	1.39
2	F	771	TRP	CB-CG	-5.78	1.39	1.50
1	E	204	TYR	CB-CG	-5.77	1.43	1.51
1	C	604	GLU	CG-CD	-5.77	1.43	1.51
2	F	367	GLU	CD-OE1	-5.75	1.19	1.25
1	C	996	TYR	CG-CD1	-5.75	1.31	1.39
1	B	1322	TYR	CB-CG	-5.74	1.43	1.51
1	D	779	PHE	CB-CG	-5.73	1.41	1.51
1	C	1110	PHE	CB-CG	-5.72	1.41	1.51
1	D	1034	VAL	CB-CG2	-5.72	1.40	1.52
1	A	1650	TYR	CD1-CE1	-5.71	1.30	1.39
1	E	1527	GLU	CD-OE2	-5.71	1.19	1.25
2	F	1554	ASN	CB-CG	-5.67	1.38	1.51
1	B	1628	GLU	CD-OE2	-5.66	1.19	1.25
2	F	411	TYR	CB-CG	-5.66	1.43	1.51
1	B	968	TYR	CG-CD1	-5.64	1.31	1.39
1	C	1595	TYR	CB-CG	-5.64	1.43	1.51
1	E	730	PHE	CB-CG	-5.64	1.41	1.51
1	E	1650	TYR	CG-CD1	-5.63	1.31	1.39
1	B	730	PHE	CB-CG	-5.63	1.41	1.51
1	E	1342	TYR	CB-CG	-5.61	1.43	1.51
2	F	664	MET	CG-SD	-5.59	1.66	1.81
1	B	2099	TYR	CB-CG	-5.59	1.43	1.51
1	D	675	TYR	CB-CG	-5.58	1.43	1.51
2	F	1840	TYR	CB-CG	-5.58	1.43	1.51
1	C	344	GLU	CG-CD	-5.57	1.43	1.51
2	F	1836	TYR	CB-CG	-5.57	1.43	1.51
1	E	141	ARG	CG-CD	-5.56	1.38	1.51
1	E	1124	ARG	CB-CG	-5.56	1.37	1.52
2	F	2093	GLU	CD-OE1	-5.56	1.19	1.25
1	A	902	TYR	CD2-CE2	-5.56	1.31	1.39
1	D	904	GLU	CD-OE1	-5.54	1.19	1.25
2	F	1455	TRP	CB-CG	-5.54	1.40	1.50
1	B	264	TYR	CB-CG	-5.52	1.43	1.51
1	C	1868	TYR	CB-CG	-5.52	1.43	1.51
1	D	612	VAL	CB-CG2	-5.51	1.41	1.52
1	B	2096	PHE	CB-CG	-5.51	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	307	GLU	CD-OE2	-5.49	1.19	1.25
1	C	2356	GLU	CD-OE1	-5.49	1.19	1.25
1	E	328	TYR	CB-CG	-5.48	1.43	1.51
1	C	1848	TYR	CB-CG	-5.47	1.43	1.51
1	A	1598	TRP	CB-CG	-5.46	1.40	1.50
1	A	2393	PHE	CB-CG	-5.45	1.42	1.51
1	C	1268	TYR	CB-CG	-5.45	1.43	1.51
1	A	1034	VAL	CB-CG2	-5.45	1.41	1.52
1	C	1650	TYR	CB-CG	-5.45	1.43	1.51
1	C	1650	TYR	CD1-CE1	-5.44	1.31	1.39
2	F	256	TRP	CD2-CE3	-5.44	1.32	1.40
2	F	174	ARG	CZ-NH2	-5.43	1.25	1.33
1	C	2096	PHE	CB-CG	-5.43	1.42	1.51
2	F	396	TRP	CB-CG	-5.42	1.40	1.50
2	F	204	TYR	CB-CG	-5.41	1.43	1.51
1	C	103	TYR	CB-CG	-5.41	1.43	1.51
1	A	604	GLU	CD-OE1	-5.40	1.19	1.25
2	F	370	TYR	CD1-CE1	-5.40	1.31	1.39
1	C	1342	TYR	CB-CG	-5.38	1.43	1.51
2	F	1383	ARG	CB-CG	-5.38	1.38	1.52
1	E	1124	ARG	CD-NE	-5.37	1.37	1.46
1	B	2103	TYR	CB-CG	-5.37	1.43	1.51
1	C	1805	TYR	CB-CG	-5.37	1.43	1.51
1	A	2159	GLU	CD-OE2	-5.36	1.19	1.25
1	B	766	TYR	CB-CG	-5.35	1.43	1.51
1	B	1005	GLU	CD-OE1	-5.35	1.19	1.25
1	C	353	TYR	CE1-CZ	-5.35	1.31	1.38
1	D	858	HIS	CB-CG	-5.35	1.40	1.50
1	E	640	TRP	CB-CG	-5.34	1.40	1.50
1	E	1121	TYR	CB-CG	-5.34	1.43	1.51
2	F	873	GLU	CD-OE1	-5.34	1.19	1.25
1	A	264	TYR	CB-CG	-5.33	1.43	1.51
2	F	842	TRP	CB-CG	-5.33	1.40	1.50
1	C	353	TYR	CD1-CE1	-5.33	1.31	1.39
1	B	1110	PHE	CB-CG	-5.33	1.42	1.51
2	F	1257	GLU	CD-OE1	-5.33	1.19	1.25
1	A	1123	TRP	CB-CG	-5.32	1.40	1.50
1	D	1218	ASN	CB-CG	-5.32	1.38	1.51
1	B	996	TYR	CB-CG	-5.31	1.43	1.51
1	B	1568	GLU	CG-CD	-5.30	1.44	1.51
1	C	1124	ARG	CB-CG	-5.30	1.38	1.52
1	B	328	TYR	CB-CG	-5.30	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1372	CYS	CB-SG	-5.29	1.73	1.81
1	C	1868	TYR	CD2-CE2	-5.29	1.31	1.39
1	A	766	TYR	CG-CD1	-5.28	1.32	1.39
1	B	2332	GLU	CD-OE1	-5.28	1.19	1.25
1	C	118	TYR	CE2-CZ	-5.27	1.31	1.38
1	E	141	ARG	CD-NE	-5.27	1.37	1.46
2	F	390	PHE	CB-CG	-5.27	1.42	1.51
1	B	1853	PHE	CB-CG	-5.27	1.42	1.51
1	B	137	TYR	CB-CG	-5.26	1.43	1.51
1	D	652	PHE	CB-CG	-5.26	1.42	1.51
1	B	2452	HIS	CB-CG	-5.25	1.40	1.50
1	C	1372	CYS	CB-SG	-5.25	1.73	1.81
1	E	1017	PHE	CB-CG	-5.24	1.42	1.51
1	A	1628	GLU	CD-OE2	-5.24	1.19	1.25
1	B	187	GLU	CD-OE1	-5.24	1.19	1.25
2	F	1764	GLU	CD-OE1	-5.23	1.19	1.25
1	E	1143	GLU	CG-CD	-5.23	1.44	1.51
1	B	1017	PHE	CB-CG	-5.23	1.42	1.51
1	B	1848	TYR	CD1-CE1	-5.22	1.31	1.39
1	D	1848	TYR	CE2-CZ	-5.22	1.31	1.38
1	C	731	TRP	CZ3-CH2	-5.21	1.31	1.40
1	D	1163	TYR	CD1-CE1	-5.21	1.31	1.39
1	C	1124	ARG	CD-NE	-5.21	1.37	1.46
2	F	495	GLU	CD-OE1	-5.20	1.20	1.25
1	A	1868	TYR	CG-CD1	-5.20	1.32	1.39
1	E	2402	TYR	CB-CG	-5.20	1.43	1.51
1	E	1021	TRP	CB-CG	-5.20	1.40	1.50
1	E	1034	VAL	CB-CG2	-5.19	1.42	1.52
2	F	96	PHE	CB-CG	-5.19	1.42	1.51
2	F	687	TRP	CB-CG	-5.19	1.41	1.50
1	A	1853	PHE	CB-CG	-5.18	1.42	1.51
1	C	1017	PHE	CB-CG	-5.17	1.42	1.51
1	B	776	PHE	CG-CD2	-5.16	1.31	1.38
1	C	1143	GLU	CG-CD	-5.15	1.44	1.51
1	D	2096	PHE	CB-CG	-5.15	1.42	1.51
2	F	859	TYR	CE2-CZ	-5.15	1.31	1.38
1	B	2265	PHE	CB-CG	-5.15	1.42	1.51
1	C	2308	GLU	CD-OE2	-5.14	1.20	1.25
1	A	1650	TYR	CB-CG	-5.14	1.44	1.51
1	E	763	GLU	CG-CD	-5.14	1.44	1.51
1	A	1086	GLU	CD-OE1	-5.14	1.20	1.25
2	F	1299	TRP	CZ3-CH2	-5.14	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	390	GLU	CD-OE1	-5.13	1.20	1.25
1	E	390	GLU	CG-CD	-5.13	1.44	1.51
1	D	1805	TYR	CB-CG	-5.13	1.44	1.51
1	C	614	GLU	CD-OE2	-5.12	1.20	1.25
1	B	534	GLU	CD-OE2	-5.12	1.20	1.25
1	B	1143	GLU	CD-OE2	-5.12	1.20	1.25
1	E	2473	GLU	CG-CD	-5.12	1.44	1.51
1	D	1236	CYS	CB-SG	-5.12	1.73	1.81
2	F	228	TYR	CB-CG	-5.11	1.44	1.51
1	D	1595	TYR	CB-CG	-5.11	1.44	1.51
1	E	109	VAL	CB-CG1	-5.11	1.42	1.52
2	F	355	GLU	CD-OE2	-5.11	1.20	1.25
1	B	205	GLU	CD-OE2	-5.11	1.20	1.25
1	E	1721	TRP	CB-CG	-5.11	1.41	1.50
1	B	1658	GLU	CD-OE1	-5.10	1.20	1.25
1	C	652	PHE	CB-CG	-5.10	1.42	1.51
1	D	1628	GLU	CD-OE2	-5.10	1.20	1.25
1	E	816	GLU	CD-OE2	-5.10	1.20	1.25
1	E	1650	TYR	CB-CG	-5.10	1.44	1.51
1	D	703	SER	CB-OG	-5.09	1.35	1.42
2	F	286	ARG	CD-NE	-5.09	1.37	1.46
1	D	2308	GLU	CD-OE2	-5.09	1.20	1.25
1	C	121	GLU	CD-OE2	-5.08	1.20	1.25
1	E	1196	TYR	CB-CG	-5.07	1.44	1.51
1	C	2435	TYR	CB-CG	-5.07	1.44	1.51
1	A	766	TYR	CD1-CE1	-5.06	1.31	1.39
1	C	875	ASN	CB-CG	-5.06	1.39	1.51
1	C	2280	TYR	CB-CG	-5.06	1.44	1.51
1	C	996	TYR	CG-CD2	-5.05	1.32	1.39
1	A	205	GLU	CD-OE2	-5.05	1.20	1.25
1	B	528	TYR	CB-CG	-5.05	1.44	1.51
1	D	695	TYR	CB-CG	-5.05	1.44	1.51
1	A	730	PHE	CB-CG	-5.04	1.42	1.51
1	B	1805	TYR	CD1-CE1	-5.04	1.31	1.39
1	A	1163	TYR	CG-CD1	-5.04	1.32	1.39
1	A	2096	PHE	CB-CG	-5.04	1.42	1.51
1	D	328	TYR	CB-CG	-5.04	1.44	1.51
1	B	1086	GLU	CD-OE1	-5.04	1.20	1.25
1	C	1163	TYR	CD1-CE1	-5.04	1.31	1.39
1	C	915	TRP	CB-CG	-5.03	1.41	1.50
2	F	174	ARG	CB-CG	-5.03	1.39	1.52
1	C	328	TYR	CB-CG	-5.03	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	193	ARG	CG-CD	-5.03	1.39	1.51
1	D	1765	SER	CA-CB	-5.02	1.45	1.52
1	E	1598	TRP	CB-CG	-5.01	1.41	1.50
2	F	887	TYR	CB-CG	-5.01	1.44	1.51
1	B	1042	GLU	CD-OE2	-5.01	1.20	1.25
2	F	495	GLU	CD-OE2	-5.01	1.20	1.25
1	A	2308	GLU	CD-OE2	-5.01	1.20	1.25
1	D	118	TYR	CE2-CZ	-5.01	1.32	1.38

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	ARG	NE-CZ-NH2	-12.65	113.97	120.30
1	E	1616	ARG	NE-CZ-NH2	-11.43	114.59	120.30
2	F	286	ARG	NE-CZ-NH1	-11.17	114.72	120.30
2	F	1585	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	E	2018	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	C	1616	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	B	1869	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	C	517	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	D	547	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	C	2018	ARG	NE-CZ-NH2	-9.68	115.46	120.30
2	F	174	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	F	2117	ARG	NE-CZ-NH1	-9.53	115.53	120.30
2	F	424	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	2018	ARG	NE-CZ-NH2	-9.33	115.63	120.30
2	F	1585	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	C	353	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	A	2018	ARG	NE-CZ-NH2	-9.10	115.75	120.30
2	F	871	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	E	1124	ARG	NE-CZ-NH2	-8.99	115.81	120.30
1	C	1124	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	E	2216	ARG	NE-CZ-NH2	-8.93	115.84	120.30
2	F	174	ARG	NE-CZ-NH1	8.89	124.74	120.30
1	B	1124	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	1650	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	E	1650	TYR	CB-CG-CD1	-8.78	115.73	121.00
1	C	1204	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	E	1305	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	D	1166	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	1322	TYR	CB-CG-CD1	-8.48	115.91	121.00
2	F	1044	ARG	NE-CZ-NH2	-8.47	116.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1650	TYR	CB-CG-CD1	-8.47	115.92	121.00
1	E	547	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	E	1159	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	2410	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	1159	ARG	NE-CZ-NH2	-8.33	116.14	120.30
1	D	487	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	C	1650	TYR	CB-CG-CD1	-8.27	116.04	121.00
2	F	302	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	807	PHE	CB-CG-CD2	8.20	126.54	120.80
1	E	1563	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	D	2512	ARG	NE-CZ-NH2	-8.13	116.23	120.30
1	E	1601	TYR	CB-CG-CD2	-7.97	116.22	121.00
1	A	1611	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	1563	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	A	1868	TYR	CB-CG-CD1	-7.95	116.23	121.00
1	B	137	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	D	1124	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	B	1794	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	E	942	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	2512	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	C	807	PHE	CB-CG-CD1	-7.82	115.32	120.80
2	F	131	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	C	2410	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	448	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	B	942	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	C	1611	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	B	1611	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	D	1794	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	2512	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	D	208	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	D	1611	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	1369	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	A	942	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	2216	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	B	2216	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	F	1383	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	766	TYR	CB-CG-CD1	-7.42	116.55	121.00
2	F	1411	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	E	2216	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	E	1868	TYR	CB-CG-CD1	-7.36	116.58	121.00
2	F	1436	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	E	1050	ARG	NE-CZ-NH1	7.30	123.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	C	1040	TYR	CB-CG-CD1	-7.24	116.65	121.00
1	B	1305	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	D	1168	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	B	1305	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	B	1166	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	2410	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	1650	TYR	CB-CG-CD1	-7.05	116.77	121.00
2	F	49	ARG	NE-CZ-NH1	7.04	123.82	120.30
2	F	2051	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	A	528	TYR	CB-CG-CD1	-7.01	116.79	121.00
1	C	1168	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	E	1305	ARG	NE-CZ-NH2	-6.97	116.82	120.30
2	F	917	ARG	NE-CZ-NH2	-6.97	116.82	120.30
1	B	1868	TYR	CB-CG-CD1	-6.94	116.83	121.00
1	B	1050	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	C	2512	ARG	NE-CZ-NH2	-6.87	116.87	120.30
2	F	1139	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	B	1601	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	1204	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	E	1286	TYR	CB-CG-CD2	-6.81	116.91	121.00
2	F	800	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	E	1072	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	1369	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	2216	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	F	625	TYR	CB-CG-CD1	-6.67	117.00	121.00
1	B	1287	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	1601	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	E	806	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	434	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	E	1711	PHE	CB-CG-CD2	6.55	125.38	120.80
2	F	2114	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	B	1040	TYR	CB-CG-CD1	-6.47	117.11	121.00
2	F	49	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	F	1001	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	C	2399	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	F	1383	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	E	1982	TYR	CB-CG-CD1	-6.41	117.15	121.00
1	E	204	TYR	CB-CG-CD2	-6.41	117.16	121.00
2	F	1205	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	E	1168	TYR	CB-CG-CD2	-6.39	117.17	121.00
1	C	1794	ARG	NE-CZ-NH2	-6.37	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	332	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	1982	TYR	CB-CG-CD1	-6.35	117.19	121.00
1	D	2512	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	F	768	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	1287	ARG	NE-CZ-NH2	-6.32	117.14	120.30
2	F	196	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	517	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	E	448	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	D	1616	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	208	ARG	NE-CZ-NH2	-6.28	117.16	120.30
2	F	859	TYR	CB-CG-CD2	-6.27	117.24	121.00
2	F	1167	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	F	976	TYR	CB-CG-CD1	-6.26	117.24	121.00
2	F	2051	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	999	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	1148	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	2266	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	D	354	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	2411	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	208	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	D	2428	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	2512	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	484	TYR	CB-CG-CD1	-6.19	117.29	121.00
2	F	131	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	1050	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	E	1358	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	1050	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	C	2512	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	1711	PHE	CB-CG-CD2	6.13	125.09	120.80
2	F	1848	ARG	NE-CZ-NH2	6.11	123.36	120.30
2	F	1367	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	2411	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	1306	TYR	CB-CG-CD2	-6.08	117.35	121.00
2	F	332	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	F	2125	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	F	1789	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	519	PHE	CB-CG-CD2	6.06	125.04	120.80
1	E	488	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	C	1166	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	2018	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	1159	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	1166	ARG	NE-CZ-NH1	5.99	123.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1412	TYR	CB-CG-CD1	-5.99	117.41	121.00
1	A	1711	PHE	CB-CG-CD2	5.98	124.99	120.80
2	F	1790	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	1369	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	1204	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	103	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	A	332	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	1711	PHE	CB-CG-CD1	-5.95	116.63	120.80
2	F	1318	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	1883	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	C	1305	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	1072	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	2118	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	1305	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	1986	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	C	421	TYR	CB-CG-CD1	-5.89	117.47	121.00
2	F	1790	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	2324	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	412	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	2411	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	412	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	2216	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	E	547	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	F	921	TYR	CB-CG-CD2	-5.68	117.59	121.00
1	A	1024	TYR	CB-CG-CD2	-5.67	117.60	121.00
2	F	259	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	B	890	ALA	C-N-CD	-5.65	108.17	120.60
2	F	754	GLU	N-CA-C	-5.64	95.77	111.00
1	A	555	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	C	942	ARG	NE-CZ-NH2	-5.63	117.49	120.30
2	F	713	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	F	1115	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	2266	TYR	CB-CG-CD2	-5.60	117.64	121.00
2	F	1044	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	1168	TYR	CB-CG-CD2	-5.59	117.65	121.00
2	F	906	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	C	1194	TYR	CB-CG-CD2	-5.57	117.66	121.00
1	D	2266	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	C	1072	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	E	1124	ARG	CB-CA-C	-5.55	99.30	110.40
1	A	1982	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	C	1027	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2217	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	F	2112	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	2324	ARG	NE-CZ-NH1	5.52	123.06	120.30
2	F	1972	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	A	136	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	353	TYR	CB-CG-CD2	5.50	124.30	121.00
1	C	1124	ARG	CB-CA-C	-5.50	99.39	110.40
1	E	2217	ARG	NE-CZ-NH2	-5.49	117.56	120.30
2	F	94	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	2512	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	E	1024	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	B	2266	TYR	CB-CG-CD2	-5.46	117.73	121.00
1	E	412	ARG	NE-CZ-NH2	-5.45	117.57	120.30
2	F	267	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	448	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	F	2100	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	D	2399	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	2217	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	672	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	825	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	B	2411	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	902	TYR	CB-CG-CD2	-5.40	117.76	121.00
1	C	1050	ARG	NE-CZ-NH1	-5.40	117.60	120.30
2	F	1848	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	C	2399	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	807	PHE	CB-CG-CD2	5.38	124.56	120.80
1	B	779	PHE	CB-CA-C	-5.38	99.65	110.40
1	A	208	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	2217	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	1272	ASP	N-CA-C	-5.37	96.51	111.00
1	D	2217	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	F	51	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	F	1425	TYR	CB-CG-CD1	-5.34	117.79	121.00
2	F	2033	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	2513	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	A	2411	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	E	2266	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	B	1711	PHE	CB-CG-CD2	5.33	124.53	120.80
1	E	2428	ASP	CB-CG-OD1	5.32	123.09	118.30
2	F	1318	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	1168	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	2005	GLY	N-CA-C	-5.30	99.85	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1040	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	354	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	E	2095	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	1286	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	C	890	ALA	C-N-CD	-5.28	108.99	120.60
1	D	1305	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	A	1040	TYR	CB-CG-CD1	-5.27	117.84	121.00
1	C	2018	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	C	308	TYR	CB-CG-CD1	-5.26	117.85	121.00
2	F	2089	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	2095	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	A	2006	GLY	N-CA-C	-5.24	100.00	113.10
1	C	1664	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	E	996	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	E	412	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	F	300	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	675	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	D	952	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	E	1072	ASP	CB-CG-OD2	-5.20	113.62	118.30
2	F	419	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	D	412	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	890	ALA	C-N-CD	-5.19	109.18	120.60
2	F	370	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	1604	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	391	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	D	1040	TYR	CB-CG-CD1	-5.16	117.90	121.00
1	B	2018	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	1124	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	F	765	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	1814	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	C	1616	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	1711	PHE	CB-CG-CD1	-5.13	117.21	120.80
1	D	1305	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	1204	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	2399	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	334	TYR	CB-CG-CD2	-5.10	117.94	121.00
2	F	1488	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	E	2399	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	1027	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	434	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	D	1794	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	F	1449	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1650	TYR	CB-CG-CD2	5.06	124.04	121.00
2	F	688	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	E	1616	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	2153	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	F	286	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	359	PHE	CB-CG-CD1	5.03	124.32	120.80
1	B	2399	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	1286	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	E	332	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	F	987	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	F	1329	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	1664	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	D	376	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	528	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	B	603	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	1196	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	C	1711	PHE	CB-CG-CD1	-5.01	117.29	120.80
1	D	137	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	E	487	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	B	1805	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	C	1604	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	766	TYR	Sidechain

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	38	0
1	B	18197	0	17794	47	0
1	C	18197	0	17794	45	0
1	D	18197	0	17794	38	0
1	E	18197	0	17794	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	17285	0	16668	43	0
All	All	108270	0	105638	240	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 1.

All (240) 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:B:1623:THR:OG1	1:B:1624:ILE:N	2.32	0.61
1:E:1774:TYR:HH	1:E:1848:TYR:HH	1.47	0.60
1:B:2319:ASP:OD2	1:B:2323:LYS:NZ	2.36	0.58
1:B:2358:ASP:OD1	1:B:2502:LYS:NZ	2.38	0.57
2:F:1416:ASP:OD1	2:F:1416:ASP:N	2.37	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:D:1148:ASP:N	1:D:1148:ASP:OD1	2.33	0.56
1:A:2207:ASP:OD2	1:A:2211:LYS:NZ	2.38	0.56
1:D:624:ASP:N	1:D:624:ASP:OD1	2.37	0.56
1:C:329:ARG:NH1	1:C:434:TYR:OH	2.39	0.56
1:C:2207:ASP:OD2	1:C:2211:LYS:NZ	2.38	0.56
1:B:624:ASP:N	1:B:624:ASP:OD1	2.37	0.56
1:B:1072:ASP:OD1	1:B:1072:ASP:N	2.36	0.56
1:D:253:GLU:O	1:D:442:LYS:NZ	2.38	0.56
2:F:73:ASP:OD1	2:F:74:CYS:N	2.39	0.56
1:A:2319:ASP:OD2	1:A:2323:LYS:NZ	2.39	0.56
1:B:1626:SER:OG	1:B:1627:MET:N	2.40	0.55
1:A:2358:ASP:OD1	1:A:2502:LYS:NZ	2.39	0.55
1:A:624:ASP:OD1	1:A:624:ASP:N	2.38	0.55
1:B:1774:TYR:OH	1:B:1848:TYR:OH	2.24	0.54
2:F:385:ASP:OD1	2:F:385:ASP:N	2.39	0.54
2:F:829:ASP:OD1	2:F:829:ASP:N	2.39	0.54
1:B:2257:ARG:NH2	1:C:2309:THR:OG1	2.40	0.54
1:D:890:ALA:O	1:D:892:GLN:N	2.42	0.53
1:A:1225:LYS:NZ	1:A:1226:LEU:O	2.40	0.53
1:D:2257:ARG:NH2	1:E:2309:THR:OG1	2.42	0.53
1:E:2358:ASP:OD1	1:E:2502:LYS:NZ	2.42	0.52
1:C:890:ALA:O	1:C:892:GLN:N	2.41	0.52
1:E:548:LYS:NZ	1:E:559:ASP:OD1	2.42	0.52
1:E:890:ALA:O	1:E:892:GLN:N	2.42	0.52
1:B:1774:TYR:HH	1:B:1848:TYR:HH	1.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:ALA:O	1:B:892:GLN:N	2.42	0.52
1:A:1120:GLU:OE2	1:A:1146:LYS:NZ	2.42	0.52
1:D:1683:ASP:OD1	1:D:1683:ASP:N	2.43	0.52
1:D:301:SER:OG	1:D:302:ASN:N	2.42	0.51
2:F:179:SER:OG	2:F:180:GLN:N	2.43	0.51
1:A:1164:LYS:NZ	1:B:1622:ASP:OD2	2.36	0.51
1:C:540:SER:OG	1:C:541:GLY:N	2.44	0.51
1:C:1291:TYR:O	1:C:1292:GLN:HB3	2.11	0.51
1:A:261:GLU:OE1	1:A:1380:LYS:NZ	2.44	0.50
1:D:2319:ASP:OD2	1:D:2323:LYS:NZ	2.45	0.50
1:E:1841:ALA:O	1:E:1842:GLN:HB2	2.11	0.50
1:D:797:ASP:OD1	1:D:798:ALA:N	2.45	0.50
1:D:848:GLN:HE21	1:D:852:GLN:HE21	1.60	0.50
1:A:890:ALA:O	1:A:892:GLN:N	2.45	0.50
1:B:540:SER:OG	1:B:541:GLY:N	2.44	0.50
1:B:1683:ASP:N	1:B:1683:ASP:OD1	2.43	0.50
2:F:754:GLU:O	2:F:755:ILE:HB	2.12	0.50
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.45	0.50
1:B:342:ASP:OD2	1:B:360:LYS:NZ	2.44	0.49
2:F:616:ASP:N	2:F:616:ASP:OD1	2.45	0.49
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.45	0.49
1:A:180:GLU:OE1	1:A:184:LYS:NZ	2.45	0.49
1:C:301:SER:OG	1:C:302:ASN:N	2.46	0.49
1:E:161:THR:O	1:E:162:LEU:HB3	2.13	0.49
1:D:2466:ASP:N	1:D:2466:ASP:OD1	2.46	0.48
1:E:176:GLU:OE2	1:E:956:LYS:NZ	2.47	0.48
1:E:2287:ASP:N	1:E:2287:ASP:OD1	2.45	0.48
2:F:1687:ASP:N	2:F:1687:ASP:OD1	2.38	0.48
1:E:2466:ASP:N	1:E:2466:ASP:OD1	2.46	0.48
2:F:153:ASP:O	2:F:174:ARG:NH2	2.46	0.48
2:F:1234:SER:OG	2:F:1235:ASP:N	2.46	0.48
1:C:1841:ALA:O	1:C:1842:GLN:HB2	2.14	0.48
1:D:521:THR:H	1:D:522:PRO:HD2	1.79	0.48
1:D:1333:TYR:CG	1:D:1334:ASN:N	2.82	0.48
1:B:2380:GLY:N	1:B:2383:THR:OG1	2.46	0.48
1:A:1774:TYR:OH	1:A:1848:TYR:OH	2.28	0.48
1:B:1841:ALA:O	1:B:1842:GLN:HB2	2.14	0.48
2:F:161:ASP:N	2:F:161:ASP:OD1	2.42	0.48
1:A:1561:ASP:OD1	1:A:1561:ASP:N	2.46	0.47
1:A:1834:SER:OG	1:A:1835:VAL:N	2.47	0.47
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1178:THR:OG1	1:B:1179:LYS:N	2.47	0.47
1:C:1178:THR:OG1	1:C:1179:LYS:N	2.46	0.47
1:B:1514:ASP:N	1:B:1514:ASP:OD1	2.46	0.47
1:D:1841:ALA:O	1:D:1842:GLN:HB2	2.13	0.47
1:B:1834:SER:OG	1:B:1835:VAL:N	2.46	0.47
1:E:1991:ASP:OD2	1:E:1993:LYS:NZ	2.45	0.47
1:A:1343:LYS:NZ	1:B:1803:SER:O	2.47	0.47
1:B:1975:SER:OG	1:B:1976:ILE:N	2.48	0.47
2:F:830:GLN:O	2:F:955:ARG:NH2	2.47	0.47
1:B:2103:TYR:O	1:B:2189:ARG:NH1	2.48	0.47
1:B:2284:LEU:O	1:B:2286:ASP:N	2.48	0.47
1:C:1333:TYR:CG	1:C:1334:ASN:N	2.82	0.47
1:E:540:SER:OG	1:E:541:GLY:N	2.47	0.47
1:E:1124:ARG:HD3	1:E:1144:TRP:CD2	2.50	0.47
2:F:431:ASP:OD1	2:F:431:ASP:N	2.44	0.47
1:B:533:ASP:OD1	1:B:533:ASP:N	2.37	0.47
1:C:872:THR:O	1:C:873:SER:HB2	2.15	0.47
1:B:477:LYS:NZ	1:B:624:ASP:OD2	2.40	0.46
1:D:290:ASP:OD1	1:D:290:ASP:N	2.43	0.46
1:E:1840:VAL:C	1:E:1841:ALA:O	2.52	0.46
1:A:2103:TYR:O	1:A:2189:ARG:NH1	2.49	0.46
1:C:1206:ASP:N	1:C:1206:ASP:OD1	2.42	0.46
1:E:270:ASN:OD1	1:E:270:ASN:N	2.46	0.46
2:F:1793:ASP:N	2:F:1793:ASP:OD1	2.47	0.46
1:A:1133:ASP:OD1	1:A:1133:ASP:N	2.40	0.46
1:C:270:ASN:OD1	1:C:270:ASN:N	2.48	0.46
1:D:1834:SER:OG	1:D:1835:VAL:N	2.49	0.46
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.46	0.46
1:B:1183:ASN:OD1	1:B:1183:ASN:N	2.44	0.46
1:C:1975:SER:OG	1:C:1976:ILE:N	2.47	0.46
1:C:1290:SER:C	1:C:1291:TYR:O	2.49	0.46
1:D:161:THR:O	1:D:162:LEU:HB3	2.16	0.46
2:F:1329:ASP:N	2:F:1329:ASP:OD1	2.43	0.46
1:B:1333:TYR:O	1:B:1334:ASN:C	2.54	0.46
1:D:342:ASP:OD2	1:D:360:LYS:NZ	2.46	0.46
1:D:2008:LYS:NZ	1:D:2267:ASP:OD2	2.43	0.46
1:E:2103:TYR:O	1:E:2189:ARG:NH1	2.49	0.45
2:F:1055:THR:OG1	2:F:1056:ASP:N	2.49	0.45
1:C:176:GLU:OE2	1:C:956:LYS:NZ	2.48	0.45
1:A:1683:ASP:N	1:A:1683:ASP:OD1	2.43	0.45
1:E:1046:ASP:OD1	1:E:1046:ASP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:TYR:CZ	1:B:391:TYR:HB2	2.52	0.45
1:C:1829:SER:OG	1:C:1830:ASP:N	2.50	0.45
1:C:1977:ASP:N	1:C:1977:ASP:OD1	2.45	0.45
1:A:842:ASP:OD1	1:A:843:ALA:N	2.50	0.45
1:C:1834:SER:OG	1:C:1835:VAL:N	2.50	0.45
1:C:1124:ARG:HD3	1:C:1144:TRP:CD2	2.52	0.45
1:C:2103:TYR:O	1:C:2189:ARG:NH1	2.50	0.45
1:D:766:TYR:CD1	1:D:771:ILE:HD11	2.52	0.45
1:E:1834:SER:OG	1:E:1835:VAL:N	2.50	0.45
1:D:329:ARG:HB3	1:D:431:TYR:CE1	2.53	0.44
1:B:250:ILE:O	1:B:442:LYS:NZ	2.50	0.44
1:D:2284:LEU:O	1:D:2286:ASP:N	2.50	0.44
2:F:754:GLU:O	2:F:755:ILE:CB	2.65	0.44
1:A:161:THR:O	1:A:162:LEU:HB3	2.17	0.44
1:E:533:ASP:OD1	1:E:533:ASP:N	2.48	0.44
1:B:1343:LYS:NZ	1:C:1803:SER:O	2.50	0.44
1:C:2457:SER:OG	1:C:2458:GLY:N	2.50	0.44
1:C:2466:ASP:N	1:C:2466:ASP:OD1	2.45	0.44
1:D:1975:SER:OG	1:D:1976:ILE:N	2.50	0.44
1:D:2365:SER:OG	1:D:2366:GLY:N	2.50	0.44
1:E:963:SER:OG	1:E:964:ARG:N	2.48	0.44
1:C:336:THR:OG1	1:C:337:ASN:N	2.49	0.44
2:F:1427:ASP:OD1	2:F:1427:ASP:C	2.55	0.44
1:A:1622:ASP:OD2	1:E:1164:LYS:NZ	2.35	0.44
1:B:963:SER:OG	1:B:964:ARG:N	2.50	0.44
1:D:439:LYS:NZ	1:D:458:GLU:OE2	2.41	0.44
2:F:904:SER:O	2:F:905:ARG:C	2.56	0.44
1:A:537:ASP:OD1	1:A:538:LEU:N	2.51	0.44
1:B:2466:ASP:OD1	1:B:2466:ASP:N	2.47	0.44
1:E:2365:SER:OG	1:E:2366:GLY:N	2.51	0.44
1:C:1683:ASP:OD1	1:C:1683:ASP:N	2.43	0.44
1:D:963:SER:OG	1:D:964:ARG:N	2.49	0.44
2:F:618:SER:OG	2:F:619:GLY:N	2.50	0.44
2:F:1591:THR:OG1	2:F:1592:ALA:N	2.51	0.44
1:A:2466:ASP:N	1:A:2466:ASP:OD1	2.50	0.43
2:F:530:ASP:N	2:F:530:ASP:OD1	2.51	0.43
2:F:209:ASP:OD1	2:F:209:ASP:N	2.46	0.43
2:F:1912:ASN:O	2:F:2125:ARG:NH2	2.51	0.43
1:D:1257:ASP:N	1:D:1257:ASP:OD1	2.46	0.43
1:A:534:GLU:OE1	1:A:534:GLU:N	2.52	0.43
1:C:1662:LYS:NZ	1:C:1830:ASP:OD2	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:ALA:HB3	1:D:694:PRO:HD3	2.01	0.43
1:E:1507:LYS:NZ	1:E:1538:ASP:OD2	2.41	0.43
2:F:253:GLN:O	2:F:259:TYR:OH	2.36	0.43
1:A:1183:ASN:OD1	1:A:1183:ASN:N	2.50	0.43
1:C:1507:LYS:NZ	1:C:1538:ASP:OD2	2.39	0.43
1:B:1138:ALA:HB3	1:B:1842:GLN:OE1	2.19	0.43
1:E:975:ASN:N	1:E:975:ASN:OD1	2.42	0.43
1:E:1183:ASN:OD1	1:E:1183:ASN:N	2.48	0.43
1:A:2347:ASP:OD1	1:A:2347:ASP:N	2.47	0.42
1:D:1291:TYR:O	1:D:1292:GLN:HB2	2.19	0.42
2:F:1370:ASP:N	2:F:1370:ASP:OD1	2.48	0.42
2:F:2090:ASN:OD1	2:F:2091:GLN:N	2.52	0.42
1:A:1524:SER:OG	1:A:1525:PHE:N	2.51	0.42
1:C:1561:ASP:N	1:C:1561:ASP:OD1	2.48	0.42
1:E:329:ARG:HB3	1:E:431:TYR:CE1	2.54	0.42
1:C:1137:ALA:O	1:C:1138:ALA:HB3	2.19	0.42
1:E:2284:LEU:O	1:E:2286:ASP:N	2.52	0.42
1:C:196:GLY:N	1:C:285:TYR:OH	2.52	0.42
1:B:1729:ASP:OD2	1:B:1730:LYS:NZ	2.52	0.42
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.52	0.42
1:C:1291:TYR:O	1:C:1292:GLN:CB	2.65	0.42
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.54	0.42
1:E:1774:TYR:OH	1:E:1848:TYR:OH	2.21	0.42
1:A:176:GLU:OE2	1:A:956:LYS:NZ	2.50	0.42
1:E:771:ILE:HD12	1:E:776:PHE:HA	2.00	0.42
1:B:1333:TYR:O	1:B:1335:GLY:N	2.53	0.42
1:C:353:TYR:CE1	1:C:397:LEU:HB2	2.54	0.42
1:E:386:GLN:OE1	1:E:391:TYR:OH	2.38	0.42
1:C:477:LYS:NZ	1:C:624:ASP:OD2	2.39	0.42
1:C:2496:LYS:NZ	1:D:2401:ASP:OD1	2.49	0.42
1:D:773:GLU:HA	1:D:776:PHE:CD1	2.55	0.42
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.46	0.42
2:F:2117:ARG:NH1	2:F:2140:LEU:O	2.53	0.42
1:A:2382:ASP:OD1	1:A:2382:ASP:N	2.47	0.42
1:B:93:ASN:OD1	1:B:93:ASN:N	2.47	0.42
1:C:1908:ASP:N	1:C:1908:ASP:OD1	2.52	0.42
1:A:488:TYR:OH	1:A:635:ASN:OD1	2.36	0.41
1:B:1124:ARG:HD2	1:B:1144:TRP:CD2	2.55	0.41
1:A:1991:ASP:OD2	1:A:1993:LYS:NZ	2.47	0.41
1:D:1977:ASP:N	1:D:1977:ASP:OD1	2.44	0.41
1:E:857:GLN:CD	1:E:857:GLN:N	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2358:ASP:OD1	1:C:2502:LYS:NZ	2.49	0.41
1:B:2382:ASP:OD1	1:B:2382:ASP:N	2.51	0.41
1:B:455:THR:OG1	1:B:456:ILE:N	2.53	0.41
1:B:1124:ARG:HG3	1:B:1144:TRP:CE3	2.55	0.41
1:C:856:HIS:NE2	1:C:895:SER:OG	2.54	0.41
1:E:299:LYS:NZ	1:E:458:GLU:OE2	2.53	0.41
1:A:1333:TYR:O	1:A:1334:ASN:C	2.58	0.41
1:A:1684:THR:OG1	1:A:1685:ASN:N	2.54	0.41
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.53	0.41
1:D:1840:VAL:C	1:D:1841:ALA:O	2.56	0.41
1:A:2365:SER:OG	1:A:2366:GLY:N	2.53	0.41
1:B:736:THR:OG1	1:B:737:LYS:N	2.50	0.41
1:D:782:LYS:N	1:D:783:PRO:HD3	2.36	0.41
2:F:772:ASP:OD1	2:F:779:ARG:NE	2.53	0.41
2:F:574:SER:OG	2:F:575:ALA:N	2.54	0.41
1:A:2103:TYR:CE1	1:A:2193:GLU:HB2	2.55	0.41
1:B:2382:ASP:OD2	1:C:2404:ALA:N	2.54	0.41
1:B:2478:ASP:OD1	1:B:2478:ASP:N	2.40	0.41
1:D:322:ASP:OD1	1:D:322:ASP:N	2.32	0.41
1:D:707:VAL:HG13	1:D:776:PHE:CD2	2.55	0.41
2:F:1484:ASP:OD2	2:F:1486:LYS:NZ	2.37	0.41
1:B:831:THR:OG1	1:B:832:ALA:N	2.54	0.41
2:F:1268:PHE:O	2:F:1272:ALA:N	2.55	0.41
2:F:1515:ASN:N	2:F:1515:ASN:OD1	2.46	0.41
2:F:2044:ASP:OD1	2:F:2044:ASP:N	2.45	0.41
1:A:465:ASN:O	1:A:466:LEU:C	2.58	0.40
1:C:1497:LYS:HB3	1:C:1558:PHE:HB2	2.02	0.40
2:F:1247:PRO:HA	2:F:1332:ASP:OD1	2.21	0.40
1:C:2287:ASP:N	1:C:2287:ASP:OD1	2.45	0.40
1:B:2459:GLN:OE1	1:B:2459:GLN:N	2.53	0.40
1:C:542:SER:OG	1:C:543:THR:N	2.49	0.40
2:F:269:ASN:OD1	2:F:269:ASN:N	2.47	0.40
2:F:283:TRP:CZ3	2:F:303:ARG:HB3	2.56	0.40
2:F:1393:ASP:OD1	2:F:1393:ASP:N	2.49	0.40
1:A:2466:ASP:OD1	1:A:2467:GLY:N	2.55	0.40
1:C:322:ASP:OD1	1:C:323:GLY:N	2.54	0.40
1:E:1153:PRO:O	1:E:1154:TYR:C	2.60	0.40
1:E:1559:ALA:HB3	1:E:1563:ARG:HG2	2.04	0.40
2:F:6:ASP:OD1	2:F:6:ASP:N	2.44	0.40
2:F:1329:ASP:OD1	2:F:1330:ARG:N	2.54	0.40
1:A:545:ASP:C	1:A:545:ASP:OD1	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ALA:HB3	1:A:694:PRO:HD3	2.03	0.40
1:E:137:TYR:CE2	1:E:139:ASP:HB2	2.57	0.40
2:F:841:THR:OG1	2:F:842:TRP:N	2.53	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%)	2240 (98%)	40 (2%)	6 (0%)	41	72
1	B	2286/2516 (91%)	2225 (97%)	54 (2%)	7 (0%)	41	72
1	C	2286/2516 (91%)	2225 (97%)	56 (2%)	5 (0%)	47	78
1	D	2286/2516 (91%)	2233 (98%)	46 (2%)	7 (0%)	41	72
1	E	2286/2516 (91%)	2239 (98%)	39 (2%)	8 (0%)	41	72
2	F	2162/2439 (89%)	2111 (98%)	46 (2%)	5 (0%)	47	78
All	All	13592/15019 (90%)	13273 (98%)	281 (2%)	38 (0%)	44	72

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	891	PRO
1	B	891	PRO
1	C	891	PRO
1	D	891	PRO
1	E	790	THR
1	E	891	PRO
1	A	991	ALA
1	A	1334	ASN
1	B	1138	ALA

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Mol	Chain	Res	Type
1	B	1334	ASN
1	C	991	ALA
1	C	1334	ASN
1	D	991	ALA
1	D	1138	ALA
1	E	991	ALA
1	E	1154	TYR
2	F	755	ILE
1	D	1292	GLN
2	F	137	HIS
2	F	602	ALA
1	B	1190	THR
1	C	1758	MET
1	E	659	TYR
1	A	890	ALA
1	A	1758	MET
1	A	1953	ASN
1	B	101	SER
1	B	2425	PRO
1	D	890	ALA
1	E	1953	ASN
2	F	530	ASP
1	B	745	ALA
1	C	350	GLY
1	D	1758	MET
1	D	1953	ASN
1	E	304	GLY
2	F	2115	GLY
1	E	890	ALA

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%)	1960 (100%)	0	100 100
1	B	1960/2157 (91%)	1959 (100%)	1 (0%)	93 98

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1960/2157 (91%)	1960 (100%)	0	100	100
1	D	1960/2157 (91%)	1957 (100%)	3 (0%)	93	98
1	E	1960/2157 (91%)	1959 (100%)	1 (0%)	93	98
2	F	1872/2108 (89%)	1871 (100%)	1 (0%)	93	98
All	All	11672/12893 (90%)	11666 (100%)	6 (0%)	93	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	211	ILE
1	D	661	LYS
1	D	968	TYR
1	D	1169	LEU
1	E	1169	LEU
2	F	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	587	ASN
1	B	679	GLN
1	C	1671	ASN
1	D	848	GLN
1	D	1951	GLN
1	E	854	GLN
1	E	1362	ASN
1	E	1599	GLN
1	E	1951	GLN
2	F	450	ASN
2	F	1546	GLN
2	F	1650	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

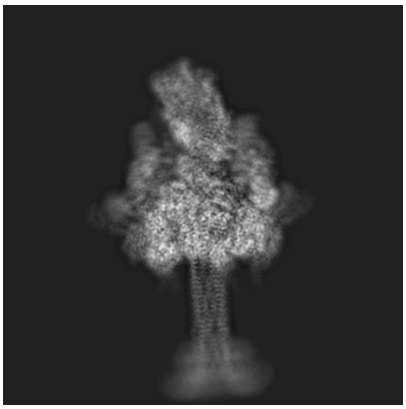
6 Map visualisation (i)

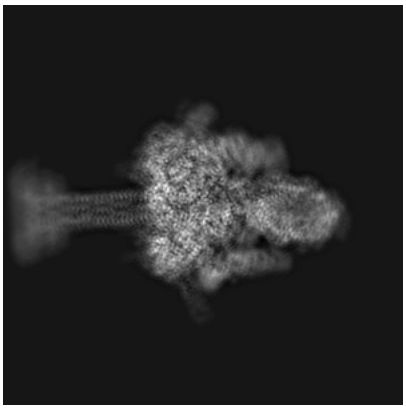
This section contains visualisations of the EMDB entry EMD-10312. These allow visual inspection of the internal detail of the map and identification of artifacts.

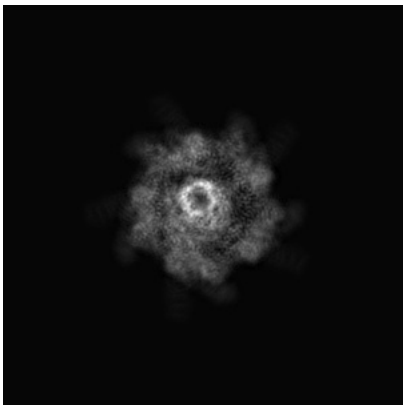
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

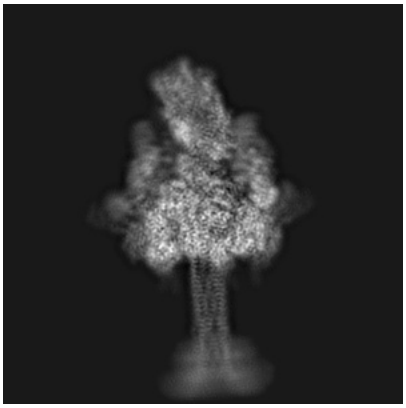
6.1.1 Primary map

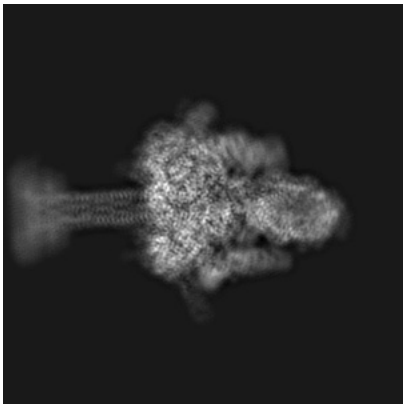

X

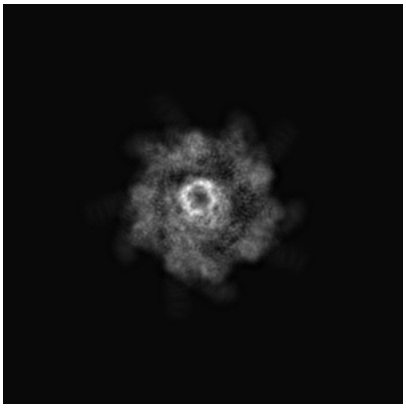

Y


Z

6.1.2 Raw map


X

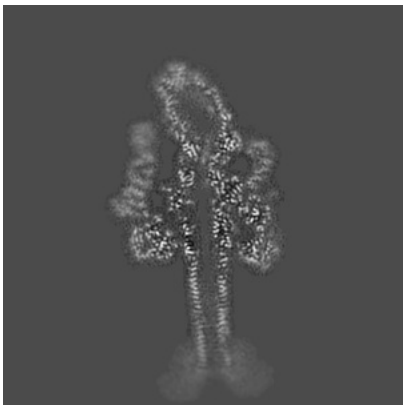

Y

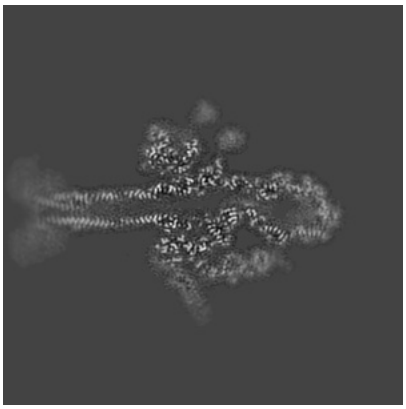

Z

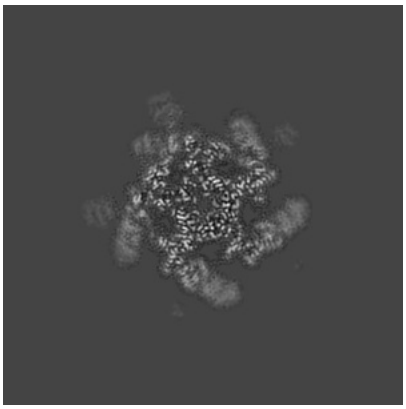
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

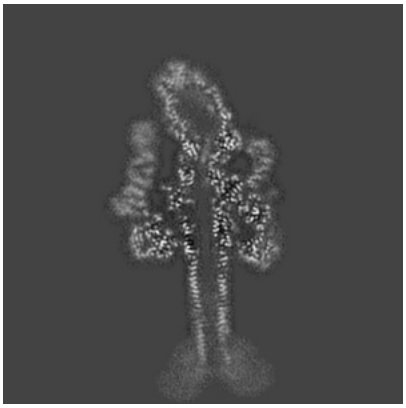
6.2.1 Primary map

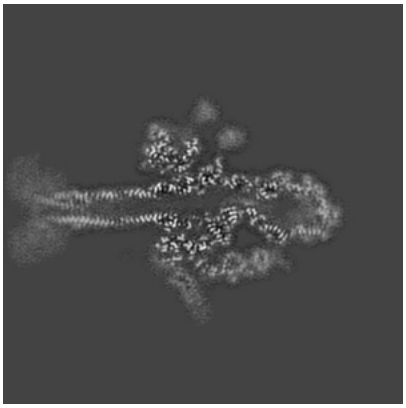

X Index: 192

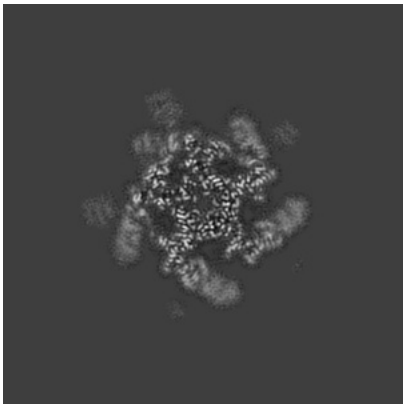

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

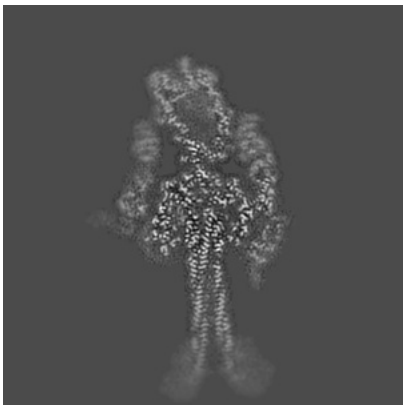

Y Index: 192


Z Index: 192

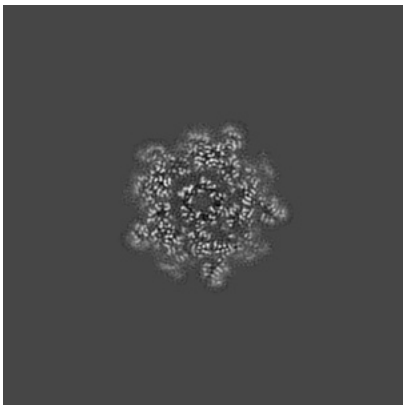
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

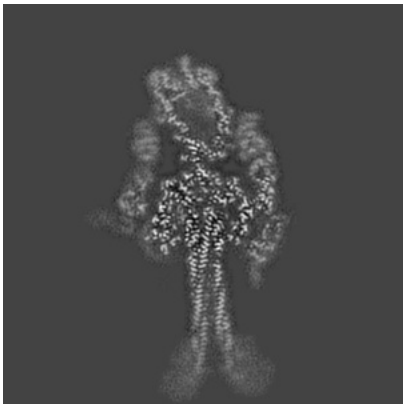
6.3.1 Primary map

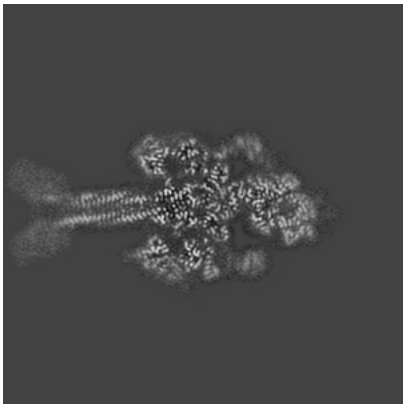

X Index: 179

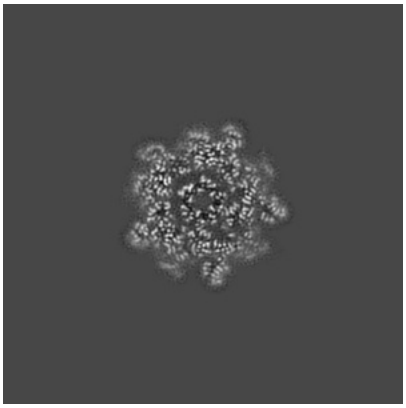
Y Index: 207


Z Index: 153

6.3.2 Raw map


X Index: 179

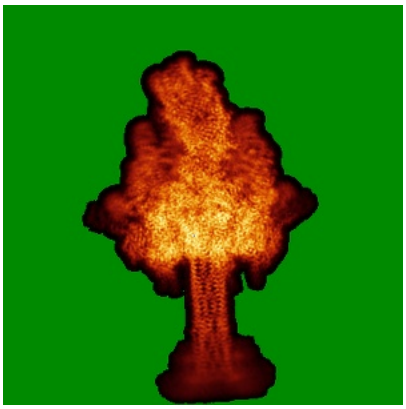

Y Index: 207

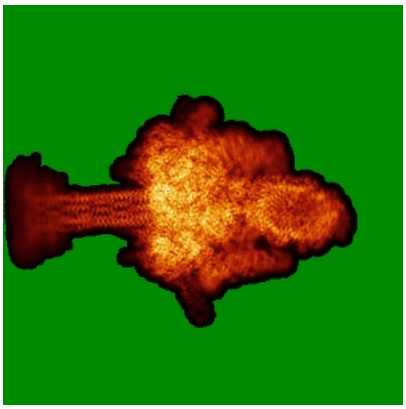

Z Index: 153

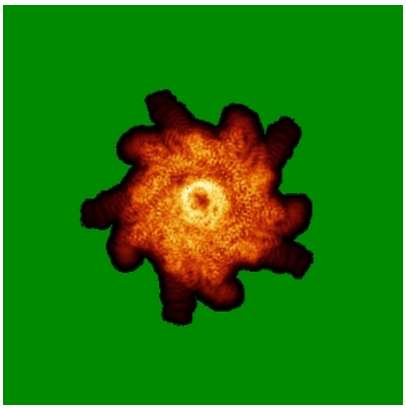
The images above show the largest variance slices of the map in three orthogonal directions.

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

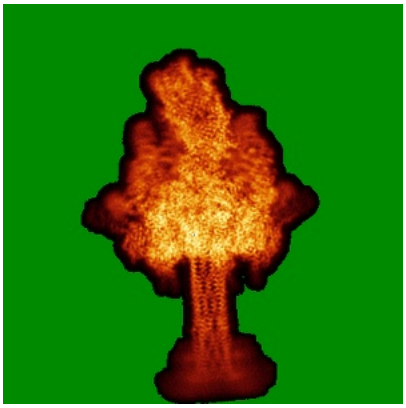
6.4.1 Primary map

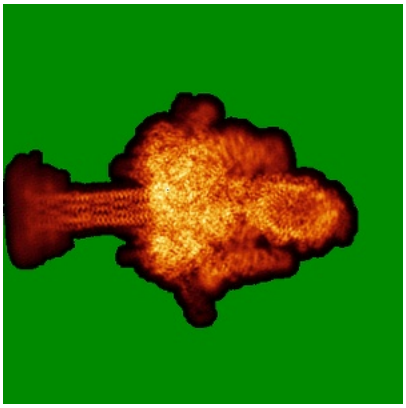

X

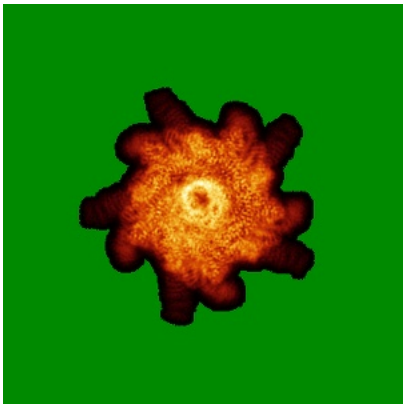

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

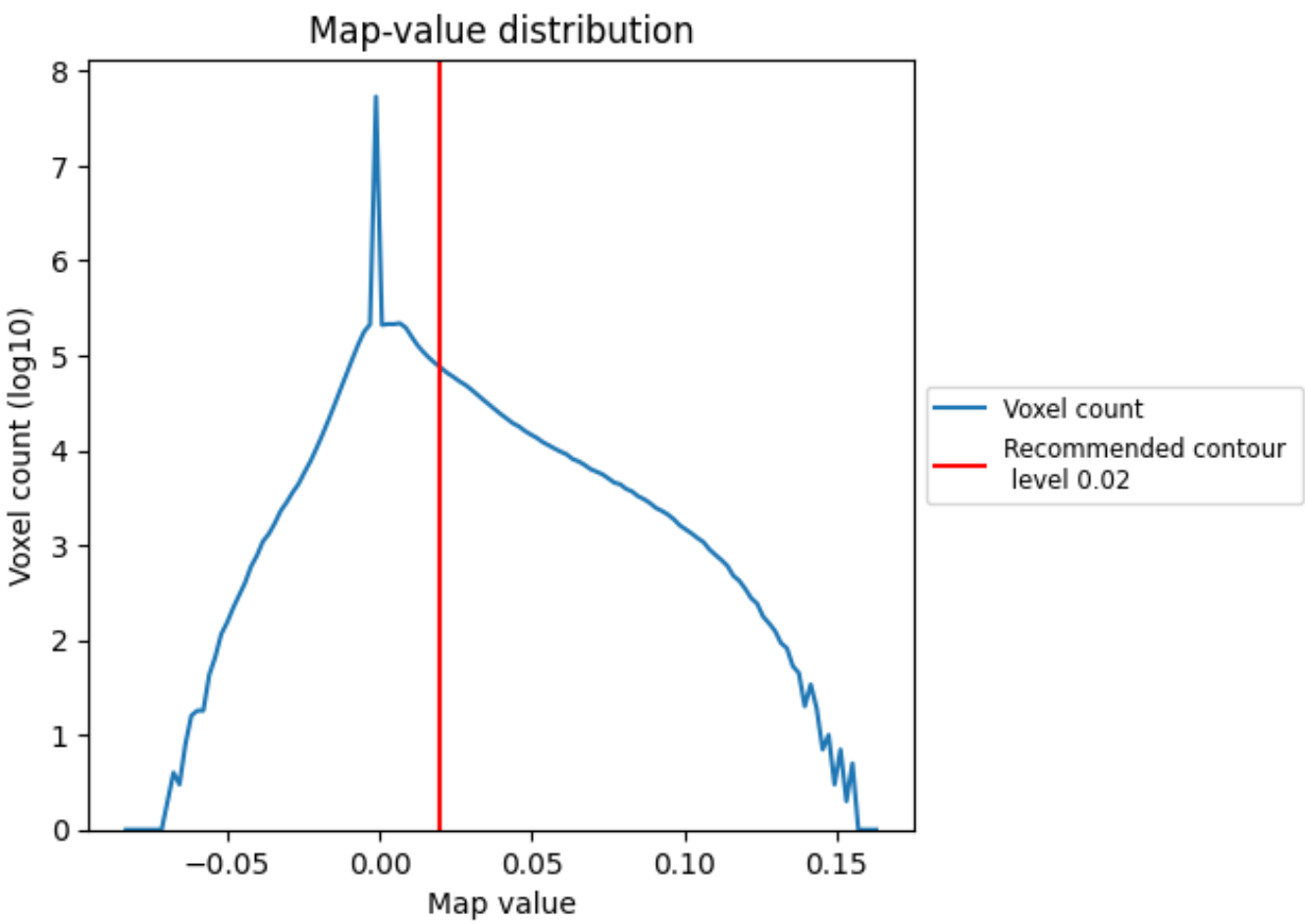
6.6 Mask visualisation (i)

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

7 Map analysis (i)

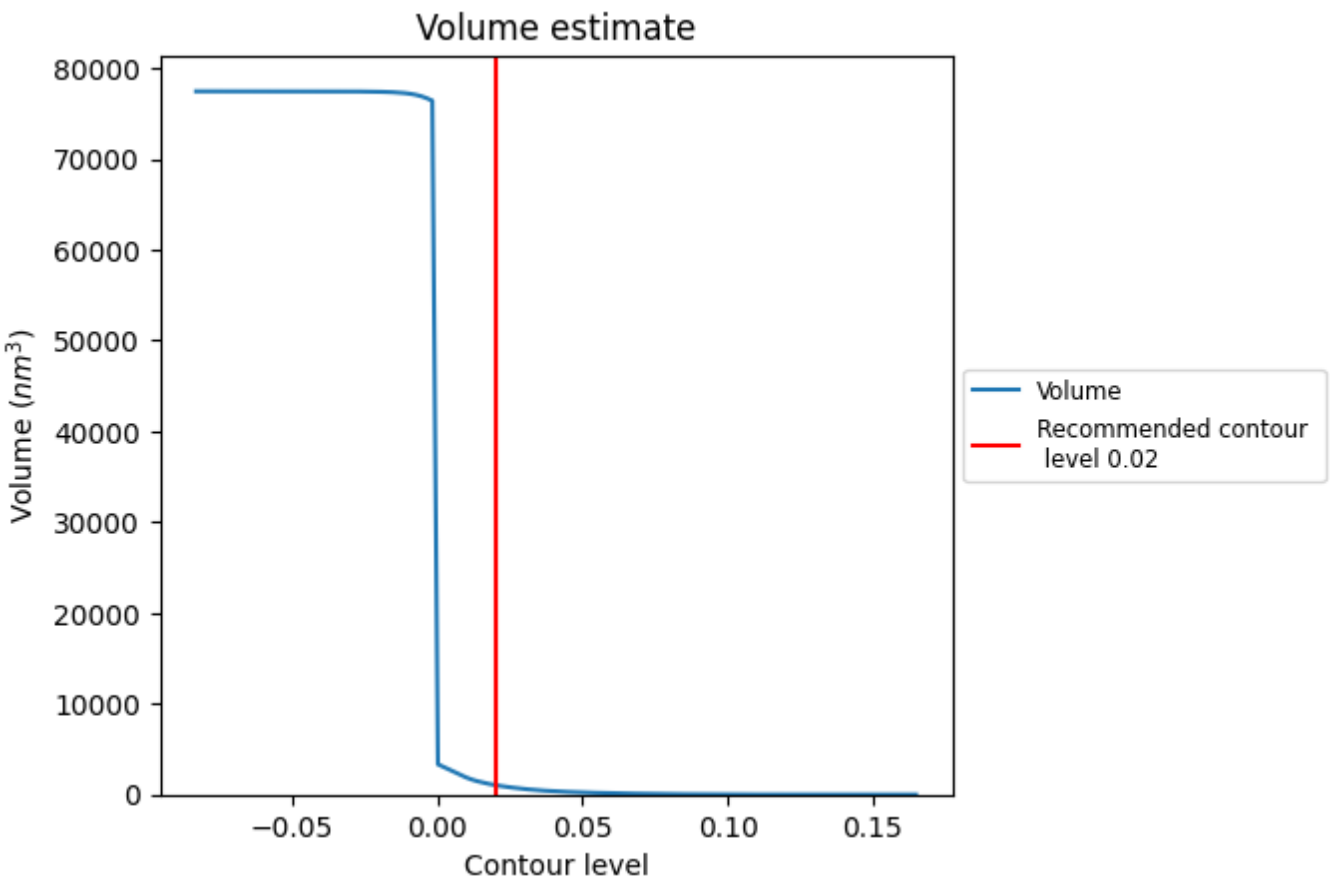
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

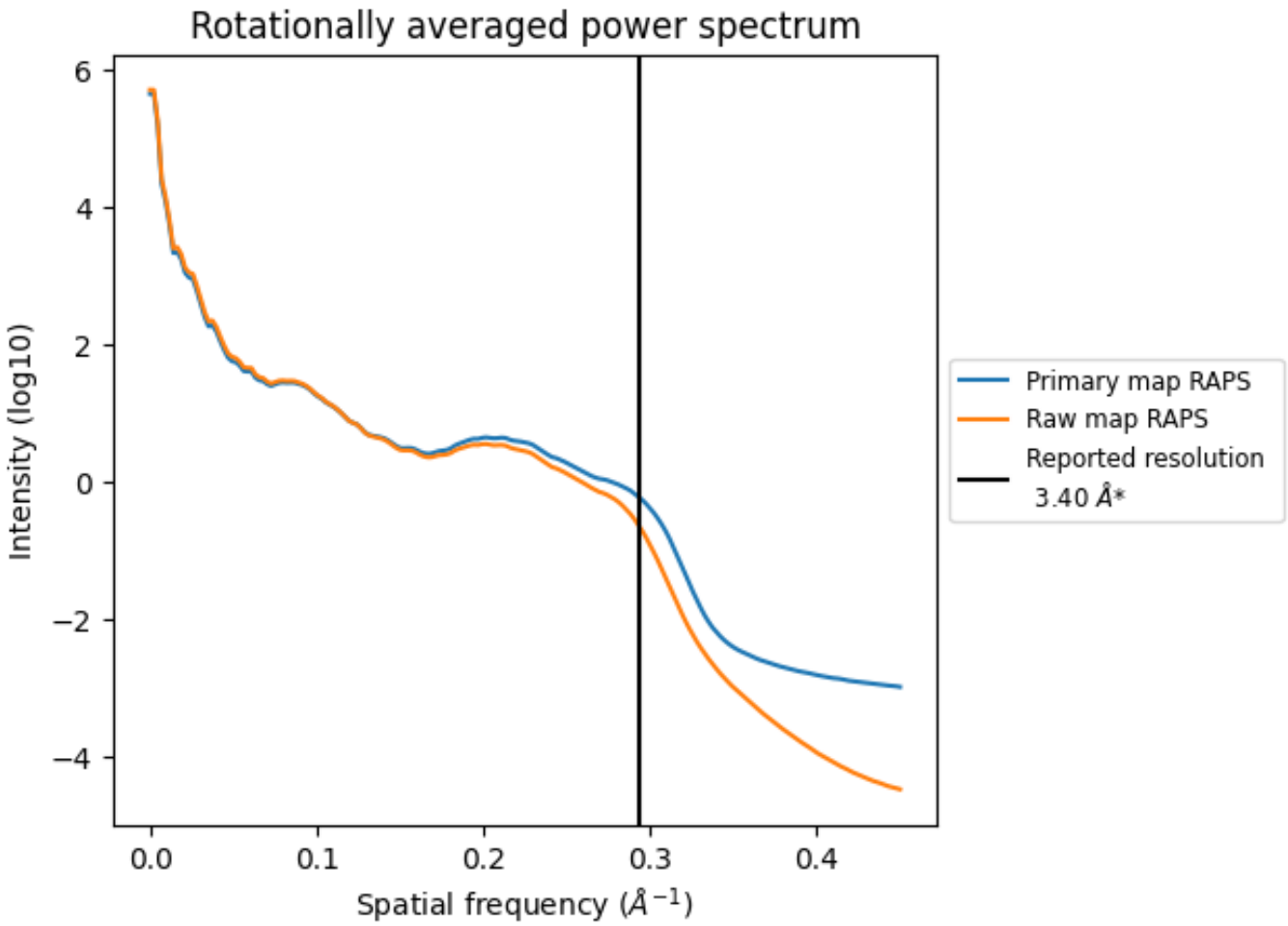
7.2 Volume estimate (i)



The volume at the recommended contour level is 1043 nm^3; this corresponds to an approximate mass of 942 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)

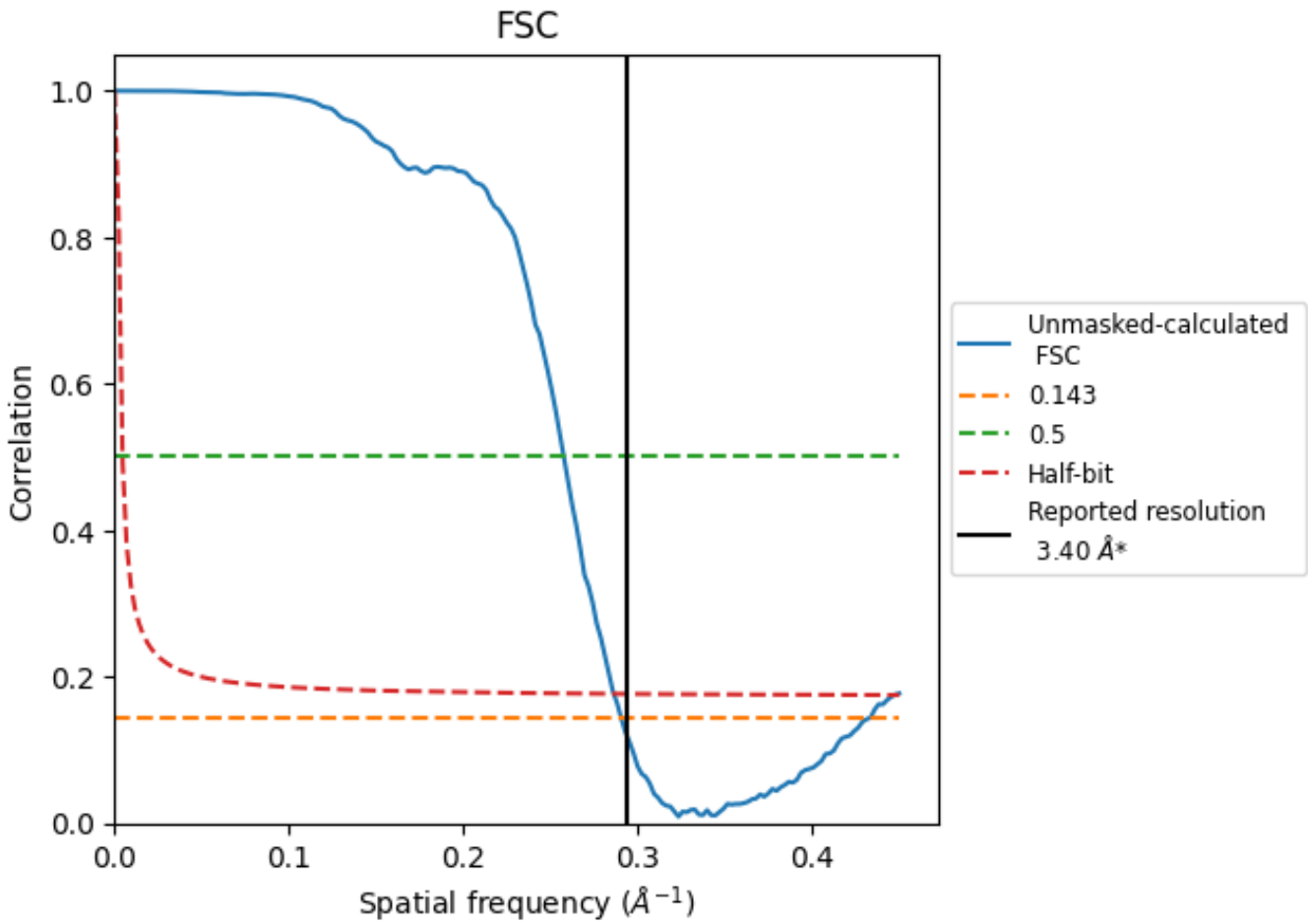


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

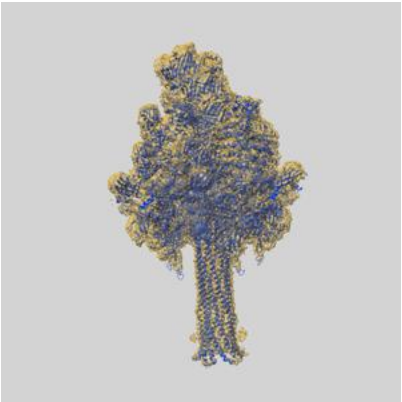
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	3.88	3.49

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

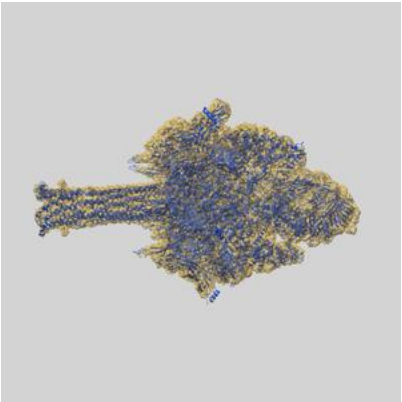
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10312 and PDB model 6SUE. Per-residue inclusion information can be found in section 3 on page 5.

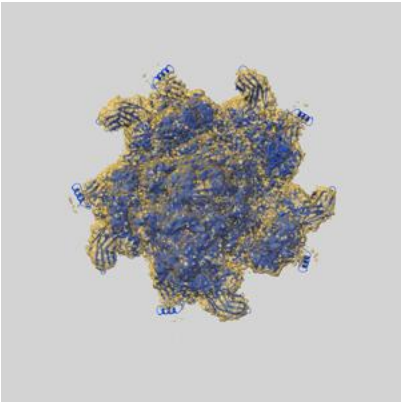
9.1 Map-model overlay (i)



X



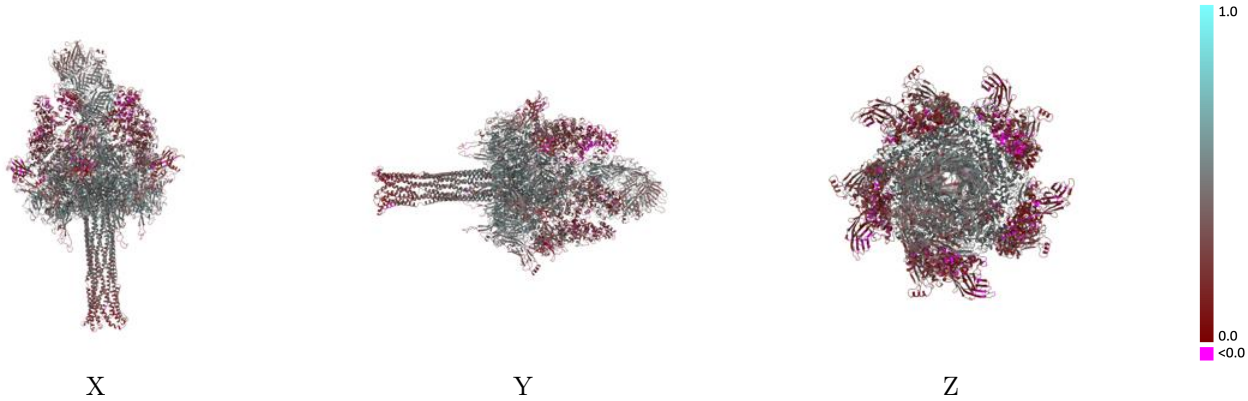
Y



Z

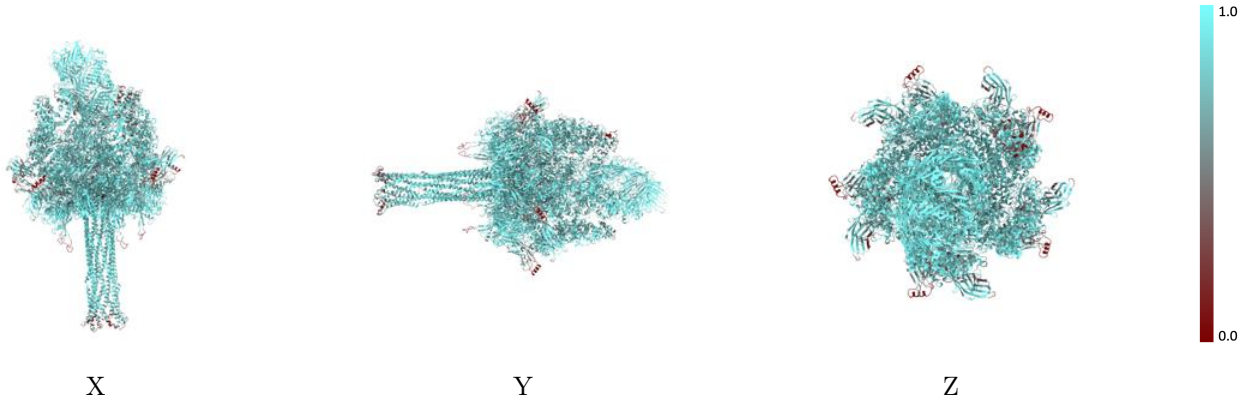
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



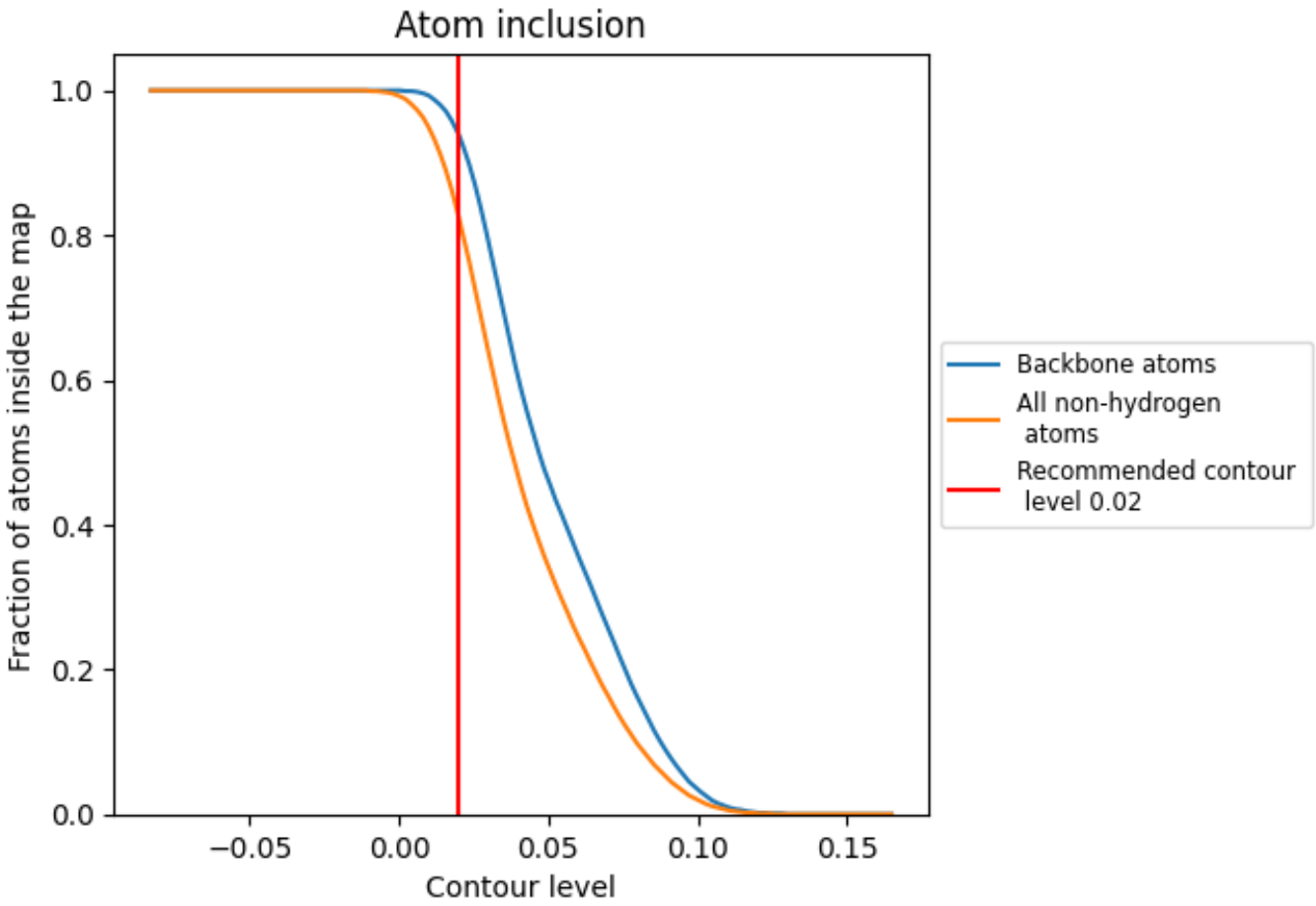
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.3850
A	0.8100	0.3810
B	0.8150	0.3740
C	0.8150	0.3730
D	0.7950	0.3600
E	0.8210	0.3870
F	0.8990	0.4340