Full wwPDB EM Validation Report ⓘ

Mar 4, 2024 – 04:41 pm GMT

PDB ID	:	8CPZ
EMDB ID	:	EMD-16791
Title	:	Photorhabdus luminescens TcdA1 prepore-to-pore intermediate, K1179W mutant
Authors	:	Nganga, P.N.; Roderer, D.; Belyy, A.; Prumbaum, D.; Raunser, S.
Deposited on	:	2023-03-03
Resolution	:	2.90 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:

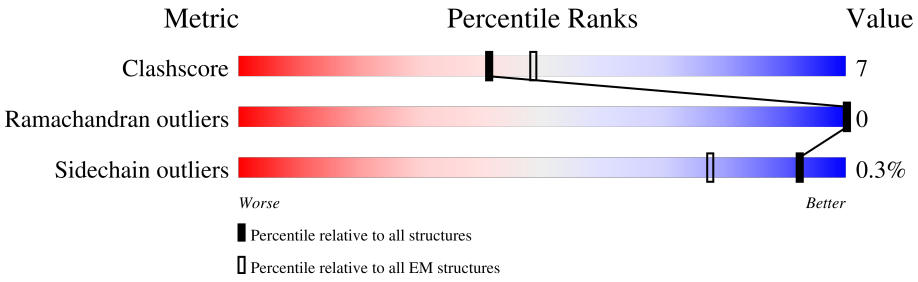
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.90 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	2535	68% 16% 16%
1	B	2535	68% 16% 16%
1	C	2535	68% 16% 16%
1	D	2535	68% 16% 16%
1	E	2535	68% 16% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 84420 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	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	B	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	C	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	D	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		
1	E	2122	Total	C	N	O	S	0	0
			16884	10699	2868	3262	55		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP Q9RN43
A	-17	ALA	-	expression tag	UNP Q9RN43
A	-16	HIS	-	expression tag	UNP Q9RN43
A	-15	HIS	-	expression tag	UNP Q9RN43
A	-14	HIS	-	expression tag	UNP Q9RN43
A	-13	HIS	-	expression tag	UNP Q9RN43
A	-12	HIS	-	expression tag	UNP Q9RN43
A	-11	HIS	-	expression tag	UNP Q9RN43
A	-10	SER	-	expression tag	UNP Q9RN43
A	-9	SER	-	expression tag	UNP Q9RN43
A	-8	GLY	-	expression tag	UNP Q9RN43
A	-7	LEU	-	expression tag	UNP Q9RN43
A	-6	GLU	-	expression tag	UNP Q9RN43
A	-5	VAL	-	expression tag	UNP Q9RN43
A	-4	LEU	-	expression tag	UNP Q9RN43
A	-3	PHE	-	expression tag	UNP Q9RN43
A	-2	GLN	-	expression tag	UNP Q9RN43
A	-1	GLY	-	expression tag	UNP Q9RN43
A	0	PRO	-	expression tag	UNP Q9RN43
A	1179	TRP	LYS	engineered mutation	UNP Q9RN43

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	initiating methionine	UNP Q9RN43
B	-17	ALA	-	expression tag	UNP Q9RN43
B	-16	HIS	-	expression tag	UNP Q9RN43
B	-15	HIS	-	expression tag	UNP Q9RN43
B	-14	HIS	-	expression tag	UNP Q9RN43
B	-13	HIS	-	expression tag	UNP Q9RN43
B	-12	HIS	-	expression tag	UNP Q9RN43
B	-11	HIS	-	expression tag	UNP Q9RN43
B	-10	SER	-	expression tag	UNP Q9RN43
B	-9	SER	-	expression tag	UNP Q9RN43
B	-8	GLY	-	expression tag	UNP Q9RN43
B	-7	LEU	-	expression tag	UNP Q9RN43
B	-6	GLU	-	expression tag	UNP Q9RN43
B	-5	VAL	-	expression tag	UNP Q9RN43
B	-4	LEU	-	expression tag	UNP Q9RN43
B	-3	PHE	-	expression tag	UNP Q9RN43
B	-2	GLN	-	expression tag	UNP Q9RN43
B	-1	GLY	-	expression tag	UNP Q9RN43
B	0	PRO	-	expression tag	UNP Q9RN43
B	1179	TRP	LYS	engineered mutation	UNP Q9RN43
C	-18	MET	-	initiating methionine	UNP Q9RN43
C	-17	ALA	-	expression tag	UNP Q9RN43
C	-16	HIS	-	expression tag	UNP Q9RN43
C	-15	HIS	-	expression tag	UNP Q9RN43
C	-14	HIS	-	expression tag	UNP Q9RN43
C	-13	HIS	-	expression tag	UNP Q9RN43
C	-12	HIS	-	expression tag	UNP Q9RN43
C	-11	HIS	-	expression tag	UNP Q9RN43
C	-10	SER	-	expression tag	UNP Q9RN43
C	-9	SER	-	expression tag	UNP Q9RN43
C	-8	GLY	-	expression tag	UNP Q9RN43
C	-7	LEU	-	expression tag	UNP Q9RN43
C	-6	GLU	-	expression tag	UNP Q9RN43
C	-5	VAL	-	expression tag	UNP Q9RN43
C	-4	LEU	-	expression tag	UNP Q9RN43
C	-3	PHE	-	expression tag	UNP Q9RN43
C	-2	GLN	-	expression tag	UNP Q9RN43
C	-1	GLY	-	expression tag	UNP Q9RN43
C	0	PRO	-	expression tag	UNP Q9RN43
C	1179	TRP	LYS	engineered mutation	UNP Q9RN43
D	-18	MET	-	initiating methionine	UNP Q9RN43
D	-17	ALA	-	expression tag	UNP Q9RN43

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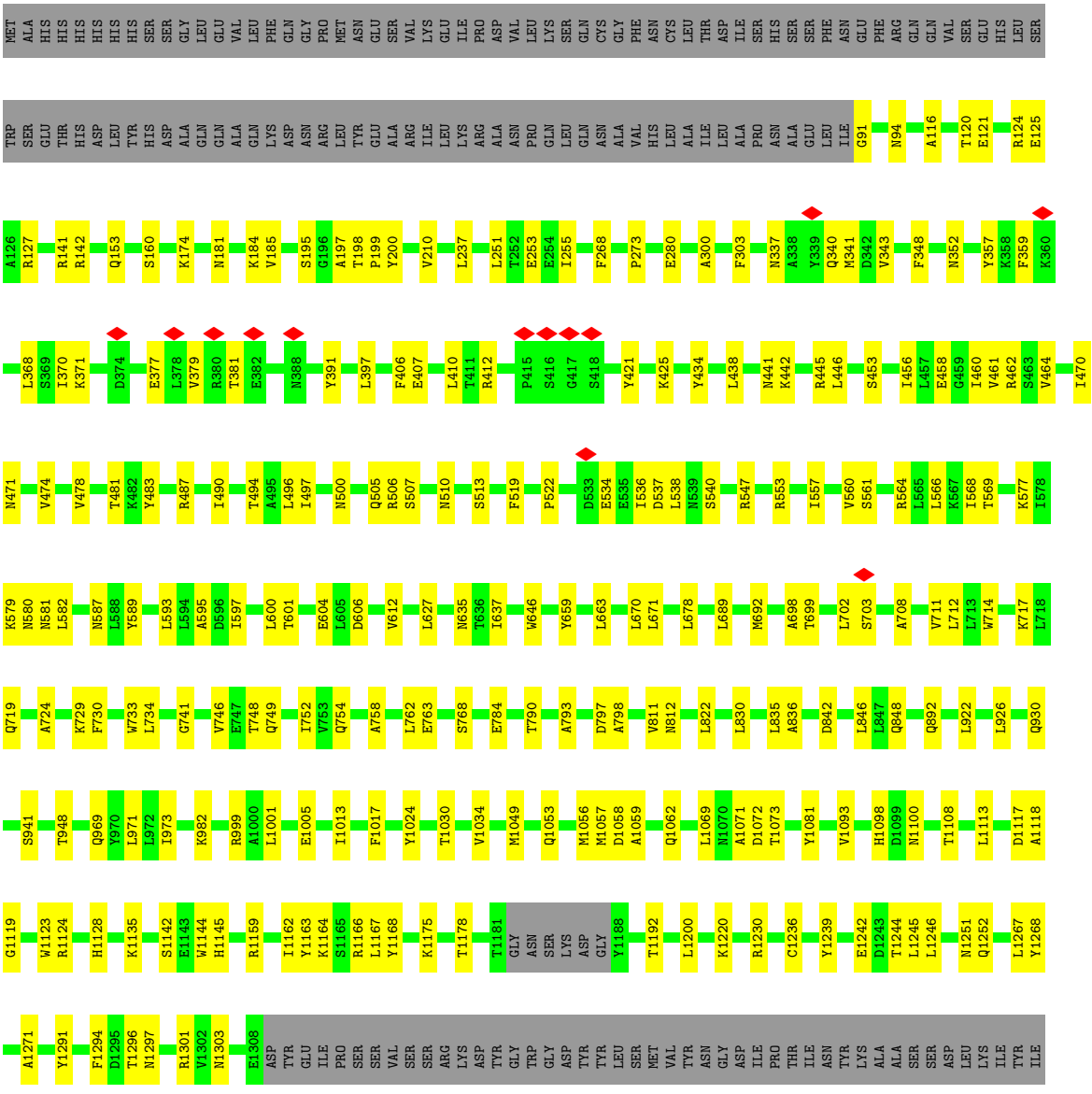
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q9RN43
D	-15	HIS	-	expression tag	UNP Q9RN43
D	-14	HIS	-	expression tag	UNP Q9RN43
D	-13	HIS	-	expression tag	UNP Q9RN43
D	-12	HIS	-	expression tag	UNP Q9RN43
D	-11	HIS	-	expression tag	UNP Q9RN43
D	-10	SER	-	expression tag	UNP Q9RN43
D	-9	SER	-	expression tag	UNP Q9RN43
D	-8	GLY	-	expression tag	UNP Q9RN43
D	-7	LEU	-	expression tag	UNP Q9RN43
D	-6	GLU	-	expression tag	UNP Q9RN43
D	-5	VAL	-	expression tag	UNP Q9RN43
D	-4	LEU	-	expression tag	UNP Q9RN43
D	-3	PHE	-	expression tag	UNP Q9RN43
D	-2	GLN	-	expression tag	UNP Q9RN43
D	-1	GLY	-	expression tag	UNP Q9RN43
D	0	PRO	-	expression tag	UNP Q9RN43
D	1179	TRP	LYS	engineered mutation	UNP Q9RN43
E	-18	MET	-	initiating methionine	UNP Q9RN43
E	-17	ALA	-	expression tag	UNP Q9RN43
E	-16	HIS	-	expression tag	UNP Q9RN43
E	-15	HIS	-	expression tag	UNP Q9RN43
E	-14	HIS	-	expression tag	UNP Q9RN43
E	-13	HIS	-	expression tag	UNP Q9RN43
E	-12	HIS	-	expression tag	UNP Q9RN43
E	-11	HIS	-	expression tag	UNP Q9RN43
E	-10	SER	-	expression tag	UNP Q9RN43
E	-9	SER	-	expression tag	UNP Q9RN43
E	-8	GLY	-	expression tag	UNP Q9RN43
E	-7	LEU	-	expression tag	UNP Q9RN43
E	-6	GLU	-	expression tag	UNP Q9RN43
E	-5	VAL	-	expression tag	UNP Q9RN43
E	-4	LEU	-	expression tag	UNP Q9RN43
E	-3	PHE	-	expression tag	UNP Q9RN43
E	-2	GLN	-	expression tag	UNP Q9RN43
E	-1	GLY	-	expression tag	UNP Q9RN43
E	0	PRO	-	expression tag	UNP Q9RN43
E	1179	TRP	LYS	engineered mutation	UNP Q9RN43

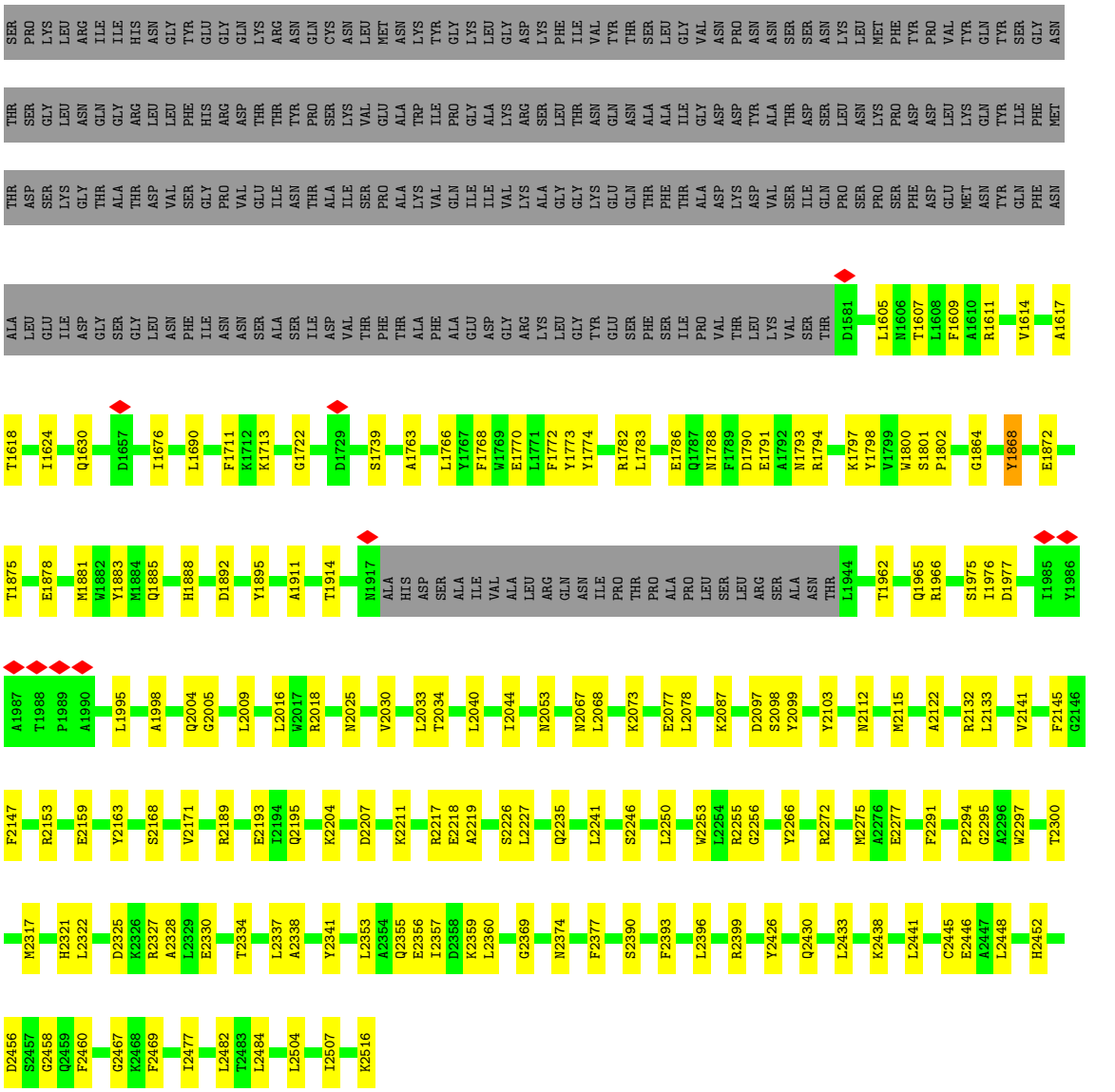
3 Residue-property plots (i)

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

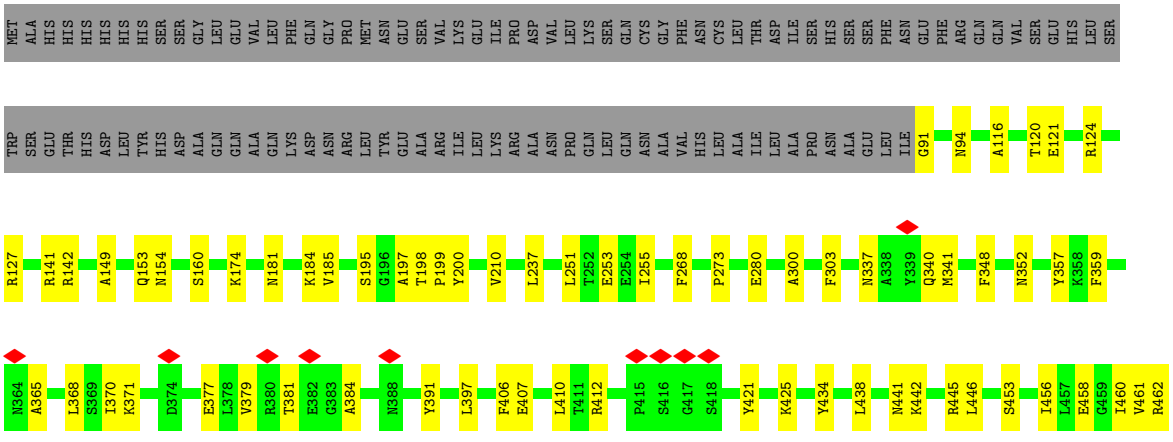
Chain A:

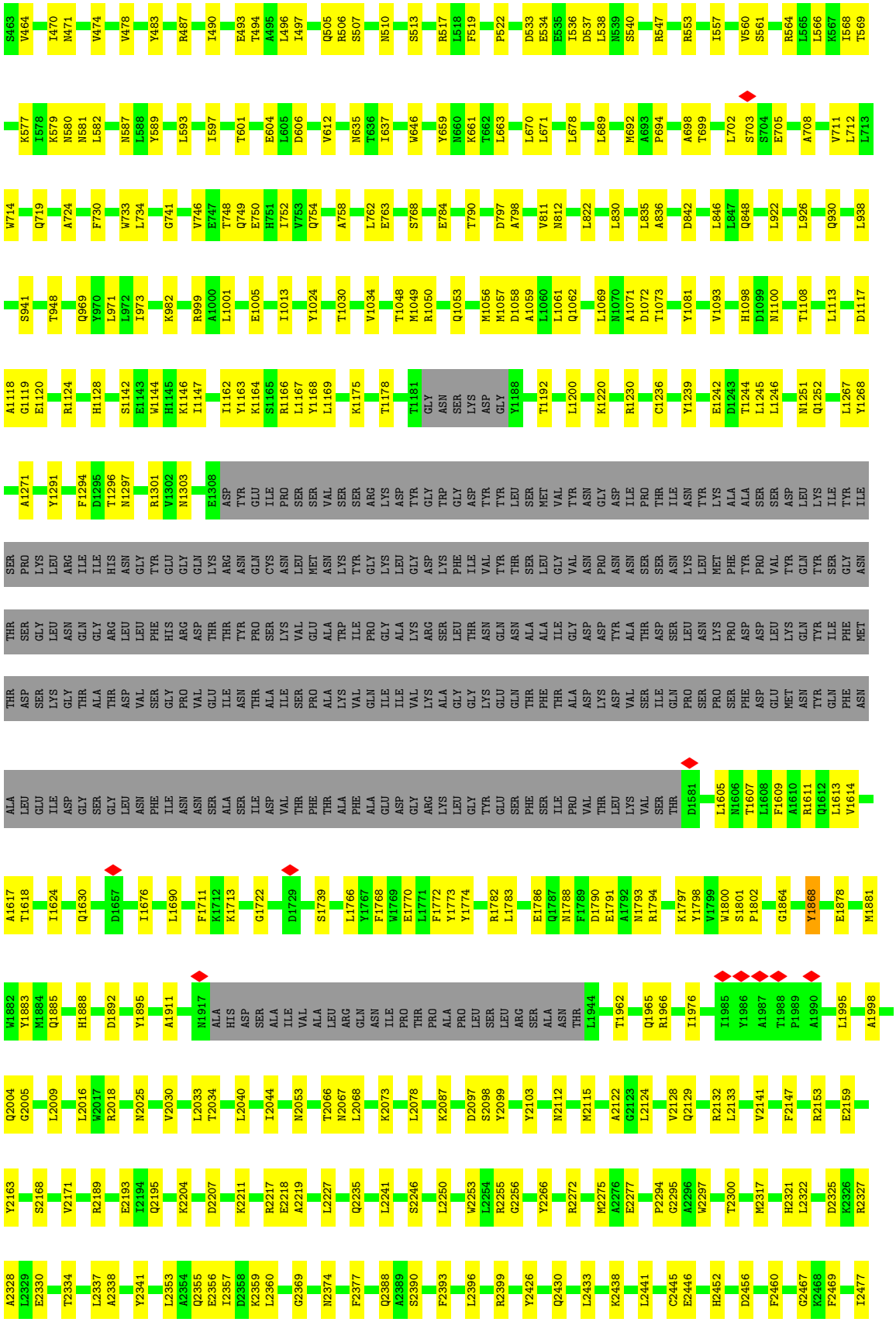




• Molecule 1: TcdA1

Chain B:

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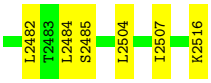
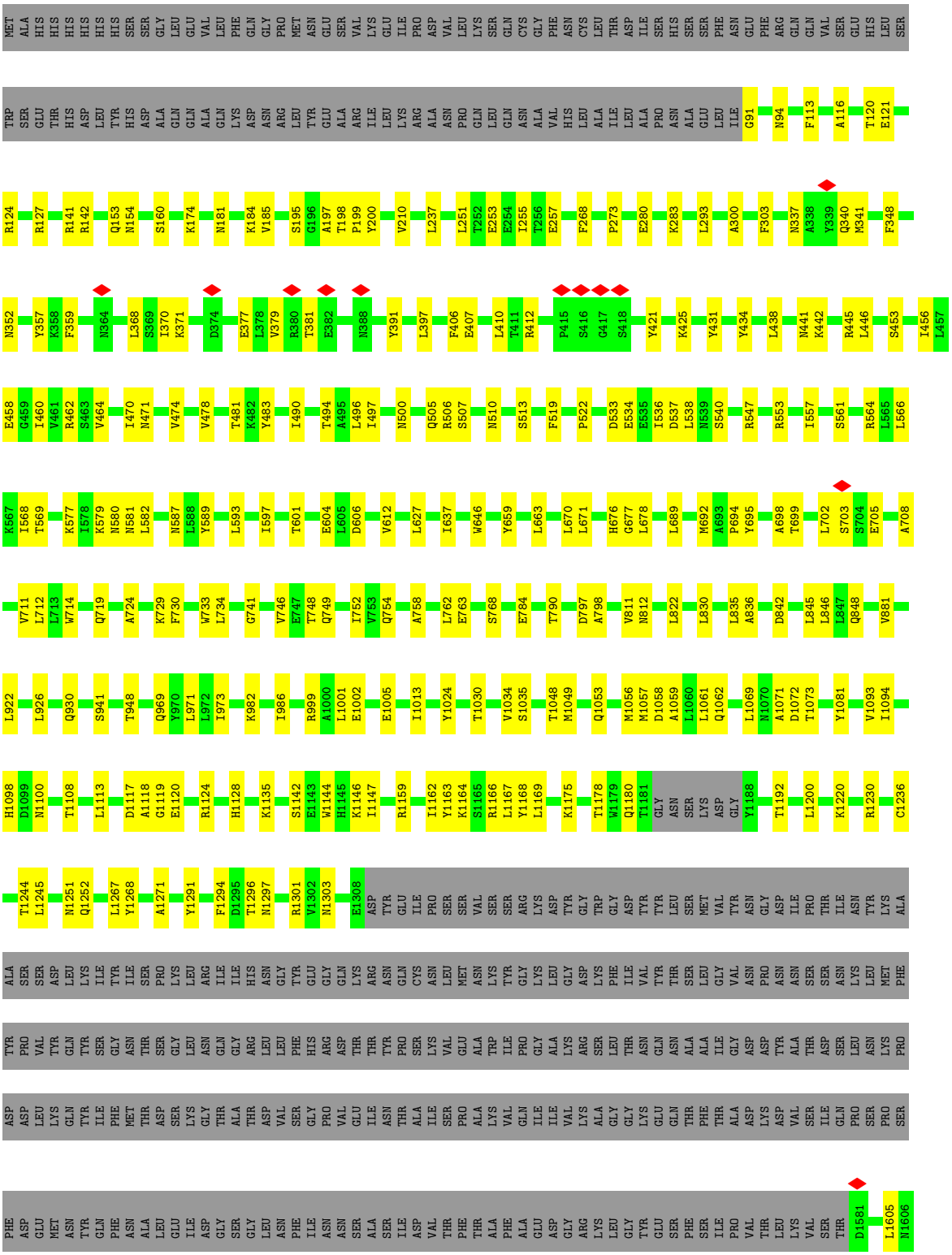
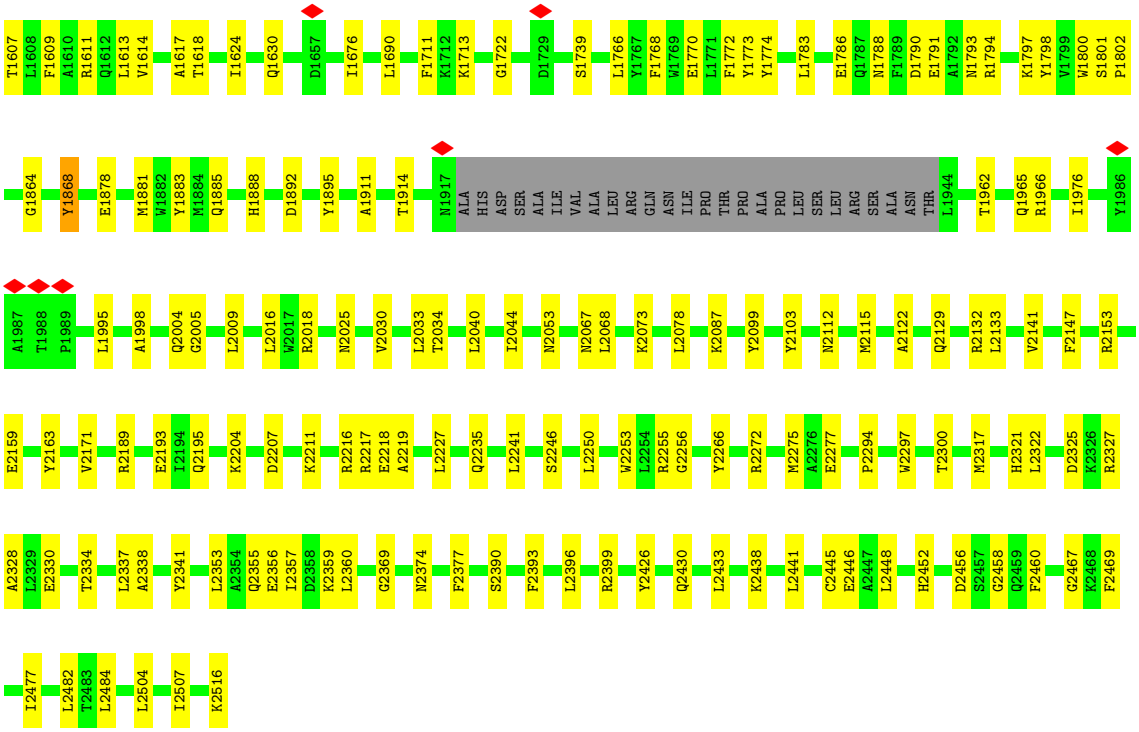
K577 I578 K579 N580 N581 L582 N587 L588 Y589 L593 I597 T601 E604 L605 D606 V612 N635 T636 I637 W646 Y659 N660 K661 T662 L663 L670 L671 L678 L689 M692 A693 P694 A698 T699 L702 S703 S704 E705 A708 V711 L712 L713
W714 Q719 A724 F730 W733 L734 G741 V746 E747 T748 Q749 E750 H751 I752 V753 Q754 A758 L762 E763 S768 E784 T790 D797 A798 V811 N812 L822 L830 L835 A836 D842 L846 L847 Q848 L922 L926 Q930 L938
S941 T948 Q969 Y970 L971 L972 I973 K982 R999 A1000 L1001 E1005 I1013 Y1024 T1030 V1034 T1048 M1049 R1050 Q1053 M1056 M1057 D1058 A1059 L1060 L1061 Q1062 L1069 N1070 A1071 D1072 T1073 Y1081 V1093 H1098 D1099 N1100 T1108 L1113 D1117
A1118 G1119 E1120 R1124 H1128 S1142 E1143 W1144 H1145 K1146 I1147 I1162 Y1163 K1164 S1165 R1166 L1167 Y1168 L1169 K1175 T1178 T1181 GLY ASN SER LYS ASP GLY Y1188 T1192 L1200 K1220 R1230 C1236 Y1239 E1242 D1243 T1244 L1245 L1246 N1251 Q1252 L1267 Y1268
A1271 Y1291 F1294 D1295 T1296 N1297 R1301 V1302 N1303 E1308 ASP TYR GLU ILE PRO SER SER VAL SER SER ARG LYS ASP TYR GLY TRP GLY ASP TYR TYR LEU SER MET VAL TYR ASN GLY ASP ILE PRO THR ILE ASN TYR LYS ALA ALA SER SER ASP LEU LYS ILE TYR ILE
SER PRO LYS LEU ARG ILE ILE HIS ASN GLY TYR GLU GLY GLN LYS ARG ASN GLN CYS ASN LEU MET ASN LYS TYR GLY LYS LEU 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 GLN ASN ALA ALA ILE GLY ASP ASP TYR ALA THR ASP SER LEU ASN LYS PRO SER 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 ALA ILE SER PRO ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN THR PHE THR ALA ASP LYS ASP VAL SER ILE GLN PRO SER PRO SER PHE ASP GLU MET ASN TYR GLN PHE ASN
ALA LEU GLU ILE ASP GLY SER GLY LEU ASN PHE ILE ASN ASN SER ALA ASP VAL THR PHE THR ALA PHE ALA GLU ASP GLY ARG LYS LEU GLY TYR GLU SER PHE SER ILE PRO VAL THR LEU LYS VAL SER THR D1581 L1605 N1606 T1607 L1608 F1609 A1610 R1611 Q1612 L1613 V1614
A1617 T1618 I1624 Q1630 D1657 I1676 L1690 F1711 K1712 K1713 G1722 D1729 S1739 L1766 Y1767 F1768 W1769 E1770 L1771 F1772 Y1773 Y1774 R1782 L1783 E1786 Q1787 N1788 F1789 D1790 E1791 A1792 N1793 R1794 K1797 Y1798 V1799 W1800 S1801 P1802 G1864 Y1868 E1878 M1881
W1882 Y1883 M1884 Q1885 H1888 D1892 Y1895 A1911 N1917 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 THR L1944 T1962 Q1965 R1966 I1976 I1985 Y1986 A1987 T1988 P1989 A1990 L1995 A1998
Q2004 G2005 L2009 L2016 W2017 R2018 N2025 V2030 L2033 T2034 L2040 I2044 N2053 T2066 N2067 L2068 K2073 L2078 K2087 D2097 S2098 Y2099 Y2103 N2112 M2115 A2122 G2123 L2124 V2128 Q2129 R2132 L2133 V2141 F2147 R2153 E2159
Y2163 S2168 V2171 R2189 E2193 I2194 Q2195 K2204 D2207 K2211 R2217 E2218 A2219 L2227 Q2235 L2241 S2246 L2250 W2253 L2254 R2255 G2256 Y2266 R2272 M2275 A2276 E2277 P2294 G2295 A2296 W2297 T2300 M2317 H2321 L2322 D2325 K2326 R2327
A2328 L2329 E2330 T2334 L2337 A2338 Y2341 L2353 A2354 Q2355 E2356 I2357 D2358 K2359 L2360 G2369 N2374 F2377 Q2388 A2389 S2390 F2393 L2396 R2399 Y2426 Q2430 L2433 K2438 L2441 C2445 E2446 H2452 D2456 F2460 G2467 K2468 F2469 I2477



• Molecule 1: TcdA1

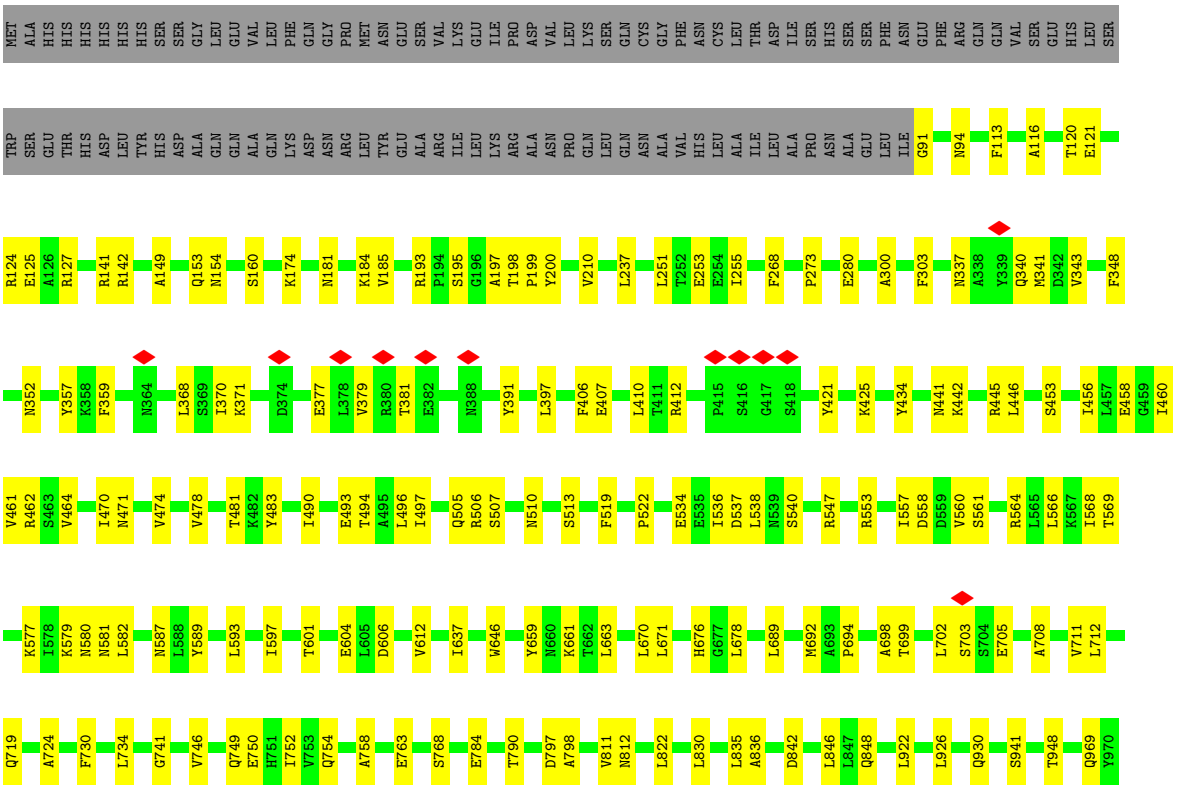
Chain C:

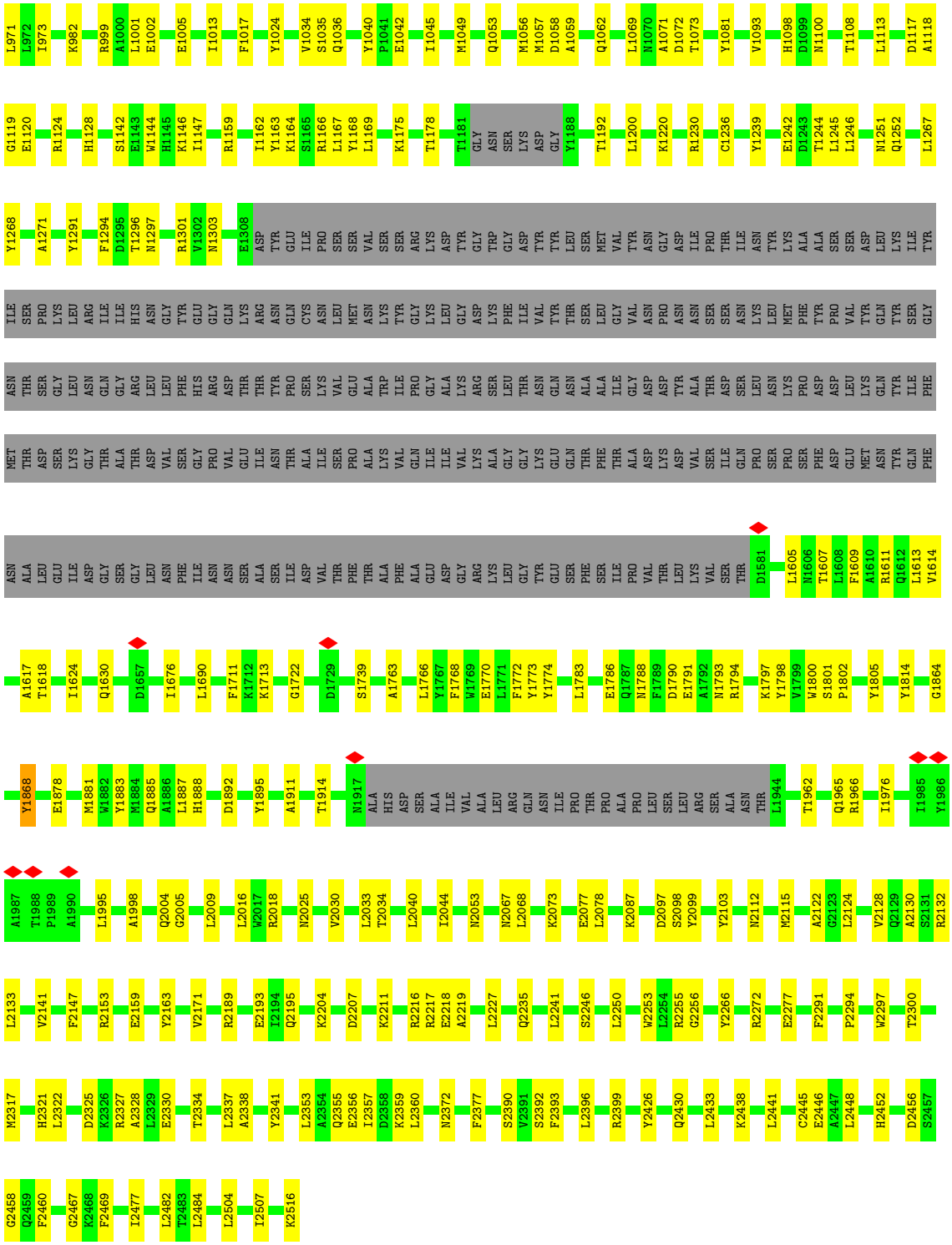




• Molecule 1: TcdA1

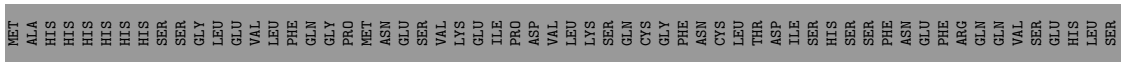
Chain D:

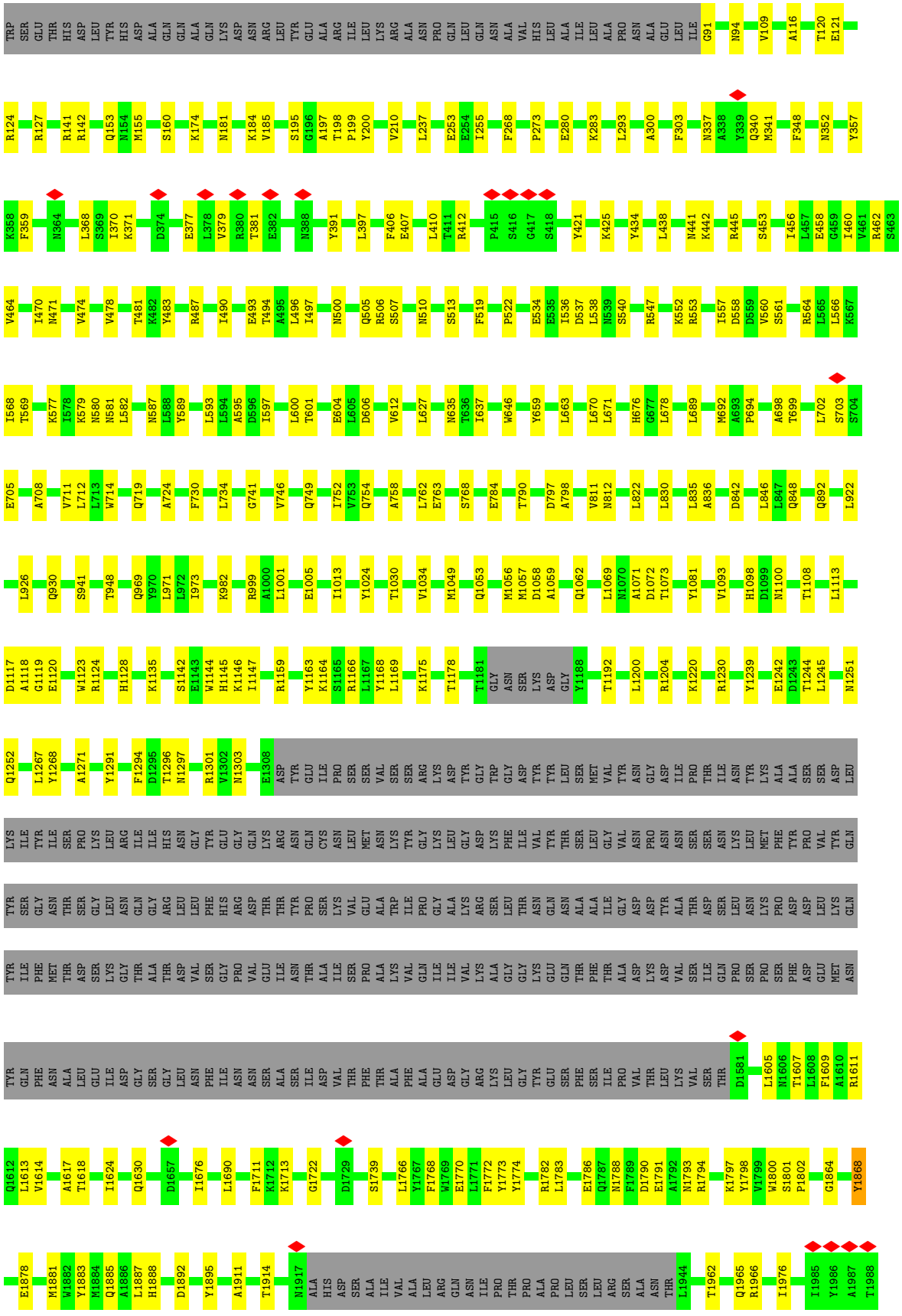


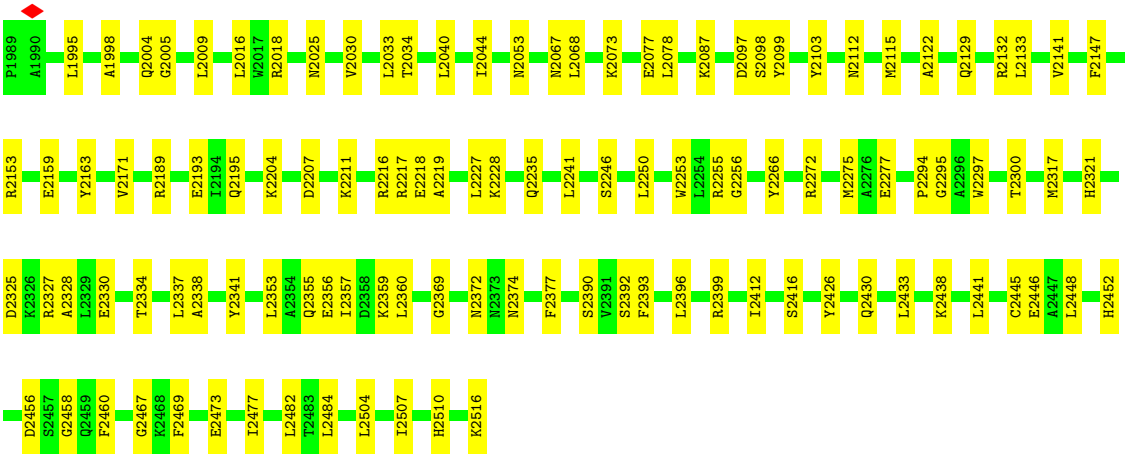


• Molecule 1: TcdA1

Chain E:




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 LEU ILE
G91 N94 V109 A116 T120 E121
R124 R127 R141 R142 Q153 N154 M155 S160 K174 N181 K184 V185 S195 G196 A197 T198 P199 Y200 V210 L237 E253 E254 I255 F268 P273 E280 K283 L293 A300 F303 N337 A338 Y339 Q340 M341 F348 N352 Y357
K358 F359 N364 L368 S369 I370 K371 D374 E377 L378 V379 R380 T381 E382 N388 Y391 L397 F406 E407 L410 T411 R412 P415 S416 G417 S418 Y421 K425 Y434 L438 N441 K442 R445 S453 I456 L457 E458 G459 I460 V461 R462 S463
V464 I470 N471 V474 V478 T481 K482 Y483 R487 T490 E493 T494 A495 L496 I497 N500 Q505 R506 S507 N510 S513 F519 P522 E534 E535 I536 D537 L538 N539 S540 R547 K552 R553 I557 D558 D559 V560 S561 R564 L565 L566 K567
I568 T569 K577 I578 K579 N580 N581 L582 N587 L588 Y589 L593 L594 A595 D596 I597 L600 T601 E604 L605 D606 V612 L627 N635 T636 I637 W646 Y659 L663 L670 L671 H676 G677 L678 L689 M692 A693 P694 A698 T699 L702 S703 S704
E705 A708 V711 L712 L713 W714 Q719 A724 F730 L734 G741 V746 Q749 I752 V753 Q754 A758 L762 E763 S768 E784 T790 D797 A798 V811 N812 L822 L830 L835 A836 D842 L846 L847 Q848 Q892 L922
L926 Q930 S941 T948 Q969 Y970 L971 L972 I973 K982 R999 A1000 L1001 E1005 I1013 Y1024 T1030 V1034 M1049 Q1053 M1056 M1057 D1058 A1059 Q1062 L1069 N1070 A1071 D1072 T1073 Y1081 V1093 H1098 D1099 N1100 T1108 L1113
D1117 A1118 G1119 E1120 W1123 R1124 H1128 K1135 S1142 E1143 W1144 H1145 K1146 I1147 R1159 Y1163 K1164 S1165 R1166 L1167 Y1168 L1169 K1175 T1178 T1181 GLY ASN SER LYS ASP GLY Y1188 T1192 L1200 R1204 K1220 R1230 Y1239 E1242 D1243 T1244 L1245 N1251
Q1252 L1267 Y1268 A1271 Y1291 F1294 D1295 T1296 N1297 R1301 V1302 N1303 E1308 ASP TYR GLU ILE PRO SER SER VAL SER SER ARG LYS ASP TYR GLY TRP GLY ASP TYR TYR LEU SER MET VAL TYR ASN GLY ASP ILE PRO THR ILE ASN TYR LYS ALA ALA SER SER ASP LEU
LYS ILE TYR ILE SER PRO LYS LEU ARG ILE ILE HIS ASN GLY TYR GLU GLY GLN LYS ARG ASN GLN CYS ASN LEU MET ASN LYS TYR GLY LYS LEU GLY ASP LYS PHE ILE VAL TYR THR SER LEU GLY VAL ASN PRO ASN ASN SER SER ASN LYS TYR 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 PHE ASP GLU 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 ALA ILE SER PRO ALA LYS VAL GLN ILE ILE VAL LYS ALA GLY GLY LYS GLU GLN THR PHE THR ALA ASP LYS ASP VAL SER ILE GLN PRO SER PRO SER PHE ASP GLU MET ASN
TYR GLN PHE ASN ALA LEU GLU ILE ASP GLY SER GLY LEU ASN PHE ILE ASN ASN SER ALA SER ILE ASP VAL THR PHE THR ALA PHE ALA GLU ASP GLY ARG LYS LEU GLY TYR GLU SER PHE SER ILE PRO VAL THR LEU LYS VAL SER THR D1581 L1605 N1606 T1607 L1608 F1609 A1610 R1611
Q1612 L1613 V1614 A1617 T1618 I1624 Q1630 D1657 I1676 L1690 F1711 K1712 K1713 G1722 D1729 S1739 L1766 Y1767 F1768 W1769 E1770 L1771 F1772 Y1773 Y1774 R1782 L1783 E1786 Q1787 N1788 F1789 D1790 E1791 A1792 N1793 R1794 K1797 Y1798 V1799 W1800 S1801 P1802 G1864 Y1868
E1878 M1881 W1882 Y1883 M1884 Q1885 A1886 L1887 H1888 D1892 Y1895 A1911 T1914 N1917 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 THR L1944 T1962 Q1965 R1966 I1976 I1985 Y1986 A1987 T1988


P1989 A1990 L1995 A1998 Q2004 G2005 L2009 L2016 W2017 R2018 N2025 V2030 L2033 T2034 L2040 I2044 M2053 N2067 L2068 K2073 E2077 L2078 K2087 D2097 S2098 Y2099 Y2103 N2112 M2115 A2122 Q2129 R2132 L2133 V2141 F2147
R2153 E2159 Y2163 V2171 R2189 E2193 T2194 Q2195 K2204 D2207 K2211 R2216 R2217 E2218 A2219 L2227 K2228 Q2235 L2241 S2246 L2250 W2253 L2254 R2255 G2256 Y2266 R2272 M2275 A2276 E2277 P2294 G2295 A2296 W2297 T2300 M2317 H2321
D2325 K2326 R2327 A2328 L2329 E2330 T2334 L2337 A2338 Y2341 L2353 A2354 Q2355 E2356 I2357 D2358 K2359 L2360 G2369 N2372 N2373 N2374 F2377 S2390 V2391 S2392 F2393 L2396 R2399 I2412 S2416 Y2426 Q2430 L2433 K2438 L2441 C2445 E2446 A2447 L2448 H2452
D2456 S2457 G2458 Q2459 F2460 G2467 K2468 F2469 E2473 I2477 L2482 T2483 L2484 L2504 I2507 H2510 K2516

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	230785	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2750	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.447	Depositor
Minimum map value	-0.144	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	425.92, 425.92, 425.92	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.21, 1.21, 1.21	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.27	0/17247	0.51	0/23428
1	B	0.27	0/17247	0.51	0/23428
1	C	0.27	0/17247	0.51	0/23428
1	D	0.27	0/17247	0.51	0/23428
1	E	0.26	0/17247	0.51	0/23428
All	All	0.27	0/86235	0.51	0/117140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	16884	0	16507	277	0
1	B	16884	0	16507	280	0
1	C	16884	0	16507	275	0
1	D	16884	0	16507	277	0
1	E	16884	0	16507	280	0
All	All	84420	0	82535	1241	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 7.

All (1241) 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:689:LEU:HD11	1:B:712:LEU:HB3	1.62	0.82
1:C:1296:THR:HG23	1:C:1301:ARG:HH12	1.46	0.81
1:C:689:LEU:HD11	1:C:712:LEU:HB3	1.61	0.81
1:E:689:LEU:HD11	1:E:712:LEU:HB3	1.62	0.81
1:D:1296:THR:HG23	1:D:1301:ARG:HH12	1.45	0.81
1:A:1296:THR:HG23	1:A:1301:ARG:HH12	1.46	0.80
1:B:1296:THR:HG23	1:B:1301:ARG:HH12	1.46	0.80
1:A:689:LEU:HD11	1:A:712:LEU:HB3	1.62	0.79
1:A:2445:CYS:SG	1:B:2327:ARG:NH1	2.56	0.79
1:D:2445:CYS:SG	1:E:2327:ARG:NH1	2.56	0.79
1:A:2327:ARG:NH1	1:E:2445:CYS:SG	2.55	0.79
1:B:2445:CYS:SG	1:C:2327:ARG:NH1	2.56	0.78
1:E:1296:THR:HG23	1:E:1301:ARG:HH12	1.46	0.78
1:D:689:LEU:HD11	1:D:712:LEU:HB3	1.63	0.78
1:B:1108:THR:HG1	1:B:1128:HIS:HE2	1.31	0.78
1:C:2445:CYS:SG	1:D:2327:ARG:NH1	2.57	0.78
1:E:1108:THR:HG1	1:E:1128:HIS:HE2	1.31	0.77
1:C:1059:ALA:HA	1:C:1062:GLN:HE21	1.50	0.75
1:E:1059:ALA:HA	1:E:1062:GLN:HE21	1.50	0.75
1:B:1797:LYS:HG3	1:B:1801:SER:HB2	1.69	0.74
1:B:1059:ALA:HA	1:B:1062:GLN:HE21	1.51	0.74
1:D:1059:ALA:HA	1:D:1062:GLN:HE21	1.51	0.74
1:A:1059:ALA:HA	1:A:1062:GLN:HE21	1.51	0.74
1:C:1108:THR:HG1	1:C:1128:HIS:HE2	1.34	0.73
1:C:1797:LYS:HG3	1:C:1801:SER:HB2	1.70	0.73
1:D:1093:VAL:HG21	1:D:1605:LEU:HD23	1.70	0.73
1:D:1797:LYS:HG3	1:D:1801:SER:HB2	1.68	0.73
1:E:1797:LYS:HG3	1:E:1801:SER:HB2	1.69	0.73
1:B:1093:VAL:HG21	1:B:1605:LEU:HD23	1.70	0.72
1:C:460:ILE:HG12	1:C:496:LEU:HD21	1.70	0.72
1:B:460:ILE:HG12	1:B:496:LEU:HD21	1.71	0.72
1:D:460:ILE:HG12	1:D:496:LEU:HD21	1.69	0.72
1:A:460:ILE:HG12	1:A:496:LEU:HD21	1.71	0.72
1:C:210:VAL:HG11	1:C:922:LEU:HB3	1.72	0.72
1:A:1797:LYS:HG3	1:A:1801:SER:HB2	1.70	0.72
1:C:1093:VAL:HG21	1:C:1605:LEU:HD23	1.71	0.72
1:B:2277:GLU:HA	1:B:2317:MET:HE1	1.73	0.71
1:E:460:ILE:HG12	1:E:496:LEU:HD21	1.70	0.71
1:D:1163:TYR:HB2	1:D:1245:LEU:HD21	1.72	0.71
1:C:462:ARG:HH11	1:C:506:ARG:HH11	1.37	0.71
1:E:1163:TYR:HB2	1:E:1245:LEU:HD21	1.72	0.71
1:A:300:ALA:HA	1:A:303:PHE:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:ALA:HA	1:B:303:PHE:CD2	2.27	0.70
1:D:300:ALA:HA	1:D:303:PHE:CD2	2.27	0.70
1:E:210:VAL:HG11	1:E:922:LEU:HB3	1.74	0.70
1:A:698:ALA:HB1	1:B:2253:TRP:HA	1.71	0.70
1:C:300:ALA:HA	1:C:303:PHE:CD2	2.26	0.70
1:C:698:ALA:HB1	1:D:2253:TRP:HA	1.73	0.70
1:B:698:ALA:HB1	1:C:2253:TRP:HA	1.72	0.70
1:C:1163:TYR:HB2	1:C:1245:LEU:HD21	1.72	0.70
1:E:1093:VAL:HG21	1:E:1605:LEU:HD23	1.72	0.70
1:A:462:ARG:HH11	1:A:506:ARG:HH11	1.39	0.70
1:A:1093:VAL:HG21	1:A:1605:LEU:HD23	1.73	0.70
1:A:2277:GLU:HA	1:A:2317:MET:HE1	1.73	0.70
1:D:2277:GLU:HA	1:D:2317:MET:HE1	1.74	0.69
1:A:210:VAL:HG11	1:A:922:LEU:HB3	1.73	0.69
1:D:462:ARG:HH11	1:D:506:ARG:HH11	1.40	0.69
1:B:210:VAL:HG11	1:B:922:LEU:HB3	1.74	0.69
1:B:1163:TYR:HB2	1:B:1245:LEU:HD21	1.72	0.69
1:D:210:VAL:HG11	1:D:922:LEU:HB3	1.73	0.69
1:E:300:ALA:HA	1:E:303:PHE:CD2	2.27	0.69
1:A:1108:THR:HG1	1:A:1128:HIS:HE2	1.40	0.69
1:A:2253:TRP:HA	1:E:698:ALA:HB1	1.75	0.69
1:B:746:VAL:HB	1:B:749:GLN:HB2	1.74	0.69
1:E:462:ARG:HH11	1:E:506:ARG:HH11	1.41	0.69
1:E:746:VAL:HB	1:E:749:GLN:HB2	1.75	0.69
1:A:1163:TYR:HB2	1:A:1245:LEU:HD21	1.73	0.69
1:D:746:VAL:HB	1:D:749:GLN:HB2	1.74	0.69
1:B:462:ARG:HH11	1:B:506:ARG:HH11	1.41	0.68
1:A:746:VAL:HB	1:A:749:GLN:HB2	1.76	0.68
1:C:2277:GLU:HA	1:C:2317:MET:HE1	1.76	0.68
1:C:746:VAL:HB	1:C:749:GLN:HB2	1.73	0.67
1:E:2277:GLU:HA	1:E:2317:MET:HE1	1.75	0.67
1:C:2356:GLU:HA	1:C:2359:LYS:HG2	1.76	0.66
1:E:2356:GLU:HA	1:E:2359:LYS:HG2	1.77	0.66
1:B:2356:GLU:HA	1:B:2359:LYS:HG2	1.77	0.66
1:C:505:GLN:HE22	1:C:582:LEU:HD13	1.61	0.66
1:D:121:GLU:HG2	1:D:124:ARG:HH21	1.61	0.66
1:D:2356:GLU:HA	1:D:2359:LYS:HG2	1.77	0.66
1:C:121:GLU:HG2	1:C:124:ARG:HH21	1.61	0.65
1:E:2068:LEU:HD22	1:E:2227:LEU:HG	1.78	0.65
1:C:1069:LEU:HD23	1:C:1786:GLU:HG3	1.78	0.65
1:A:2255:ARG:NH2	1:E:703:SER:O	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ALA:HB1	1:E:2253:TRP:HA	1.79	0.65
1:A:121:GLU:HG2	1:A:124:ARG:HH21	1.62	0.64
1:A:659:TYR:HB2	1:A:754:GLN:HG2	1.79	0.64
1:B:703:SER:O	1:C:2255:ARG:NH2	2.28	0.64
1:D:2068:LEU:HD22	1:D:2227:LEU:HG	1.79	0.64
1:A:2068:LEU:HD22	1:A:2227:LEU:HG	1.78	0.64
1:D:659:TYR:HB2	1:D:754:GLN:HG2	1.78	0.64
1:A:703:SER:O	1:B:2255:ARG:NH2	2.28	0.64
1:D:698:ALA:HB2	1:E:2256:GLY:HA3	1.79	0.64
1:A:2356:GLU:HA	1:A:2359:LYS:HG2	1.78	0.64
1:A:91:GLY:N	1:A:94:ASN:HD22	1.96	0.63
1:A:505:GLN:HE22	1:A:582:LEU:HD13	1.64	0.63
1:B:2068:LEU:HD22	1:B:2227:LEU:HG	1.79	0.63
1:B:659:TYR:HB2	1:B:754:GLN:HG2	1.80	0.63
1:E:91:GLY:N	1:E:94:ASN:HD22	1.96	0.63
1:C:703:SER:O	1:D:2255:ARG:NH2	2.29	0.63
1:E:568:ILE:HD11	1:E:606:ASP:HB2	1.81	0.63
1:A:519:PHE:O	1:A:553:ARG:NH2	2.31	0.63
1:A:1069:LEU:HD23	1:A:1786:GLU:HG3	1.80	0.63
1:B:121:GLU:HG2	1:B:124:ARG:HH21	1.64	0.63
1:D:505:GLN:HE22	1:D:582:LEU:HD13	1.64	0.63
1:E:2025:ASN:OD1	1:E:2272:ARG:NH1	2.30	0.63
1:D:1864:GLY:HA3	1:D:1883:TYR:CE1	2.34	0.63
1:E:121:GLU:HG2	1:E:124:ARG:HH21	1.62	0.63
1:E:519:PHE:O	1:E:553:ARG:NH2	2.31	0.63
1:C:670:LEU:HA	1:C:699:THR:HG21	1.81	0.62
1:A:1864:GLY:HA3	1:A:1883:TYR:CE1	2.34	0.62
1:A:368:LEU:N	1:A:381:THR:O	2.27	0.62
1:C:698:ALA:HB2	1:D:2256:GLY:HA3	1.81	0.62
1:D:703:SER:O	1:E:2255:ARG:NH2	2.28	0.62
1:E:1069:LEU:HD23	1:E:1786:GLU:HG3	1.81	0.62
1:C:91:GLY:N	1:C:94:ASN:HD22	1.97	0.62
1:C:659:TYR:HB2	1:C:754:GLN:HG2	1.80	0.62
1:E:1783:LEU:HD12	1:E:1788:ASN:HB3	1.81	0.62
1:A:2073:LYS:HZ1	1:E:2219:ALA:HA	1.64	0.62
1:B:368:LEU:N	1:B:381:THR:O	2.27	0.62
1:B:505:GLN:HE22	1:B:582:LEU:HD13	1.64	0.62
1:E:1864:GLY:HA3	1:E:1883:TYR:CE1	2.34	0.62
1:A:698:ALA:HB2	1:B:2256:GLY:HA3	1.81	0.62
1:B:1885:GLN:HA	1:B:1888:HIS:CE1	2.35	0.62
1:C:568:ILE:HD11	1:C:606:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1164:LYS:HE2	1:B:1611:ARG:HG2	1.81	0.61
1:A:2256:GLY:HA3	1:E:698:ALA:HB2	1.81	0.61
1:B:1864:GLY:HA3	1:B:1883:TYR:CE1	2.34	0.61
1:B:2067:ASN:HB3	1:B:2227:LEU:HD21	1.82	0.61
1:D:1069:LEU:HD23	1:D:1786:GLU:HG3	1.81	0.61
1:A:458:GLU:OE2	1:A:506:ARG:NH1	2.30	0.61
1:B:1783:LEU:HD12	1:B:1788:ASN:HB3	1.81	0.61
1:A:1885:GLN:HA	1:A:1888:HIS:CE1	2.35	0.61
1:B:2016:LEU:O	1:C:2327:ARG:NH2	2.34	0.61
1:E:505:GLN:HE22	1:E:582:LEU:HD13	1.66	0.61
1:C:2068:LEU:HD22	1:C:2227:LEU:HG	1.80	0.61
1:D:1783:LEU:HD12	1:D:1788:ASN:HB3	1.82	0.61
1:B:2219:ALA:HA	1:C:2073:LYS:HZ1	1.66	0.61
1:C:1783:LEU:HD12	1:C:1788:ASN:HB3	1.82	0.61
1:B:91:GLY:N	1:B:94:ASN:HD22	1.97	0.61
1:B:2153:ARG:NH1	1:B:2159:GLU:OE1	2.31	0.61
1:D:1885:GLN:HA	1:D:1888:HIS:CE1	2.35	0.61
1:D:2438:LYS:HG3	1:D:2446:GLU:HG3	1.83	0.61
1:E:2504:LEU:HD21	1:E:2507:ILE:HD11	1.82	0.61
1:C:2016:LEU:O	1:D:2327:ARG:NH2	2.34	0.61
1:C:2504:LEU:HD21	1:C:2507:ILE:HD11	1.82	0.61
1:C:1864:GLY:HA3	1:C:1883:TYR:CE1	2.35	0.61
1:C:2218:GLU:OE1	1:D:2073:LYS:NZ	2.34	0.61
1:A:568:ILE:HD11	1:A:606:ASP:HB2	1.83	0.61
1:B:2438:LYS:HG3	1:B:2446:GLU:HG3	1.83	0.61
1:B:2504:LEU:HD21	1:B:2507:ILE:HD11	1.81	0.61
1:C:519:PHE:O	1:C:553:ARG:NH2	2.34	0.61
1:E:1885:GLN:HA	1:E:1888:HIS:CE1	2.35	0.61
1:B:568:ILE:HD11	1:B:606:ASP:HB2	1.81	0.60
1:C:253:GLU:O	1:C:442:LYS:NZ	2.28	0.60
1:A:1611:ARG:HG2	1:E:1164:LYS:HE2	1.83	0.60
1:D:2504:LEU:HD21	1:D:2507:ILE:HD11	1.83	0.60
1:E:2393:PHE:HA	1:E:2396:LEU:HD12	1.83	0.60
1:A:1783:LEU:HD12	1:A:1788:ASN:HB3	1.83	0.60
1:B:2460:PHE:CE1	1:C:2330:GLU:HB3	2.36	0.60
1:D:670:LEU:HA	1:D:699:THR:HG21	1.84	0.60
1:D:2025:ASN:OD1	1:D:2272:ARG:NH1	2.30	0.60
1:A:2330:GLU:HB3	1:E:2460:PHE:CE1	2.36	0.60
1:B:698:ALA:HB2	1:C:2256:GLY:HA3	1.82	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HD12	1.84	0.60
1:D:1794:ARG:NH2	1:D:1798:TYR:OH	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2393:PHE:HA	1:D:2396:LEU:HD12	1.82	0.60
1:E:2438:LYS:HG3	1:E:2446:GLU:HG3	1.82	0.60
1:B:458:GLU:OE2	1:B:506:ARG:NH1	2.31	0.60
1:C:1885:GLN:HA	1:C:1888:HIS:CE1	2.36	0.60
1:E:659:TYR:HB2	1:E:754:GLN:HG2	1.83	0.60
1:E:830:LEU:HD21	1:E:835:LEU:HD12	1.83	0.60
1:B:2393:PHE:HA	1:B:2396:LEU:HD12	1.83	0.60
1:C:2025:ASN:OD1	1:C:2272:ARG:NH1	2.32	0.60
1:C:2438:LYS:HG3	1:C:2446:GLU:HG3	1.82	0.60
1:D:2460:PHE:CE1	1:E:2330:GLU:HB3	2.37	0.60
1:A:2460:PHE:CE1	1:B:2330:GLU:HB3	2.37	0.60
1:B:1069:LEU:HD23	1:B:1786:GLU:HG3	1.83	0.60
1:C:2460:PHE:CE1	1:D:2330:GLU:HB3	2.37	0.60
1:D:519:PHE:O	1:D:553:ARG:NH2	2.34	0.60
1:D:1607:THR:HG21	1:D:1768:PHE:HZ	1.66	0.60
1:B:670:LEU:HA	1:B:699:THR:HG21	1.82	0.60
1:D:568:ILE:HD11	1:D:606:ASP:HB2	1.83	0.60
1:A:2504:LEU:HD21	1:A:2507:ILE:HD11	1.82	0.59
1:C:337:ASN:ND2	1:C:421:TYR:O	2.25	0.59
1:B:2218:GLU:OE1	1:C:2073:LYS:NZ	2.33	0.59
1:D:91:GLY:N	1:D:94:ASN:HD22	2.00	0.59
1:A:830:LEU:HD21	1:A:835:LEU:HD12	1.84	0.59
1:A:2016:LEU:O	1:B:2327:ARG:NH2	2.35	0.59
1:C:741:GLY:HA2	1:E:2005:GLY:HA2	1.85	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HD12	1.83	0.59
1:A:670:LEU:HA	1:A:699:THR:HG21	1.83	0.59
1:D:2219:ALA:HA	1:E:2073:LYS:HZ1	1.67	0.59
1:D:2016:LEU:O	1:E:2327:ARG:NH2	2.34	0.59
1:A:2005:GLY:HA2	1:D:741:GLY:HA2	1.85	0.59
1:A:2393:PHE:HA	1:A:2396:LEU:HD12	1.85	0.59
1:A:2218:GLU:OE1	1:B:2073:LYS:NZ	2.35	0.58
1:C:540:SER:HB2	1:D:848:GLN:NE2	2.18	0.58
1:E:368:LEU:N	1:E:381:THR:O	2.27	0.58
1:A:741:GLY:HA2	1:C:2005:GLY:HA2	1.86	0.58
1:B:540:SER:HB2	1:C:848:GLN:NE2	2.18	0.58
1:C:2067:ASN:HB3	1:C:2227:LEU:HD21	1.84	0.58
1:E:337:ASN:ND2	1:E:421:TYR:O	2.25	0.58
1:A:848:GLN:NE2	1:E:540:SER:HB2	2.18	0.58
1:B:2005:GLY:HA2	1:E:741:GLY:HA2	1.85	0.58
1:E:1607:THR:HG21	1:E:1768:PHE:HZ	1.67	0.58
1:C:830:LEU:HD21	1:C:835:LEU:HD12	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1607:THR:HG21	1:C:1768:PHE:HZ	1.67	0.58
1:D:540:SER:HB2	1:E:848:GLN:NE2	2.18	0.58
1:A:2438:LYS:HG3	1:A:2446:GLU:HG3	1.86	0.58
1:B:741:GLY:HA2	1:D:2005:GLY:HA2	1.86	0.58
1:E:198:THR:O	1:E:445:ARG:NH1	2.37	0.58
1:A:540:SER:HB2	1:B:848:GLN:NE2	2.18	0.58
1:B:1607:THR:HG21	1:B:1768:PHE:HZ	1.67	0.58
1:D:2218:GLU:OE1	1:E:2073:LYS:NZ	2.34	0.58
1:D:2246:SER:HA	1:D:2250:LEU:HD23	1.85	0.58
1:A:2112:ASN:HA	1:A:2115:MET:HG2	1.86	0.58
1:C:2393:PHE:HA	1:C:2396:LEU:HD12	1.84	0.58
1:A:1607:THR:HG21	1:A:1768:PHE:HZ	1.69	0.58
1:B:519:PHE:O	1:B:553:ARG:NH2	2.37	0.58
1:B:2246:SER:HA	1:B:2250:LEU:HD23	1.85	0.58
1:E:458:GLU:OE2	1:E:506:ARG:NH1	2.30	0.58
1:E:2040:LEU:O	1:E:2044:ILE:HG12	2.04	0.58
1:A:2327:ARG:NH2	1:E:2016:LEU:O	2.36	0.58
1:B:1794:ARG:NH2	1:B:1798:TYR:OH	2.37	0.58
1:C:505:GLN:NE2	1:C:582:LEU:HD13	2.19	0.58
1:D:2153:ARG:NH1	1:D:2159:GLU:OE1	2.32	0.57
1:C:458:GLU:OE2	1:C:506:ARG:NH1	2.31	0.57
1:C:1966:ARG:HD2	1:C:1976:ILE:HG13	1.86	0.57
1:C:2219:ALA:HA	1:D:2073:LYS:HZ1	1.69	0.57
1:D:612:VAL:HG22	1:D:637:ILE:HD12	1.86	0.57
1:D:2067:ASN:HB3	1:D:2227:LEU:HD21	1.86	0.57
1:D:2112:ASN:HA	1:D:2115:MET:HG2	1.86	0.57
1:A:2246:SER:HA	1:A:2250:LEU:HD23	1.85	0.57
1:B:505:GLN:NE2	1:B:582:LEU:HD13	2.19	0.57
1:B:2040:LEU:O	1:B:2044:ILE:HG12	2.05	0.57
1:C:2246:SER:HA	1:C:2250:LEU:HD23	1.84	0.57
1:D:505:GLN:NE2	1:D:582:LEU:HD13	2.20	0.57
1:E:670:LEU:HA	1:E:699:THR:HG21	1.85	0.57
1:E:2246:SER:HA	1:E:2250:LEU:HD23	1.86	0.57
1:A:2040:LEU:O	1:A:2044:ILE:HG12	2.05	0.57
1:B:2353:LEU:HD23	1:B:2357:ILE:HD11	1.87	0.57
1:C:1220:LYS:HE2	1:C:1267:LEU:HB3	1.85	0.57
1:C:2040:LEU:O	1:C:2044:ILE:HG12	2.05	0.57
1:C:2112:ASN:HA	1:C:2115:MET:HG2	1.85	0.57
1:C:2153:ARG:NH1	1:C:2159:GLU:OE1	2.32	0.57
1:E:2067:ASN:HB3	1:E:2227:LEU:HD21	1.87	0.57
1:E:2112:ASN:HA	1:E:2115:MET:HG2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:ASP:OD1	1:B:798:ALA:N	2.38	0.57
1:B:2112:ASN:HA	1:B:2115:MET:HG2	1.87	0.57
1:A:2353:LEU:HD23	1:A:2357:ILE:HD11	1.87	0.56
1:B:646:TRP:CZ2	1:B:768:SER:HB3	2.40	0.56
1:D:2040:LEU:O	1:D:2044:ILE:HG12	2.05	0.56
1:A:836:ALA:HB2	1:A:846:LEU:HD12	1.87	0.56
1:A:2153:ARG:NH1	1:A:2159:GLU:OE1	2.32	0.56
1:C:2353:LEU:HD23	1:C:2357:ILE:HD11	1.88	0.56
1:D:337:ASN:ND2	1:D:421:TYR:O	2.25	0.56
1:D:458:GLU:OE2	1:D:506:ARG:NH1	2.32	0.56
1:D:646:TRP:CZ2	1:D:768:SER:HB3	2.40	0.56
1:D:797:ASP:OD1	1:D:798:ALA:N	2.38	0.56
1:D:1164:LYS:HE2	1:E:1611:ARG:HG2	1.85	0.56
1:D:2353:LEU:HD23	1:D:2357:ILE:HD11	1.87	0.56
1:E:1072:ASP:OD1	1:E:1073:THR:N	2.38	0.56
1:E:2353:LEU:HD23	1:E:2357:ILE:HD11	1.87	0.56
1:A:1966:ARG:HD2	1:A:1976:ILE:HG13	1.87	0.56
1:B:1072:ASP:OD1	1:B:1073:THR:N	2.38	0.56
1:E:836:ALA:HB2	1:E:846:LEU:HD12	1.87	0.56
1:B:1966:ARG:HD2	1:B:1976:ILE:HG13	1.87	0.56
1:E:797:ASP:OD1	1:E:798:ALA:N	2.38	0.56
1:E:2153:ARG:NH1	1:E:2159:GLU:OE1	2.33	0.56
1:C:797:ASP:OD1	1:C:798:ALA:N	2.38	0.56
1:C:2103:TYR:CE1	1:C:2189:ARG:HG2	2.40	0.56
1:D:836:ALA:HB2	1:D:846:LEU:HD12	1.88	0.56
1:A:337:ASN:ND2	1:A:421:TYR:O	2.25	0.56
1:B:836:ALA:HB2	1:B:846:LEU:HD12	1.88	0.56
1:B:2433:LEU:HA	1:B:2484:LEU:HA	1.88	0.56
1:D:1072:ASP:OD1	1:D:1073:THR:N	2.39	0.56
1:A:646:TRP:CZ2	1:A:768:SER:HB3	2.41	0.56
1:A:2067:ASN:HB3	1:A:2227:LEU:HD21	1.87	0.56
1:B:337:ASN:ND2	1:B:421:TYR:O	2.25	0.56
1:C:646:TRP:CZ2	1:C:768:SER:HB3	2.41	0.56
1:D:1271:ALA:HB1	1:E:1611:ARG:HD3	1.88	0.56
1:A:797:ASP:OD1	1:A:798:ALA:N	2.38	0.56
1:C:612:VAL:HG22	1:C:637:ILE:HD12	1.88	0.56
1:A:341:MET:HE2	1:A:359:PHE:CE1	2.42	0.55
1:A:505:GLN:NE2	1:A:582:LEU:HD13	2.20	0.55
1:C:836:ALA:HB2	1:C:846:LEU:HD12	1.88	0.55
1:C:2341:TYR:OH	1:C:2390:SER:O	2.20	0.55
1:D:2433:LEU:HA	1:D:2484:LEU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:646:TRP:CZ2	1:E:768:SER:HB3	2.41	0.55
1:C:1164:LYS:HE2	1:D:1611:ARG:HG2	1.87	0.55
1:D:2204:LYS:HG2	1:E:2087:LYS:HD2	1.88	0.55
1:E:2433:LEU:HA	1:E:2484:LEU:HA	1.87	0.55
1:A:1252:GLN:HB3	1:A:1297:ASN:OD1	2.06	0.55
1:E:557:ILE:HB	1:E:561:SER:OG	2.07	0.55
1:E:1966:ARG:HD2	1:E:1976:ILE:HG13	1.87	0.55
1:A:2025:ASN:OD1	1:A:2272:ARG:NH1	2.33	0.55
1:B:1058:ASP:O	1:B:1062:GLN:HG3	2.06	0.55
1:E:505:GLN:NE2	1:E:582:LEU:HD13	2.20	0.55
1:A:1072:ASP:OD1	1:A:1073:THR:N	2.39	0.55
1:B:341:MET:HE1	1:B:359:PHE:CE1	2.42	0.55
1:C:198:THR:O	1:C:445:ARG:NH1	2.39	0.55
1:D:1117:ASP:OD1	1:D:1118:ALA:N	2.38	0.55
1:A:612:VAL:HG22	1:A:637:ILE:HD12	1.87	0.55
1:D:341:MET:HE2	1:D:359:PHE:CE1	2.42	0.55
1:E:120:THR:O	1:E:124:ARG:HG3	2.07	0.55
1:E:253:GLU:O	1:E:442:LYS:NZ	2.30	0.55
1:A:2103:TYR:CE1	1:A:2189:ARG:HG2	2.42	0.55
1:B:1164:LYS:HE2	1:C:1611:ARG:HG2	1.87	0.55
1:B:1252:GLN:HB3	1:B:1297:ASN:OD1	2.07	0.55
1:D:368:LEU:N	1:D:381:THR:O	2.27	0.55
1:B:1868:TYR:HB3	1:B:1976:ILE:HD12	1.89	0.55
1:C:120:THR:O	1:C:124:ARG:HG3	2.07	0.55
1:C:368:LEU:HG	1:C:370:ILE:HD11	1.89	0.55
1:A:2433:LEU:HA	1:A:2484:LEU:HA	1.88	0.55
1:C:1252:GLN:HB3	1:C:1297:ASN:OD1	2.07	0.55
1:D:1630:GLN:HG2	1:D:1772:PHE:CE2	2.42	0.55
1:A:557:ILE:HB	1:A:561:SER:OG	2.07	0.54
1:B:2025:ASN:OD1	1:B:2272:ARG:NH1	2.35	0.54
1:B:2103:TYR:CE1	1:B:2189:ARG:HG2	2.43	0.54
1:C:341:MET:HE2	1:C:359:PHE:CE1	2.42	0.54
1:C:2103:TYR:CE1	1:C:2193:GLU:HG2	2.43	0.54
1:D:1966:ARG:HD2	1:D:1976:ILE:HG13	1.87	0.54
1:A:811:VAL:HG22	1:A:822:LEU:HD21	1.89	0.54
1:B:120:THR:O	1:B:124:ARG:HG3	2.07	0.54
1:C:368:LEU:N	1:C:381:THR:O	2.27	0.54
1:D:120:THR:O	1:D:124:ARG:HG3	2.06	0.54
1:D:1058:ASP:O	1:D:1062:GLN:HG3	2.07	0.54
1:A:120:THR:O	1:A:124:ARG:HG3	2.07	0.54
1:A:368:LEU:HG	1:A:370:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:ARG:NH2	1:A:1798:TYR:OH	2.39	0.54
1:C:1072:ASP:OD1	1:C:1073:THR:N	2.39	0.54
1:C:2337:LEU:HB3	1:C:2507:ILE:HB	1.89	0.54
1:D:1252:GLN:HB3	1:D:1297:ASN:OD1	2.07	0.54
1:E:300:ALA:HA	1:E:303:PHE:HD2	1.73	0.54
1:E:612:VAL:HG22	1:E:637:ILE:HD12	1.88	0.54
1:A:1630:GLN:HG2	1:A:1772:PHE:CE2	2.42	0.54
1:E:1252:GLN:HB3	1:E:1297:ASN:OD1	2.07	0.54
1:B:510:ASN:OD1	1:C:153:GLN:NE2	2.38	0.54
1:C:2433:LEU:HA	1:C:2484:LEU:HA	1.88	0.54
1:B:198:THR:O	1:B:445:ARG:NH1	2.41	0.54
1:B:368:LEU:HG	1:B:370:ILE:HD11	1.89	0.54
1:D:2426:TYR:HB3	1:E:2334:THR:HG21	1.88	0.54
1:A:195:SER:HB3	1:A:198:THR:OG1	2.08	0.54
1:A:300:ALA:HA	1:A:303:PHE:HD2	1.72	0.54
1:A:848:GLN:HE22	1:E:540:SER:HB2	1.73	0.54
1:C:195:SER:HB3	1:C:198:THR:OG1	2.08	0.54
1:E:1630:GLN:HG2	1:E:1772:PHE:CE2	2.42	0.54
1:A:198:THR:O	1:A:445:ARG:NH1	2.40	0.54
1:A:1271:ALA:HB1	1:B:1611:ARG:HD3	1.90	0.54
1:E:341:MET:HE2	1:E:359:PHE:CE1	2.43	0.54
1:D:368:LEU:HG	1:D:370:ILE:HD11	1.89	0.54
1:D:811:VAL:HG22	1:D:822:LEU:HD21	1.89	0.54
1:A:1058:ASP:O	1:A:1062:GLN:HG3	2.06	0.54
1:C:557:ILE:HB	1:C:561:SER:OG	2.07	0.54
1:D:557:ILE:HB	1:D:561:SER:OG	2.07	0.54
1:E:2337:LEU:HB3	1:E:2507:ILE:HB	1.90	0.54
1:A:2103:TYR:CE1	1:A:2193:GLU:HG2	2.43	0.53
1:B:612:VAL:HG22	1:B:637:ILE:HD12	1.89	0.53
1:C:2053:ASN:ND2	1:C:2241:LEU:HD11	2.23	0.53
1:D:2141:VAL:HG21	1:E:1175:LYS:HE2	1.90	0.53
1:E:2103:TYR:CE1	1:E:2189:ARG:HG2	2.44	0.53
1:C:300:ALA:HA	1:C:303:PHE:HD2	1.72	0.53
1:E:197:ALA:N	1:E:948:THR:HG21	2.23	0.53
1:A:1071:ALA:HB2	1:A:1791:GLU:OE2	2.09	0.53
1:C:2426:TYR:HB3	1:D:2334:THR:HG21	1.90	0.53
1:E:195:SER:HB3	1:E:198:THR:OG1	2.08	0.53
1:E:368:LEU:HG	1:E:370:ILE:HD11	1.89	0.53
1:E:811:VAL:HG22	1:E:822:LEU:HD21	1.90	0.53
1:B:557:ILE:HB	1:B:561:SER:OG	2.07	0.53
1:C:268:PHE:HZ	1:C:441:ASN:HB2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1058:ASP:O	1:C:1062:GLN:HG3	2.09	0.53
1:C:1271:ALA:HB1	1:D:1611:ARG:HD3	1.90	0.53
1:D:198:THR:O	1:D:445:ARG:NH1	2.41	0.53
1:D:540:SER:HB2	1:E:848:GLN:HE22	1.74	0.53
1:D:1220:LYS:HE2	1:D:1267:LEU:HB3	1.91	0.53
1:E:2341:TYR:OH	1:E:2390:SER:O	2.21	0.53
1:C:926:LEU:HD22	1:C:930:GLN:HB3	1.91	0.53
1:D:1790:ASP:OD1	1:D:1791:GLU:N	2.42	0.53
1:D:2103:TYR:CE1	1:D:2189:ARG:HG2	2.43	0.53
1:A:197:ALA:N	1:A:948:THR:HG21	2.24	0.53
1:B:540:SER:HB2	1:C:848:GLN:HE22	1.73	0.53
1:B:719:GLN:HB3	1:B:724:ALA:HB1	1.90	0.53
1:B:2141:VAL:HG21	1:C:1175:LYS:HE2	1.91	0.53
1:B:2426:TYR:HB3	1:C:2334:THR:HG21	1.89	0.53
1:C:540:SER:HB2	1:D:848:GLN:HE22	1.74	0.53
1:B:1271:ALA:HB1	1:C:1611:ARG:HD3	1.90	0.53
1:D:197:ALA:N	1:D:948:THR:HG21	2.23	0.53
1:D:300:ALA:HA	1:D:303:PHE:HD2	1.73	0.53
1:E:2122:ALA:HA	1:E:2171:VAL:HG23	1.91	0.53
1:B:195:SER:HB3	1:B:198:THR:OG1	2.08	0.53
1:B:1790:ASP:OD1	1:B:1791:GLU:N	2.42	0.53
1:B:2204:LYS:HG2	1:C:2087:LYS:HD2	1.90	0.53
1:E:671:LEU:HD22	1:E:734:LEU:HD21	1.90	0.53
1:A:1220:LYS:HE2	1:A:1267:LEU:HB3	1.90	0.53
1:C:510:ASN:OD1	1:D:153:GLN:NE2	2.39	0.53
1:C:671:LEU:HD22	1:C:734:LEU:HD21	1.90	0.53
1:E:1058:ASP:O	1:E:1062:GLN:HG3	2.08	0.53
1:A:540:SER:HB2	1:B:848:GLN:HE22	1.74	0.53
1:A:1611:ARG:HD3	1:E:1271:ALA:HB1	1.91	0.53
1:E:462:ARG:NH1	1:E:506:ARG:HH11	2.07	0.53
1:A:2426:TYR:HB3	1:B:2334:THR:HG21	1.91	0.52
1:B:197:ALA:N	1:B:948:THR:HG21	2.23	0.52
1:C:1071:ALA:HB2	1:C:1791:GLU:OE2	2.09	0.52
1:D:195:SER:HB3	1:D:198:THR:OG1	2.08	0.52
1:D:1868:TYR:HB3	1:D:1976:ILE:HD12	1.91	0.52
1:A:2219:ALA:HA	1:B:2073:LYS:HZ1	1.73	0.52
1:B:268:PHE:HZ	1:B:441:ASN:HB2	1.75	0.52
1:B:300:ALA:HA	1:B:303:PHE:HD2	1.73	0.52
1:B:671:LEU:HD22	1:B:734:LEU:HD21	1.90	0.52
1:C:141:ARG:HH22	1:C:1005:GLU:CD	2.13	0.52
1:C:1790:ASP:OD1	1:C:1791:GLU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:THR:HG22	1:E:604:GLU:OE1	2.10	0.52
1:E:1220:LYS:HE2	1:E:1267:LEU:HB3	1.91	0.52
1:E:1722:GLY:O	1:E:1739:SER:HB2	2.10	0.52
1:A:1790:ASP:OD1	1:A:1791:GLU:N	2.42	0.52
1:B:2053:ASN:ND2	1:B:2241:LEU:HD11	2.24	0.52
1:B:2122:ALA:HA	1:B:2171:VAL:HG23	1.91	0.52
1:B:2341:TYR:OH	1:B:2390:SER:O	2.22	0.52
1:D:671:LEU:HD22	1:D:734:LEU:HD21	1.90	0.52
1:D:812:ASN:HA	1:E:1998:ALA:HB2	1.91	0.52
1:E:2053:ASN:ND2	1:E:2241:LEU:HD11	2.24	0.52
1:C:1794:ARG:NH2	1:C:1798:TYR:OH	2.42	0.52
1:D:268:PHE:HZ	1:D:441:ASN:HB2	1.74	0.52
1:D:1878:GLU:HA	1:D:1881:MET:HG3	1.91	0.52
1:E:1878:GLU:HA	1:E:1881:MET:HG3	1.90	0.52
1:A:2334:THR:HG21	1:E:2426:TYR:HB3	1.90	0.52
1:B:1117:ASP:OD1	1:B:1118:ALA:N	2.39	0.52
1:B:1630:GLN:HG2	1:B:1772:PHE:CE2	2.44	0.52
1:C:197:ALA:N	1:C:948:THR:HG21	2.24	0.52
1:E:1117:ASP:OD1	1:E:1118:ALA:N	2.39	0.52
1:C:811:VAL:HG22	1:C:822:LEU:HD21	1.91	0.52
1:E:926:LEU:HD22	1:E:930:GLN:HB3	1.92	0.52
1:A:719:GLN:HB3	1:A:724:ALA:HB1	1.90	0.52
1:A:812:ASN:HA	1:B:1998:ALA:HB2	1.91	0.52
1:B:237:LEU:HD11	1:B:483:TYR:HB2	1.91	0.52
1:B:1230:ARG:NH2	1:B:1251:ASN:OD1	2.43	0.52
1:D:462:ARG:NH1	1:D:506:ARG:HH11	2.07	0.52
1:A:2141:VAL:HG21	1:B:1175:LYS:HE2	1.92	0.52
1:B:462:ARG:NH1	1:B:506:ARG:HH11	2.08	0.52
1:C:462:ARG:NH1	1:C:506:ARG:HH11	2.06	0.52
1:C:601:THR:HG22	1:C:604:GLU:OE1	2.10	0.52
1:E:719:GLN:HB3	1:E:724:ALA:HB1	1.89	0.52
1:E:2103:TYR:CE1	1:E:2193:GLU:HG2	2.45	0.52
1:A:253:GLU:O	1:A:442:LYS:NZ	2.28	0.52
1:A:268:PHE:HZ	1:A:441:ASN:HB2	1.75	0.52
1:A:601:THR:HG22	1:A:604:GLU:OE1	2.10	0.52
1:C:1630:GLN:HG2	1:C:1772:PHE:CE2	2.45	0.52
1:C:1878:GLU:HA	1:C:1881:MET:HG3	1.91	0.52
1:E:497:ILE:HG21	1:E:589:TYR:HD2	1.74	0.52
1:A:237:LEU:HD11	1:A:483:TYR:HB2	1.92	0.52
1:A:926:LEU:HD22	1:A:930:GLN:HB3	1.92	0.52
1:A:1878:GLU:HA	1:A:1881:MET:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:THR:HG22	1:B:604:GLU:OE1	2.10	0.52
1:B:678:LEU:HD11	1:B:692:MET:HA	1.92	0.52
1:B:811:VAL:HG22	1:B:822:LEU:HD21	1.91	0.52
1:B:2266:TYR:CZ	1:B:2297:TRP:HB2	2.45	0.52
1:B:1722:GLY:O	1:B:1739:SER:HB2	2.11	0.51
1:C:1146:LYS:NZ	1:C:1147:ILE:O	2.40	0.51
1:C:1722:GLY:O	1:C:1739:SER:HB2	2.10	0.51
1:D:1071:ALA:HB2	1:D:1791:GLU:OE2	2.10	0.51
1:A:671:LEU:HD22	1:A:734:LEU:HD21	1.92	0.51
1:A:1614:VAL:O	1:A:1618:THR:HG23	2.11	0.51
1:B:537:ASP:HA	1:B:577:LYS:HA	1.91	0.51
1:B:564:ARG:NH2	1:C:842:ASP:OD1	2.43	0.51
1:B:2337:LEU:HB3	1:B:2507:ILE:HB	1.93	0.51
1:C:2338:ALA:HA	1:C:2353:LEU:HD13	1.92	0.51
1:E:1794:ARG:NH2	1:E:1798:TYR:OH	2.43	0.51
1:A:537:ASP:HA	1:A:577:LYS:HA	1.92	0.51
1:A:1722:GLY:O	1:A:1739:SER:HB2	2.10	0.51
1:B:1614:VAL:O	1:B:1618:THR:HG23	2.11	0.51
1:A:678:LEU:HD11	1:A:692:MET:HA	1.92	0.51
1:C:2004:GLN:H	1:C:2300:THR:HG22	1.76	0.51
1:D:2341:TYR:OH	1:D:2390:SER:O	2.22	0.51
1:E:1071:ALA:HB2	1:E:1791:GLU:OE2	2.11	0.51
1:A:2204:LYS:HG2	1:B:2087:LYS:HD2	1.92	0.51
1:D:601:THR:HG22	1:D:604:GLU:OE1	2.10	0.51
1:E:1230:ARG:NH2	1:E:1251:ASN:OD1	2.43	0.51
1:A:141:ARG:HH22	1:A:1005:GLU:CD	2.13	0.51
1:A:2053:ASN:ND2	1:A:2241:LEU:HD11	2.25	0.51
1:A:2266:TYR:CZ	1:A:2297:TRP:HB2	2.46	0.51
1:B:536:ILE:HD13	1:B:547:ARG:HB2	1.93	0.51
1:C:1868:TYR:HB3	1:C:1976:ILE:HD12	1.93	0.51
1:D:237:LEU:HD11	1:D:483:TYR:HB2	1.93	0.51
1:A:842:ASP:OD1	1:E:564:ARG:NH2	2.44	0.51
1:A:153:GLN:NE2	1:E:510:ASN:OD1	2.39	0.51
1:A:724:ALA:O	1:A:729:LYS:NZ	2.32	0.51
1:A:1024:TYR:O	1:A:1030:THR:OG1	2.23	0.51
1:B:141:ARG:HH22	1:B:1005:GLU:CD	2.13	0.51
1:B:1878:GLU:HA	1:B:1881:MET:HG3	1.92	0.51
1:B:2132:ARG:HH11	1:B:2163:TYR:HB3	1.76	0.51
1:D:926:LEU:HD22	1:D:930:GLN:HB3	1.93	0.51
1:D:2122:ALA:HA	1:D:2171:VAL:HG23	1.93	0.51
1:E:141:ARG:HH22	1:E:1005:GLU:CD	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:268:PHE:HZ	1:E:441:ASN:HB2	1.74	0.51
1:E:2266:TYR:CZ	1:E:2297:TRP:HB2	2.45	0.51
1:B:2103:TYR:CE1	1:B:2193:GLU:HG2	2.45	0.51
1:D:2337:LEU:HB3	1:D:2507:ILE:HB	1.92	0.51
1:E:370:ILE:HG13	1:E:410:LEU:HG	1.93	0.51
1:E:1790:ASP:OD1	1:E:1791:GLU:N	2.43	0.51
1:A:2122:ALA:HA	1:A:2171:VAL:HG23	1.93	0.51
1:C:719:GLN:HB3	1:C:724:ALA:HB1	1.92	0.51
1:D:2103:TYR:CE1	1:D:2193:GLU:HG2	2.46	0.51
1:A:453:SER:HB3	1:A:456:ILE:HG12	1.93	0.50
1:A:462:ARG:NH1	1:A:506:ARG:HH11	2.06	0.50
1:A:2087:LYS:HD2	1:E:2204:LYS:HG2	1.92	0.50
1:D:1722:GLY:O	1:D:1739:SER:HB2	2.10	0.50
1:D:2053:ASN:ND2	1:D:2241:LEU:HD11	2.26	0.50
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.47	0.50
1:A:2341:TYR:OH	1:A:2390:SER:O	2.21	0.50
1:B:497:ILE:HG21	1:B:589:TYR:HD2	1.76	0.50
1:C:370:ILE:HG13	1:C:410:LEU:HG	1.94	0.50
1:D:537:ASP:HA	1:D:577:LYS:HA	1.94	0.50
1:E:1291:TYR:HA	1:E:1294:PHE:CE2	2.47	0.50
1:C:536:ILE:HD13	1:C:547:ARG:HB2	1.94	0.50
1:D:702:LEU:HD22	1:D:708:ALA:HB2	1.93	0.50
1:C:678:LEU:HD11	1:C:692:MET:HA	1.94	0.50
1:D:1230:ARG:NH2	1:D:1251:ASN:OD1	2.45	0.50
1:A:2073:LYS:NZ	1:E:2218:GLU:OE1	2.34	0.50
1:B:460:ILE:HG21	1:B:478:VAL:HG12	1.94	0.50
1:D:370:ILE:HG13	1:D:410:LEU:HG	1.94	0.50
1:D:1291:TYR:HA	1:D:1294:PHE:CE2	2.47	0.50
1:E:470:ILE:HA	1:E:474:VAL:HG11	1.93	0.50
1:E:1614:VAL:O	1:E:1618:THR:HG23	2.11	0.50
1:B:1291:TYR:HA	1:B:1294:PHE:CE2	2.47	0.50
1:B:2033:LEU:HD11	1:B:2266:TYR:HA	1.94	0.50
1:C:812:ASN:HA	1:D:1998:ALA:HB2	1.93	0.50
1:C:1230:ARG:NH2	1:C:1251:ASN:OD1	2.45	0.50
1:A:510:ASN:OD1	1:B:153:GLN:NE2	2.40	0.50
1:A:1291:TYR:HA	1:A:1294:PHE:CE2	2.47	0.50
1:A:1998:ALA:HB2	1:E:812:ASN:HA	1.92	0.50
1:A:2337:LEU:HB3	1:A:2507:ILE:HB	1.93	0.50
1:C:470:ILE:HA	1:C:474:VAL:HG11	1.94	0.50
1:C:702:LEU:HD22	1:C:708:ALA:HB2	1.93	0.50
1:B:926:LEU:HD22	1:B:930:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:MET:CE	1:C:410:LEU:HD22	2.42	0.50
1:C:2122:ALA:HA	1:C:2171:VAL:HG23	1.94	0.50
1:C:2204:LYS:HG2	1:D:2087:LYS:HD2	1.93	0.50
1:E:471:ASN:H	1:E:474:VAL:HG12	1.76	0.50
1:A:371:LYS:HG2	1:A:377:GLU:HA	1.94	0.50
1:A:2004:GLN:H	1:A:2300:THR:HG22	1.76	0.50
1:B:370:ILE:HG13	1:B:410:LEU:HG	1.93	0.50
1:C:497:ILE:HG21	1:C:589:TYR:HD2	1.76	0.50
1:D:2393:PHE:HE1	1:D:2482:LEU:HB2	1.77	0.50
1:E:198:THR:HB	1:E:199:PRO:HA	1.94	0.50
1:E:453:SER:HB3	1:E:456:ILE:HG12	1.94	0.50
1:A:341:MET:CE	1:A:410:LEU:HD22	2.42	0.49
1:B:1220:LYS:HE2	1:B:1267:LEU:HB3	1.93	0.49
1:D:141:ARG:HH22	1:D:1005:GLU:CD	2.13	0.49
1:D:371:LYS:HG2	1:D:377:GLU:HA	1.93	0.49
1:E:210:VAL:HG22	1:E:926:LEU:HD11	1.94	0.49
1:E:702:LEU:HD22	1:E:708:ALA:HB2	1.93	0.49
1:A:470:ILE:HA	1:A:474:VAL:HG11	1.93	0.49
1:B:470:ILE:HA	1:B:474:VAL:HG11	1.94	0.49
1:C:522:PRO:O	1:C:553:ARG:NH1	2.45	0.49
1:C:564:ARG:NH2	1:D:842:ASP:OD1	2.45	0.49
1:C:2266:TYR:CZ	1:C:2297:TRP:HB2	2.48	0.49
1:E:2393:PHE:HE1	1:E:2482:LEU:HB2	1.77	0.49
1:A:1230:ARG:NH2	1:A:1251:ASN:OD1	2.45	0.49
1:A:1962:THR:OG1	1:A:1966:ARG:NH2	2.45	0.49
1:C:471:ASN:H	1:C:474:VAL:HG12	1.77	0.49
1:D:471:ASN:H	1:D:474:VAL:HG12	1.77	0.49
1:A:702:LEU:HD22	1:A:708:ALA:HB2	1.93	0.49
1:A:1098:HIS:HE1	1:A:1100:ASN:HB3	1.78	0.49
1:B:1071:ALA:HB2	1:B:1791:GLU:OE2	2.11	0.49
1:C:537:ASP:HA	1:C:577:LYS:HA	1.93	0.49
1:D:470:ILE:HA	1:D:474:VAL:HG11	1.93	0.49
1:A:341:MET:HE1	1:A:410:LEU:HD22	1.93	0.49
1:A:1175:LYS:HE2	1:E:2141:VAL:HG21	1.94	0.49
1:B:1098:HIS:HE1	1:B:1100:ASN:HB3	1.78	0.49
1:C:1614:VAL:O	1:C:1618:THR:HG23	2.11	0.49
1:D:198:THR:HB	1:D:199:PRO:HA	1.94	0.49
1:D:460:ILE:HG21	1:D:478:VAL:HG12	1.95	0.49
1:E:407:GLU:HA	1:E:425:LYS:HA	1.94	0.49
1:A:1117:ASP:OD1	1:A:1118:ALA:N	2.38	0.49
1:A:2099:TYR:CE2	1:A:2195:GLN:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:LYS:HG2	1:B:377:GLU:HA	1.93	0.49
1:D:1614:VAL:O	1:D:1618:THR:HG23	2.11	0.49
1:A:370:ILE:HG13	1:A:410:LEU:HG	1.94	0.49
1:A:714:TRP:CZ3	1:A:762:LEU:HD22	2.48	0.49
1:B:341:MET:CE	1:B:410:LEU:HD22	2.42	0.49
1:C:371:LYS:HG2	1:C:377:GLU:HA	1.93	0.49
1:C:1291:TYR:HA	1:C:1294:PHE:CE2	2.47	0.49
1:D:1108:THR:OG1	1:D:1128:HIS:NE2	2.37	0.49
1:E:341:MET:CE	1:E:410:LEU:HD22	2.42	0.49
1:E:371:LYS:HG2	1:E:377:GLU:HA	1.93	0.49
1:A:2132:ARG:HH11	1:A:2163:TYR:HB3	1.77	0.49
1:B:453:SER:HB3	1:B:456:ILE:HG12	1.94	0.49
1:D:536:ILE:HD13	1:D:547:ARG:HB2	1.94	0.49
1:D:1962:THR:OG1	1:D:1966:ARG:NH2	2.46	0.49
1:E:237:LEU:HD11	1:E:483:TYR:HB2	1.95	0.49
1:E:678:LEU:HD11	1:E:692:MET:HA	1.93	0.49
1:A:497:ILE:HG21	1:A:589:TYR:HD2	1.77	0.49
1:A:564:ARG:NH2	1:B:842:ASP:OD1	2.46	0.49
1:B:198:THR:HB	1:B:199:PRO:HA	1.94	0.49
1:C:453:SER:HB3	1:C:456:ILE:HG12	1.94	0.49
1:D:453:SER:HB3	1:D:456:ILE:HG12	1.93	0.49
1:D:564:ARG:NH2	1:E:842:ASP:OD1	2.46	0.49
1:A:2338:ALA:HA	1:A:2353:LEU:HD13	1.94	0.49
1:B:471:ASN:H	1:B:474:VAL:HG12	1.77	0.49
1:C:210:VAL:HG22	1:C:926:LEU:HD11	1.95	0.49
1:E:2099:TYR:CE2	1:E:2195:GLN:HB3	2.48	0.49
1:A:536:ILE:HD13	1:A:547:ARG:HB2	1.94	0.48
1:B:702:LEU:HD22	1:B:708:ALA:HB2	1.94	0.48
1:B:1962:THR:OG1	1:B:1966:ARG:NH2	2.46	0.48
1:D:2235:GLN:HG3	1:E:1995:LEU:HB2	1.96	0.48
1:E:1868:TYR:HB3	1:E:1976:ILE:HD12	1.95	0.48
1:A:471:ASN:H	1:A:474:VAL:HG12	1.78	0.48
1:B:2338:ALA:HA	1:B:2353:LEU:HD13	1.95	0.48
1:C:714:TRP:CZ3	1:C:762:LEU:HD22	2.48	0.48
1:D:341:MET:CE	1:D:410:LEU:HD22	2.42	0.48
1:D:2099:TYR:CE2	1:D:2195:GLN:HB3	2.49	0.48
1:C:1098:HIS:HE1	1:C:1100:ASN:HB3	1.78	0.48
1:C:2393:PHE:HE1	1:C:2482:LEU:HB2	1.78	0.48
1:D:1098:HIS:HE1	1:D:1100:ASN:HB3	1.79	0.48
1:E:537:ASP:HA	1:E:577:LYS:HA	1.95	0.48
1:A:198:THR:HB	1:A:199:PRO:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2393:PHE:HE1	1:B:2482:LEU:HB2	1.78	0.48
1:C:2132:ARG:HH11	1:C:2163:TYR:HB3	1.79	0.48
1:D:719:GLN:HB3	1:D:724:ALA:HB1	1.95	0.48
1:E:1098:HIS:HE1	1:E:1100:ASN:HB3	1.78	0.48
1:A:407:GLU:HA	1:A:425:LYS:HA	1.94	0.48
1:B:2099:TYR:CE2	1:B:2195:GLN:HB3	2.48	0.48
1:C:198:THR:HB	1:C:199:PRO:HA	1.94	0.48
1:C:460:ILE:HG21	1:C:478:VAL:HG12	1.96	0.48
1:D:678:LEU:HD11	1:D:692:MET:HA	1.95	0.48
1:D:2004:GLN:H	1:D:2300:THR:HG22	1.78	0.48
1:E:460:ILE:HG21	1:E:478:VAL:HG12	1.96	0.48
1:A:2393:PHE:HE1	1:A:2482:LEU:HB2	1.77	0.48
1:D:210:VAL:HG22	1:D:926:LEU:HD11	1.96	0.48
1:E:497:ILE:HG21	1:E:589:TYR:CD2	2.49	0.48
1:A:160:SER:HA	1:A:982:LYS:HA	1.96	0.48
1:A:1124:ARG:HD2	1:A:1144:TRP:CE2	2.49	0.48
1:D:510:ASN:OD1	1:E:153:GLN:NE2	2.40	0.48
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.49	0.48
1:E:1124:ARG:HD2	1:E:1144:TRP:CE2	2.49	0.48
1:A:464:VAL:HG21	1:A:474:VAL:HA	1.96	0.48
1:B:197:ALA:H	1:B:948:THR:HG21	1.79	0.47
1:D:2338:ALA:HA	1:D:2353:LEU:HD13	1.95	0.47
1:A:460:ILE:HG21	1:A:478:VAL:HG12	1.96	0.47
1:D:464:VAL:HG21	1:D:474:VAL:HA	1.97	0.47
1:A:522:PRO:O	1:A:553:ARG:NH1	2.46	0.47
1:C:341:MET:HE1	1:C:410:LEU:HD22	1.96	0.47
1:C:2033:LEU:HD11	1:C:2266:TYR:HA	1.96	0.47
1:D:348:PHE:CE1	1:D:352:ASN:HB3	2.50	0.47
1:D:407:GLU:HA	1:D:425:LYS:HA	1.96	0.47
1:D:497:ILE:HG21	1:D:589:TYR:HD2	1.79	0.47
1:E:2338:ALA:HA	1:E:2353:LEU:HD13	1.95	0.47
1:C:1117:ASP:OD1	1:C:1118:ALA:N	2.39	0.47
1:D:127:ARG:HG3	1:D:127:ARG:HH11	1.79	0.47
1:E:714:TRP:CZ3	1:E:762:LEU:HD22	2.49	0.47
1:A:1868:TYR:HB3	1:A:1976:ILE:HD12	1.96	0.47
1:B:2004:GLN:H	1:B:2300:THR:HG22	1.79	0.47
1:B:1124:ARG:HD2	1:B:1144:TRP:CE2	2.50	0.47
1:B:2469:PHE:H	1:C:2327:ARG:NH2	2.13	0.47
1:C:2078:LEU:HD13	1:C:2217:ARG:HA	1.97	0.47
1:E:127:ARG:HG3	1:E:127:ARG:HH11	1.79	0.47
1:E:2132:ARG:HH11	1:E:2163:TYR:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.80	0.47
1:A:2469:PHE:H	1:B:2327:ARG:NH2	2.13	0.47
1:D:2033:LEU:HD11	1:D:2266:TYR:HA	1.96	0.47
1:E:536:ILE:HD13	1:E:547:ARG:HB2	1.96	0.47
1:A:2033:LEU:HD11	1:A:2266:TYR:HA	1.96	0.47
1:B:538:LEU:HB2	1:B:566:LEU:HD22	1.97	0.47
1:C:160:SER:HA	1:C:982:LYS:HA	1.97	0.47
1:C:1962:THR:OG1	1:C:1966:ARG:NH2	2.47	0.47
1:E:2004:GLN:H	1:E:2300:THR:HG22	1.79	0.47
1:A:348:PHE:CE1	1:A:352:ASN:HB3	2.50	0.47
1:B:407:GLU:HA	1:B:425:LYS:HA	1.97	0.47
1:B:714:TRP:CZ3	1:B:762:LEU:HD22	2.50	0.47
1:B:812:ASN:HA	1:C:1998:ALA:HB2	1.96	0.47
1:C:2469:PHE:H	1:D:2327:ARG:NH2	2.13	0.47
1:A:1001:LEU:HD23	1:A:1013:ILE:HD12	1.97	0.46
1:C:497:ILE:HG21	1:C:589:TYR:CD2	2.50	0.46
1:C:1617:ALA:HA	1:C:1624:ILE:HD11	1.97	0.46
1:D:341:MET:HE1	1:D:410:LEU:HD22	1.97	0.46
1:D:1617:ALA:HA	1:D:1624:ILE:HD11	1.97	0.46
1:B:1244:THR:HG21	1:B:1268:TYR:CD1	2.50	0.46
1:D:1001:LEU:HD23	1:D:1013:ILE:HD12	1.96	0.46
1:A:1617:ALA:HA	1:A:1624:ILE:HD11	1.97	0.46
1:B:341:MET:HE3	1:B:410:LEU:HD22	1.96	0.46
1:A:730:PHE:HE1	1:A:752:ILE:HG23	1.81	0.46
1:D:593:LEU:O	1:D:597:ILE:HG12	2.16	0.46
1:E:348:PHE:CE1	1:E:352:ASN:HB3	2.50	0.46
1:B:127:ARG:HG3	1:B:127:ARG:HH11	1.80	0.46
1:B:2321:HIS:NE2	1:B:2325:ASP:OD2	2.49	0.46
1:D:522:PRO:O	1:D:553:ARG:NH1	2.45	0.46
1:E:2033:LEU:HD11	1:E:2266:TYR:HA	1.96	0.46
1:B:474:VAL:O	1:B:478:VAL:HG13	2.16	0.46
1:C:348:PHE:CE1	1:C:352:ASN:HB3	2.50	0.46
1:D:1244:THR:HG21	1:D:1268:TYR:CD1	2.50	0.46
1:D:2132:ARG:HH11	1:D:2163:TYR:HB3	1.80	0.46
1:E:1617:ALA:HA	1:E:1624:ILE:HD11	1.98	0.46
1:B:593:LEU:O	1:B:597:ILE:HG12	2.16	0.46
1:C:237:LEU:HD11	1:C:483:TYR:HB2	1.98	0.46
1:C:407:GLU:HA	1:C:425:LYS:HA	1.96	0.46
1:E:174:LYS:HG2	1:E:185:VAL:HG21	1.96	0.46
1:E:370:ILE:HD13	1:E:379:VAL:HG13	1.98	0.46
1:E:1024:TYR:O	1:E:1030:THR:OG1	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:VAL:HG22	1:B:926:LEU:HD11	1.98	0.46
1:B:497:ILE:HG21	1:B:589:TYR:CD2	2.50	0.46
1:C:127:ARG:HG3	1:C:127:ARG:HH11	1.79	0.46
1:A:1118:ALA:O	1:D:2133:LEU:HD22	2.16	0.46
1:A:1244:THR:HG21	1:A:1268:TYR:CD1	2.51	0.46
1:B:2009:LEU:HG	1:B:2294:PRO:HB3	1.98	0.46
1:C:1113:LEU:HD11	1:C:1119:GLY:HA3	1.98	0.46
1:D:969:GLN:HB3	1:D:999:ARG:NH1	2.31	0.46
1:B:348:PHE:CE1	1:B:352:ASN:HB3	2.50	0.46
1:B:1617:ALA:HA	1:B:1624:ILE:HD11	1.97	0.46
1:C:1124:ARG:NE	1:C:1142:SER:O	2.48	0.46
1:C:2321:HIS:NE2	1:C:2325:ASP:OD2	2.49	0.46
1:E:522:PRO:O	1:E:553:ARG:NH1	2.48	0.46
1:A:497:ILE:HG21	1:A:589:TYR:CD2	2.51	0.45
1:B:357:TYR:CE2	1:B:391:TYR:HB2	2.51	0.45
1:C:1168:TYR:HD2	1:C:1200:LEU:HD11	1.81	0.45
1:C:2099:TYR:CE2	1:C:2195:GLN:HB3	2.50	0.45
1:D:357:TYR:CE2	1:D:391:TYR:HB2	2.51	0.45
1:A:2337:LEU:HD23	1:A:2507:ILE:HG13	1.99	0.45
1:C:1001:LEU:HD23	1:C:1013:ILE:HD12	1.98	0.45
1:C:2441:LEU:HG	1:C:2445:CYS:HB2	1.98	0.45
1:D:534:GLU:OE2	1:D:580:ASN:ND2	2.49	0.45
1:D:2469:PHE:H	1:E:2327:ARG:NH2	2.15	0.45
1:A:255:ILE:HD12	1:A:438:LEU:HD13	1.99	0.45
1:B:1024:TYR:CD1	1:B:1034:VAL:HG21	2.52	0.45
1:C:174:LYS:HG2	1:C:185:VAL:HG21	1.98	0.45
1:C:370:ILE:HD13	1:C:379:VAL:HG13	1.99	0.45
1:C:1892:ASP:OD1	1:C:1892:ASP:N	2.50	0.45
1:D:1711:PHE:CE2	1:D:1713:LYS:HB3	2.52	0.45
1:E:197:ALA:H	1:E:948:THR:HG21	1.79	0.45
1:A:593:LEU:O	1:A:597:ILE:HG12	2.16	0.45
1:B:370:ILE:HD13	1:B:379:VAL:HG13	1.99	0.45
1:B:1711:PHE:CE2	1:B:1713:LYS:HB3	2.52	0.45
1:C:464:VAL:HG21	1:C:474:VAL:HA	1.98	0.45
1:D:1024:TYR:CG	1:D:1034:VAL:HG21	2.52	0.45
1:E:969:GLN:HB3	1:E:999:ARG:NH1	2.31	0.45
1:E:1146:LYS:NZ	1:E:1147:ILE:O	2.42	0.45
1:E:2441:LEU:HG	1:E:2445:CYS:HB2	1.98	0.45
1:A:370:ILE:HD13	1:A:379:VAL:HG13	1.99	0.45
1:B:1001:LEU:HD23	1:B:1013:ILE:HD12	1.99	0.45
1:B:1146:LYS:NZ	1:B:1147:ILE:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1147:ILE:HD13	1:C:1169:LEU:HD11	1.99	0.45
1:D:174:LYS:HG2	1:D:185:VAL:HG21	1.98	0.45
1:D:370:ILE:HD13	1:D:379:VAL:HG13	1.99	0.45
1:E:1244:THR:HG21	1:E:1268:TYR:CD1	2.51	0.45
1:E:2337:LEU:HD23	1:E:2507:ILE:HG13	1.99	0.45
1:A:500:ASN:HB2	1:A:627:LEU:HD13	1.98	0.45
1:A:1024:TYR:CG	1:A:1034:VAL:HG21	2.52	0.45
1:A:1711:PHE:CE2	1:A:1713:LYS:HB3	2.51	0.45
1:A:2393:PHE:CE1	1:A:2482:LEU:HB2	2.52	0.45
1:B:1113:LEU:HD11	1:B:1119:GLY:HA3	1.99	0.45
1:B:1124:ARG:NE	1:B:1142:SER:O	2.49	0.45
1:B:1178:THR:HG22	1:B:1192:THR:HG23	1.99	0.45
1:C:2141:VAL:HG21	1:D:1175:LYS:HE2	1.99	0.45
1:D:1892:ASP:OD1	1:D:1892:ASP:N	2.50	0.45
1:B:181:ASN:HD21	1:B:184:LYS:HG2	1.82	0.45
1:B:2235:GLN:HG3	1:C:1995:LEU:HB2	1.98	0.45
1:C:969:GLN:HB3	1:C:999:ARG:NH1	2.31	0.45
1:C:1244:THR:HG21	1:C:1268:TYR:CD1	2.51	0.45
1:C:2393:PHE:HB3	1:C:2477:ILE:O	2.17	0.45
1:E:1711:PHE:CE2	1:E:1713:LYS:HB3	2.52	0.45
1:A:2441:LEU:HG	1:A:2445:CYS:HB2	1.98	0.45
1:B:730:PHE:HE1	1:B:752:ILE:HG23	1.82	0.45
1:B:969:GLN:HB3	1:B:999:ARG:NH1	2.32	0.45
1:B:2441:LEU:HG	1:B:2445:CYS:HB2	1.98	0.45
1:C:2393:PHE:CE1	1:C:2482:LEU:HB2	2.52	0.45
1:D:2393:PHE:HB3	1:D:2477:ILE:O	2.17	0.45
1:E:464:VAL:HG21	1:E:474:VAL:HA	1.99	0.45
1:A:357:TYR:CE2	1:A:391:TYR:HB2	2.52	0.45
1:D:197:ALA:H	1:D:948:THR:HG21	1.81	0.45
1:E:200:TYR:CE1	1:E:941:SER:HB3	2.52	0.45
1:E:1024:TYR:CD1	1:E:1034:VAL:HG21	2.51	0.45
1:A:2147:PHE:CD1	1:E:2147:PHE:HB3	2.52	0.45
1:B:1236:CYS:H	1:B:1303:ASN:ND2	2.15	0.45
1:B:1892:ASP:N	1:B:1892:ASP:OD1	2.50	0.45
1:C:357:TYR:CE2	1:C:391:TYR:HB2	2.52	0.45
1:C:724:ALA:O	1:C:729:LYS:NZ	2.32	0.45
1:C:1024:TYR:CG	1:C:1034:VAL:HG21	2.52	0.45
1:D:507:SER:HB3	1:D:513:SER:HB2	1.99	0.45
1:D:2441:LEU:HG	1:D:2445:CYS:HB2	1.99	0.45
1:E:474:VAL:O	1:E:478:VAL:HG13	2.17	0.45
1:E:2393:PHE:CE1	1:E:2482:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ASN:HD21	1:A:184:LYS:HG2	1.82	0.44
1:B:522:PRO:O	1:B:553:ARG:NH1	2.50	0.44
1:B:659:TYR:CE2	1:B:758:ALA:HB2	2.52	0.44
1:C:593:LEU:O	1:C:597:ILE:HG12	2.17	0.44
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.52	0.44
1:C:1711:PHE:CE2	1:C:1713:LYS:HB3	2.52	0.44
1:C:2133:LEU:HD22	1:E:1118:ALA:O	2.16	0.44
1:E:141:ARG:NH2	1:E:1005:GLU:OE2	2.44	0.44
1:E:507:SER:HB3	1:E:513:SER:HB2	2.00	0.44
1:E:593:LEU:O	1:E:597:ILE:HG12	2.16	0.44
1:A:210:VAL:HG22	1:A:926:LEU:HD11	1.99	0.44
1:B:340:GLN:OE1	1:B:412:ARG:NH2	2.50	0.44
1:B:1766:LEU:O	1:B:1770:GLU:HB2	2.17	0.44
1:B:2133:LEU:HD22	1:D:1118:ALA:O	2.17	0.44
1:C:2219:ALA:HA	1:D:2073:LYS:NZ	2.33	0.44
1:D:2393:PHE:CE1	1:D:2482:LEU:HB2	2.52	0.44
1:E:1056:MET:HG3	1:E:1081:TYR:CE1	2.52	0.44
1:E:1135:LYS:HA	1:E:1135:LYS:HD3	1.81	0.44
1:B:534:GLU:OE2	1:B:580:ASN:ND2	2.50	0.44
1:B:1147:ILE:HD13	1:B:1169:LEU:HD11	1.99	0.44
1:B:2129:GLN:NE2	1:D:1120:GLU:OE2	2.51	0.44
1:C:251:LEU:HD13	1:C:446:LEU:HD13	1.99	0.44
1:C:2360:LEU:HB3	1:C:2377:PHE:HE1	1.82	0.44
1:D:538:LEU:HB2	1:D:566:LEU:HD22	1.99	0.44
1:E:2018:ARG:NH2	1:E:2473:GLU:OE2	2.51	0.44
1:A:1056:MET:HG3	1:A:1081:TYR:CE1	2.53	0.44
1:B:160:SER:HA	1:B:982:LYS:HA	1.98	0.44
1:B:1056:MET:HG3	1:B:1081:TYR:CE1	2.53	0.44
1:B:2393:PHE:CE1	1:B:2482:LEU:HB2	2.53	0.44
1:E:160:SER:HA	1:E:982:LYS:HA	1.98	0.44
1:E:195:SER:OG	1:E:948:THR:HG22	2.18	0.44
1:A:2207:ASP:O	1:A:2211:LYS:HG2	2.18	0.44
1:A:2393:PHE:HB3	1:A:2477:ILE:O	2.18	0.44
1:B:1024:TYR:O	1:B:1030:THR:OG1	2.27	0.44
1:B:2078:LEU:HD13	1:B:2217:ARG:HA	2.00	0.44
1:B:2219:ALA:HA	1:C:2073:LYS:NZ	2.33	0.44
1:E:181:ASN:HD21	1:E:184:LYS:HG2	1.83	0.44
1:E:1001:LEU:HD23	1:E:1013:ILE:HD12	1.99	0.44
1:A:197:ALA:H	1:A:948:THR:HG21	1.82	0.44
1:A:2219:ALA:HA	1:B:2073:LYS:NZ	2.32	0.44
1:E:1962:THR:OG1	1:E:1966:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ARG:HE	1:B:973:ILE:HD11	1.82	0.44
1:B:784:GLU:HG3	1:B:790:THR:HA	1.98	0.44
1:B:2147:PHE:HB3	1:C:2147:PHE:CD1	2.52	0.44
1:C:197:ALA:H	1:C:948:THR:HG21	1.82	0.44
1:C:255:ILE:HD12	1:C:438:LEU:HD13	1.99	0.44
1:C:2207:ASP:O	1:C:2211:LYS:HG2	2.18	0.44
1:D:2030:VAL:O	1:D:2034:THR:HG23	2.18	0.44
1:D:2147:PHE:HB3	1:E:2147:PHE:CD1	2.52	0.44
1:D:2219:ALA:HA	1:E:2073:LYS:NZ	2.33	0.44
1:E:357:TYR:CE2	1:E:391:TYR:HB2	2.52	0.44
1:E:2078:LEU:HD13	1:E:2217:ARG:HA	2.00	0.44
1:A:474:VAL:O	1:A:478:VAL:HG13	2.18	0.44
1:B:174:LYS:HG2	1:B:185:VAL:HG21	2.00	0.44
1:C:507:SER:HB3	1:C:513:SER:HB2	2.00	0.44
1:D:784:GLU:HG3	1:D:790:THR:HA	1.99	0.44
1:D:2078:LEU:HD13	1:D:2217:ARG:HA	2.00	0.44
1:D:2321:HIS:NE2	1:D:2325:ASP:OD2	2.51	0.44
1:A:507:SER:HB3	1:A:513:SER:HB2	2.00	0.44
1:A:2235:GLN:HG3	1:B:1995:LEU:HB2	2.00	0.44
1:B:124:ARG:HG2	1:B:1911:ALA:HB1	2.00	0.44
1:C:273:PRO:HG3	1:C:434:TYR:CE1	2.52	0.44
1:C:1178:THR:HG22	1:C:1192:THR:HG23	2.00	0.44
1:C:2129:GLN:NE2	1:E:1120:GLU:OE2	2.51	0.44
1:E:1124:ARG:NE	1:E:1142:SER:O	2.51	0.44
1:E:1892:ASP:OD1	1:E:1892:ASP:N	2.50	0.44
1:E:2207:ASP:O	1:E:2211:LYS:HG2	2.18	0.44
1:A:784:GLU:HG3	1:A:790:THR:HA	2.00	0.43
1:A:969:GLN:HB3	1:A:999:ARG:NH1	2.32	0.43
1:A:1113:LEU:HD11	1:A:1119:GLY:HA3	2.00	0.43
1:A:2133:LEU:HD22	1:C:1118:ALA:O	2.17	0.43
1:B:273:PRO:HG3	1:B:434:TYR:CE1	2.53	0.43
1:B:2360:LEU:HB3	1:B:2377:PHE:HE1	1.83	0.43
1:C:255:ILE:HG12	1:C:442:LYS:HE3	2.00	0.43
1:C:474:VAL:O	1:C:478:VAL:HG13	2.18	0.43
1:D:659:TYR:CE2	1:D:758:ALA:HB2	2.53	0.43
1:D:1002:GLU:OE1	1:E:1888:HIS:NE2	2.50	0.43
1:E:487:ARG:HE	1:E:635:ASN:HD21	1.66	0.43
1:A:174:LYS:HG2	1:A:185:VAL:HG21	1.99	0.43
1:B:464:VAL:HG21	1:B:474:VAL:HA	2.01	0.43
1:E:730:PHE:HE1	1:E:752:ILE:HG23	1.83	0.43
1:E:2009:LEU:HG	1:E:2294:PRO:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:ILE:HD12	1:A:494:THR:HG22	2.00	0.43
1:A:2030:VAL:O	1:A:2034:THR:HG23	2.18	0.43
1:A:2327:ARG:NH2	1:E:2469:PHE:H	2.16	0.43
1:C:1135:LYS:HA	1:C:1135:LYS:HD3	1.82	0.43
1:C:1766:LEU:O	1:C:1770:GLU:HB2	2.17	0.43
1:D:255:ILE:HG12	1:D:442:LYS:HE3	2.00	0.43
1:D:1773:TYR:HD2	1:D:1774:TYR:CD1	2.36	0.43
1:D:2337:LEU:HD23	1:D:2507:ILE:HG13	1.99	0.43
1:E:2321:HIS:NE2	1:E:2325:ASP:OD2	2.51	0.43
1:E:2393:PHE:HB3	1:E:2477:ILE:O	2.19	0.43
1:A:1178:THR:HG22	1:A:1192:THR:HG23	2.01	0.43
1:A:1236:CYS:H	1:A:1303:ASN:ND2	2.17	0.43
1:A:2321:HIS:NE2	1:A:2325:ASP:OD2	2.52	0.43
1:A:2452:HIS:CE1	1:A:2456:ASP:HB2	2.54	0.43
1:B:195:SER:OG	1:B:948:THR:HG22	2.18	0.43
1:C:534:GLU:OE2	1:C:580:ASN:ND2	2.51	0.43
1:C:2337:LEU:HD23	1:C:2507:ILE:HG13	2.00	0.43
1:D:113:PHE:HE1	1:D:1035:SER:HG	1.64	0.43
1:D:474:VAL:O	1:D:478:VAL:HG13	2.18	0.43
1:E:255:ILE:HG12	1:E:442:LYS:HE3	2.00	0.43
1:A:280:GLU:OE2	1:B:1895:TYR:HB2	2.19	0.43
1:A:534:GLU:OE2	1:A:580:ASN:ND2	2.51	0.43
1:B:1048:THR:HG23	1:B:1061:LEU:HD11	2.00	0.43
1:B:2030:VAL:O	1:B:2034:THR:HG23	2.18	0.43
1:C:2147:PHE:HB3	1:D:2147:PHE:CD1	2.52	0.43
1:D:1053:GLN:HE21	1:D:1057:MET:HG3	1.83	0.43
1:D:1159:ARG:HD3	1:D:1303:ASN:ND2	2.33	0.43
1:E:659:TYR:CE2	1:E:758:ALA:HB2	2.53	0.43
1:A:1766:LEU:O	1:A:1770:GLU:HB2	2.18	0.43
1:B:280:GLU:OE2	1:C:1895:TYR:HB2	2.18	0.43
1:B:487:ARG:HE	1:B:635:ASN:HD21	1.66	0.43
1:B:2452:HIS:CE1	1:B:2456:ASP:HB2	2.54	0.43
1:D:181:ASN:HD21	1:D:184:LYS:HG2	1.83	0.43
1:D:497:ILE:HG21	1:D:589:TYR:CD2	2.54	0.43
1:D:2360:LEU:HB3	1:D:2377:PHE:HE1	1.83	0.43
1:D:2448:LEU:HB2	1:D:2458:GLY:HA3	2.00	0.43
1:E:255:ILE:HD12	1:E:438:LEU:HD13	1.99	0.43
1:E:569:THR:HG21	1:E:587:ASN:HB3	2.01	0.43
1:E:1168:TYR:HD2	1:E:1200:LEU:HD11	1.83	0.43
1:A:1773:TYR:HD2	1:A:1774:TYR:CD1	2.37	0.43
1:A:1895:TYR:HB2	1:E:280:GLU:OE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2207:ASP:O	1:B:2211:LYS:HG2	2.18	0.43
1:C:124:ARG:HD3	1:C:1914:THR:OG1	2.18	0.43
1:C:280:GLU:OE2	1:D:1895:TYR:HB2	2.19	0.43
1:C:730:PHE:HE1	1:C:752:ILE:HG23	1.82	0.43
1:C:1236:CYS:H	1:C:1303:ASN:ND2	2.16	0.43
1:D:1236:CYS:H	1:D:1303:ASN:ND2	2.16	0.43
1:D:1887:LEU:HD12	1:D:1887:LEU:HA	1.90	0.43
1:E:694:PRO:HA	1:E:705:GLU:OE1	2.19	0.43
1:A:659:TYR:CE2	1:A:758:ALA:HB2	2.53	0.43
1:A:1159:ARG:HD3	1:A:1303:ASN:ND2	2.33	0.43
1:A:1793:ASN:O	1:A:1797:LYS:HB2	2.19	0.43
1:A:2078:LEU:HD13	1:A:2217:ARG:HA	2.01	0.43
1:B:1118:ALA:O	1:E:2133:LEU:HD22	2.18	0.43
1:C:142:ARG:HE	1:C:973:ILE:HD11	1.84	0.43
1:C:659:TYR:CE2	1:C:758:ALA:HB2	2.53	0.43
1:C:1166:ARG:HB2	1:D:1614:VAL:HG11	2.01	0.43
1:C:2009:LEU:HG	1:C:2294:PRO:HB3	2.01	0.43
1:C:2452:HIS:CE1	1:C:2456:ASP:HB2	2.54	0.43
1:D:340:GLN:OE1	1:D:412:ARG:NH2	2.51	0.43
1:D:1168:TYR:HD2	1:D:1200:LEU:HD11	1.83	0.43
1:E:490:ILE:HD12	1:E:494:THR:HG22	2.01	0.43
1:E:558:ASP:OD1	1:E:558:ASP:N	2.47	0.43
1:E:1766:LEU:O	1:E:1770:GLU:HB2	2.19	0.43
1:E:2030:VAL:O	1:E:2034:THR:HG23	2.18	0.43
1:A:273:PRO:HG3	1:A:434:TYR:CE1	2.54	0.43
1:A:340:GLN:OE1	1:A:412:ARG:NH2	2.52	0.43
1:A:1024:TYR:CD1	1:A:1034:VAL:HG21	2.54	0.43
1:A:2009:LEU:HG	1:A:2294:PRO:HB3	2.00	0.43
1:B:116:ALA:O	1:B:120:THR:HG23	2.19	0.43
1:B:2393:PHE:HB3	1:B:2477:ILE:O	2.18	0.43
1:C:2030:VAL:O	1:C:2034:THR:HG23	2.18	0.43
1:D:1124:ARG:NE	1:D:1142:SER:O	2.51	0.43
1:D:1124:ARG:NH2	1:D:1763:ALA:O	2.50	0.43
1:E:534:GLU:OE2	1:E:580:ASN:ND2	2.52	0.43
1:E:1178:THR:HG22	1:E:1192:THR:HG23	2.00	0.43
1:E:2416:SER:HB2	1:E:2510:HIS:HB2	2.00	0.43
1:A:1614:VAL:HG11	1:E:1166:ARG:HB2	2.01	0.43
1:B:251:LEU:HD13	1:B:446:LEU:HD13	2.01	0.43
1:D:280:GLU:OE2	1:E:1895:TYR:HB2	2.19	0.43
1:D:397:LEU:HD13	1:D:406:PHE:CZ	2.54	0.43
1:D:2207:ASP:O	1:D:2211:LYS:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:SER:OG	1:A:948:THR:HG22	2.19	0.42
1:A:343:VAL:HG23	1:A:357:TYR:HB3	2.01	0.42
1:A:1135:LYS:HA	1:A:1135:LYS:HD3	1.81	0.42
1:B:1162:ILE:HD13	1:B:1167:LEU:HA	2.01	0.42
1:B:2337:LEU:HD23	1:B:2507:ILE:HG13	2.01	0.42
1:D:1147:ILE:HD13	1:D:1169:LEU:HD11	2.01	0.42
1:E:1773:TYR:HD2	1:E:1774:TYR:CD1	2.37	0.42
1:A:538:LEU:HB2	1:A:566:LEU:HD22	2.01	0.42
1:A:848:GLN:OE1	1:A:892:GLN:NE2	2.53	0.42
1:A:2355:GLN:HG2	1:A:2356:GLU:OE1	2.19	0.42
1:C:569:THR:HG21	1:C:587:ASN:HB3	2.01	0.42
1:D:141:ARG:NH2	1:D:1005:GLU:OE2	2.44	0.42
1:E:124:ARG:HG2	1:E:1911:ALA:HB1	2.00	0.42
1:E:538:LEU:HB2	1:E:566:LEU:HD22	2.01	0.42
1:E:2355:GLN:HG2	1:E:2356:GLU:OE1	2.19	0.42
1:A:1892:ASP:OD1	1:A:1892:ASP:N	2.50	0.42
1:A:2073:LYS:NZ	1:E:2219:ALA:HA	2.33	0.42
1:C:181:ASN:HD21	1:C:184:LYS:HG2	1.84	0.42
1:D:2130:ALA:HB2	1:E:1204:ARG:HH22	1.82	0.42
1:E:540:SER:OG	1:E:560:VAL:HA	2.20	0.42
1:E:2360:LEU:HB3	1:E:2377:PHE:HE1	1.84	0.42
1:A:1872:GLU:OE2	1:A:1875:THR:OG1	2.34	0.42
1:B:507:SER:HB3	1:B:513:SER:HB2	2.00	0.42
1:C:2018:ARG:N	1:C:2467:GLY:O	2.52	0.42
1:C:2369:GLY:HA3	1:C:2374:ASN:HA	2.01	0.42
1:D:160:SER:HA	1:D:982:LYS:HA	2.00	0.42
1:D:730:PHE:HE1	1:D:752:ILE:HG23	1.83	0.42
1:D:2009:LEU:HG	1:D:2294:PRO:HB3	2.01	0.42
1:E:273:PRO:HG3	1:E:434:TYR:CE1	2.53	0.42
1:E:340:GLN:OE1	1:E:412:ARG:NH2	2.51	0.42
1:E:1800:TRP:CZ2	1:E:1802:PRO:HG3	2.54	0.42
1:E:2372:ASN:HB2	1:E:2392:SER:HB2	2.02	0.42
1:A:1168:TYR:HD2	1:A:1200:LEU:HD11	1.85	0.42
1:A:1995:LEU:HB2	1:E:2235:GLN:HG3	2.01	0.42
1:A:2360:LEU:HB3	1:A:2377:PHE:HE1	1.85	0.42
1:C:116:ALA:O	1:C:120:THR:HG23	2.19	0.42
1:C:340:GLN:OE1	1:C:412:ARG:NH2	2.52	0.42
1:D:1146:LYS:NZ	1:D:1147:ILE:O	2.42	0.42
1:D:1800:TRP:CZ2	1:D:1802:PRO:HG3	2.54	0.42
1:E:579:LYS:HG3	1:E:581:ASN:H	1.85	0.42
1:A:124:ARG:HD3	1:A:1914:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:LYS:HG3	1:A:581:ASN:H	1.84	0.42
1:A:1166:ARG:HB2	1:B:1614:VAL:HG11	2.02	0.42
1:A:2295:GLY:HA3	1:D:676:HIS:CD2	2.54	0.42
1:B:2355:GLN:HG2	1:B:2356:GLU:OE1	2.19	0.42
1:C:538:LEU:HB2	1:C:566:LEU:HD22	2.00	0.42
1:D:1056:MET:HG3	1:D:1081:TYR:CE1	2.54	0.42
1:D:2452:HIS:CE1	1:D:2456:ASP:HB2	2.54	0.42
1:E:1609:PHE:CZ	1:E:1613:LEU:HD13	2.55	0.42
1:A:569:THR:HG21	1:A:587:ASN:HB3	2.00	0.42
1:A:2448:LEU:HB2	1:A:2458:GLY:HA3	2.02	0.42
1:B:255:ILE:HG12	1:B:442:LYS:HE3	2.01	0.42
1:B:1168:TYR:HD2	1:B:1200:LEU:HD11	1.84	0.42
1:C:154:ASN:HB3	1:C:986:ILE:HG13	2.02	0.42
1:C:579:LYS:HG3	1:C:581:ASN:H	1.84	0.42
1:D:1166:ARG:HB2	1:E:1614:VAL:HG11	2.02	0.42
1:D:2355:GLN:HG2	1:D:2356:GLU:OE1	2.20	0.42
1:E:2033:LEU:CD1	1:E:2266:TYR:HA	2.50	0.42
1:E:2328:ALA:HB2	1:E:2516:LYS:HB3	2.02	0.42
1:A:2033:LEU:CD1	1:A:2266:TYR:HA	2.50	0.42
1:C:711:VAL:HG11	1:C:763:GLU:OE2	2.20	0.42
1:D:368:LEU:HG	1:D:370:ILE:CD1	2.50	0.42
1:E:397:LEU:HD13	1:E:406:PHE:CZ	2.55	0.42
1:E:1053:GLN:HE21	1:E:1057:MET:HG3	1.85	0.42
1:E:2228:LYS:HE3	1:E:2228:LYS:HB2	1.87	0.42
1:A:1239:TYR:CD1	1:A:1242:GLU:HB3	2.54	0.42
1:A:2004:GLN:N	1:A:2300:THR:HG22	2.34	0.42
1:A:2077:GLU:OE2	1:E:2216:ARG:NH2	2.52	0.42
1:A:2277:GLU:OE2	1:A:2291:PHE:HB2	2.20	0.42
1:B:1773:TYR:HD2	1:B:1774:TYR:CD1	2.37	0.42
1:B:1800:TRP:CZ2	1:B:1802:PRO:HG3	2.55	0.42
1:C:141:ARG:NH2	1:C:1005:GLU:OE2	2.43	0.42
1:C:368:LEU:HG	1:C:370:ILE:CD1	2.50	0.42
1:C:1793:ASN:O	1:C:1797:LYS:HB2	2.20	0.42
1:D:490:ILE:HD12	1:D:494:THR:HG22	2.01	0.42
1:D:579:LYS:HG3	1:D:581:ASN:H	1.85	0.42
1:D:1793:ASN:O	1:D:1797:LYS:HB2	2.20	0.42
1:A:1607:THR:HG22	1:A:1609:PHE:H	1.84	0.42
1:A:1800:TRP:CZ2	1:A:1802:PRO:HG3	2.55	0.42
1:B:2018:ARG:N	1:B:2467:GLY:O	2.50	0.42
1:C:195:SER:OG	1:C:948:THR:HG22	2.20	0.42
1:C:2355:GLN:HG2	1:C:2356:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:ARG:HG2	1:D:1911:ALA:HB1	2.02	0.42
1:D:1178:THR:HG22	1:D:1192:THR:HG23	2.01	0.42
1:E:711:VAL:HG11	1:E:763:GLU:OE2	2.20	0.42
1:A:116:ALA:O	1:A:120:THR:HG23	2.20	0.41
1:A:142:ARG:HE	1:A:973:ILE:HD11	1.84	0.41
1:A:1123:TRP:NE1	1:A:1145:HIS:HB2	2.35	0.41
1:A:1162:ILE:HD13	1:A:1167:LEU:HA	2.01	0.41
1:A:2275:MET:SD	1:B:2322:LEU:HD22	2.60	0.41
1:B:493:GLU:O	1:B:497:ILE:HG12	2.20	0.41
1:B:711:VAL:HG11	1:B:763:GLU:OE2	2.20	0.41
1:B:1024:TYR:CG	1:B:1034:VAL:HG21	2.55	0.41
1:C:1676:ILE:HD12	1:C:1690:LEU:HD13	2.02	0.41
1:C:1773:TYR:HD2	1:C:1774:TYR:CD1	2.38	0.41
1:C:2275:MET:SD	1:D:2322:LEU:HD22	2.60	0.41
1:E:2452:HIS:CE1	1:E:2456:ASP:HB2	2.54	0.41
1:A:251:LEU:HD13	1:A:446:LEU:HD13	2.02	0.41
1:B:255:ILE:HD12	1:B:438:LEU:HD13	2.02	0.41
1:B:397:LEU:HD13	1:B:406:PHE:CZ	2.56	0.41
1:C:1024:TYR:O	1:C:1030:THR:OG1	2.26	0.41
1:C:1098:HIS:CE1	1:C:1100:ASN:HB3	2.55	0.41
1:C:1159:ARG:HD3	1:C:1303:ASN:ND2	2.35	0.41
1:D:195:SER:OG	1:D:948:THR:HG22	2.20	0.41
1:D:663:LEU:HD22	1:D:749:GLN:NE2	2.35	0.41
1:D:1676:ILE:HD12	1:D:1690:LEU:HD13	2.02	0.41
1:E:1123:TRP:NE1	1:E:1145:HIS:HB2	2.35	0.41
1:A:255:ILE:HG12	1:A:442:LYS:HE3	2.01	0.41
1:A:1053:GLN:HE21	1:A:1057:MET:HG3	1.86	0.41
1:A:2322:LEU:HD22	1:E:2275:MET:SD	2.60	0.41
1:B:200:TYR:CE1	1:B:941:SER:HB3	2.54	0.41
1:B:493:GLU:OE2	1:B:517:ARG:NH1	2.34	0.41
1:B:2033:LEU:CD1	1:B:2266:TYR:HA	2.50	0.41
1:B:2433:LEU:HB3	1:B:2484:LEU:HD13	2.02	0.41
1:C:283:LYS:HB2	1:C:293:LEU:HD22	2.02	0.41
1:C:784:GLU:HG3	1:C:790:THR:HA	2.02	0.41
1:C:1024:TYR:CD1	1:C:1034:VAL:HG21	2.55	0.41
1:C:1162:ILE:HD13	1:C:1167:LEU:HA	2.02	0.41
1:C:2235:GLN:HG3	1:D:1995:LEU:HB2	2.01	0.41
1:B:141:ARG:NH2	1:B:1005:GLU:OE2	2.45	0.41
1:B:368:LEU:HG	1:B:370:ILE:CD1	2.50	0.41
1:B:490:ILE:HD12	1:B:494:THR:HG22	2.01	0.41
1:B:533:ASP:HA	1:B:579:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:VAL:HG23	1:D:357:TYR:HB3	2.02	0.41
1:D:1766:LEU:O	1:D:1770:GLU:HB2	2.19	0.41
1:E:1024:TYR:CG	1:E:1034:VAL:HG21	2.55	0.41
1:E:1887:LEU:HD12	1:E:1887:LEU:HA	1.90	0.41
1:A:124:ARG:HG2	1:A:1911:ALA:HB1	2.03	0.41
1:B:579:LYS:HG3	1:B:581:ASN:H	1.84	0.41
1:B:1053:GLN:HE21	1:B:1057:MET:HG3	1.84	0.41
1:B:1120:GLU:OE2	1:E:2129:GLN:NE2	2.54	0.41
1:B:1782:ARG:HE	1:B:1782:ARG:HB3	1.76	0.41
1:C:694:PRO:HA	1:C:705:GLU:OE1	2.20	0.41
1:C:971:LEU:O	1:C:973:ILE:HG12	2.21	0.41
1:C:1053:GLN:HE21	1:C:1057:MET:HG3	1.85	0.41
1:D:694:PRO:HA	1:D:705:GLU:OE1	2.20	0.41
1:D:1024:TYR:CD1	1:D:1034:VAL:HG21	2.56	0.41
1:D:1239:TYR:HD2	1:D:1246:LEU:HD11	1.85	0.41
1:E:124:ARG:HD3	1:E:1914:THR:OG1	2.20	0.41
1:E:1113:LEU:HD11	1:E:1119:GLY:HA3	2.02	0.41
1:E:1159:ARG:HD3	1:E:1303:ASN:ND2	2.34	0.41
1:A:1617:ALA:CA	1:A:1624:ILE:HD11	2.51	0.41
1:A:2018:ARG:N	1:A:2467:GLY:O	2.52	0.41
1:A:2097:ASP:OD1	1:A:2098:SER:N	2.54	0.41
1:A:2145:PHE:CE2	1:C:1180:GLN:HG3	2.56	0.41
1:B:1609:PHE:CZ	1:B:1613:LEU:HD13	2.56	0.41
1:C:490:ILE:HD12	1:C:494:THR:HG22	2.02	0.41
1:D:116:ALA:O	1:D:120:THR:HG23	2.20	0.41
1:E:1147:ILE:HD13	1:E:1169:LEU:HD11	2.02	0.41
1:A:200:TYR:CE1	1:A:941:SER:HB3	2.55	0.41
1:A:711:VAL:HG11	1:A:763:GLU:OE2	2.20	0.41
1:A:717:LYS:HB3	1:A:793:ALA:HB2	2.03	0.41
1:A:1124:ARG:NE	1:A:1142:SER:O	2.54	0.41
1:A:2147:PHE:HB3	1:B:2147:PHE:CD1	2.54	0.41
1:B:149:ALA:O	1:B:154:ASN:ND2	2.50	0.41
1:B:694:PRO:HA	1:B:705:GLU:OE1	2.20	0.41
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.93	0.41
1:B:971:LEU:O	1:B:973:ILE:HG12	2.20	0.41
1:C:677:GLY:HA3	1:C:695:TYR:CZ	2.56	0.41
1:C:2448:LEU:HB2	1:C:2458:GLY:HA3	2.02	0.41
1:D:124:ARG:HD3	1:D:1914:THR:OG1	2.20	0.41
1:D:200:TYR:CE1	1:D:941:SER:HB3	2.56	0.41
1:D:461:VAL:HA	1:D:474:VAL:HG21	2.03	0.41
1:D:478:VAL:O	1:D:481:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ARG:HE	1:E:973:ILE:HD11	1.85	0.41
1:E:478:VAL:O	1:E:481:THR:HG22	2.21	0.41
1:E:493:GLU:O	1:E:497:ILE:HG12	2.21	0.41
1:E:784:GLU:HG3	1:E:790:THR:HA	2.02	0.41
1:E:1098:HIS:CE1	1:E:1100:ASN:HB3	2.55	0.41
1:A:125:GLU:HG3	1:A:1017:PHE:CG	2.56	0.41
1:A:397:LEU:HD13	1:A:406:PHE:CZ	2.56	0.41
1:B:253:GLU:O	1:B:442:LYS:NZ	2.29	0.41
1:B:458:GLU:HA	1:B:461:VAL:HG12	2.03	0.41
1:B:1607:THR:HG22	1:B:1609:PHE:H	1.86	0.41
1:B:1676:ILE:HD12	1:B:1690:LEU:HD13	2.01	0.41
1:C:200:TYR:CE1	1:C:941:SER:HB3	2.54	0.41
1:C:1056:MET:HG3	1:C:1081:TYR:CE1	2.56	0.41
1:C:2216:ARG:NH2	1:D:2077:GLU:OE2	2.54	0.41
1:D:125:GLU:HG3	1:D:1017:PHE:CG	2.56	0.41
1:D:193:ARG:NH2	1:D:253:GLU:OE1	2.54	0.41
1:D:273:PRO:HG3	1:D:434:TYR:CE1	2.55	0.41
1:D:569:THR:HG21	1:D:587:ASN:HB3	2.02	0.41
1:D:711:VAL:HG11	1:D:763:GLU:OE2	2.20	0.41
1:D:1162:ILE:HD13	1:D:1167:LEU:HA	2.02	0.41
1:D:2033:LEU:CD1	1:D:2266:TYR:HA	2.51	0.41
1:E:1793:ASN:O	1:E:1797:LYS:HB2	2.20	0.41
1:E:2433:LEU:HB3	1:E:2484:LEU:HD13	2.03	0.41
1:A:595:ALA:HB1	1:A:600:LEU:O	2.21	0.41
1:A:971:LEU:O	1:A:973:ILE:HG12	2.21	0.41
1:A:1098:HIS:CE1	1:A:1100:ASN:HB3	2.55	0.41
1:A:1782:ARG:HE	1:A:1782:ARG:HB3	1.76	0.41
1:A:2168:SER:HA	1:A:2171:VAL:HG12	2.03	0.41
1:A:2226:SER:HB2	1:B:2066:THR:HG21	2.03	0.41
1:B:365:ALA:HB3	1:B:384:ALA:HA	2.03	0.41
1:B:663:LEU:HD22	1:B:749:GLN:NE2	2.35	0.41
1:B:1098:HIS:CE1	1:B:1100:ASN:HB3	2.55	0.41
1:B:1239:TYR:CD1	1:B:1242:GLU:HB3	2.55	0.41
1:C:257:GLU:OE1	1:C:431:TYR:OH	2.33	0.41
1:C:397:LEU:HD13	1:C:406:PHE:CZ	2.55	0.41
1:C:733:TRP:NE1	1:C:748:THR:HB	2.36	0.41
1:C:845:LEU:HD21	1:C:881:VAL:HG13	2.03	0.41
1:C:1607:THR:HG22	1:C:1609:PHE:H	1.86	0.41
1:C:2033:LEU:CD1	1:C:2266:TYR:HA	2.50	0.41
1:D:971:LEU:O	1:D:973:ILE:HG12	2.20	0.41
1:D:1036:GLN:O	1:D:1040:TYR:N	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1805:TYR:HD2	1:D:1814:TYR:CE1	2.39	0.41
1:D:2018:ARG:N	1:D:2467:GLY:O	2.52	0.41
1:D:2372:ASN:HB2	1:D:2392:SER:HB2	2.03	0.41
1:D:2433:LEU:HB3	1:D:2484:LEU:HD13	2.03	0.41
1:E:109:VAL:HG23	1:E:155:MET:HE3	2.03	0.41
1:E:368:LEU:HG	1:E:370:ILE:CD1	2.50	0.41
1:E:500:ASN:HB2	1:E:627:LEU:HD13	2.03	0.41
1:E:595:ALA:HB1	1:E:600:LEU:O	2.21	0.41
1:E:1239:TYR:CD1	1:E:1242:GLU:HB3	2.56	0.41
1:E:2369:GLY:HA3	1:E:2374:ASN:HA	2.03	0.41
1:A:1239:TYR:HD2	1:A:1246:LEU:HD11	1.86	0.41
1:A:1607:THR:HG21	1:A:1768:PHE:CZ	2.54	0.41
1:A:1676:ILE:HD12	1:A:1690:LEU:HD13	2.03	0.41
1:B:540:SER:OG	1:B:560:VAL:HA	2.21	0.41
1:B:2275:MET:SD	1:C:2322:LEU:HD22	2.61	0.41
1:C:113:PHE:HE1	1:C:1035:SER:HG	1.67	0.41
1:C:1002:GLU:OE1	1:D:1888:HIS:NE2	2.52	0.41
1:D:142:ARG:HE	1:D:973:ILE:HD11	1.86	0.41
1:D:251:LEU:HD13	1:D:446:LEU:HD13	2.02	0.41
1:D:493:GLU:O	1:D:497:ILE:HG12	2.20	0.41
1:D:558:ASP:N	1:D:558:ASP:OD1	2.47	0.41
1:D:661:LYS:HB2	1:D:750:GLU:HB2	2.03	0.41
1:D:1113:LEU:HD11	1:D:1119:GLY:HA3	2.02	0.41
1:D:1239:TYR:CD1	1:D:1242:GLU:HB3	2.55	0.41
1:E:341:MET:HE1	1:E:410:LEU:HD22	2.02	0.41
1:E:552:LYS:NZ	1:E:558:ASP:HA	2.36	0.41
1:E:663:LEU:HD22	1:E:749:GLN:NE2	2.36	0.41
1:E:848:GLN:OE1	1:E:892:GLN:NE2	2.54	0.41
1:A:1124:ARG:NH2	1:A:1763:ALA:O	2.49	0.40
1:B:1239:TYR:HD2	1:B:1246:LEU:HD11	1.86	0.40
1:B:1793:ASN:O	1:B:1797:LYS:HB2	2.20	0.40
1:B:2369:GLY:HA3	1:B:2374:ASN:HA	2.03	0.40
1:C:478:VAL:O	1:C:481:THR:HG22	2.20	0.40
1:C:533:ASP:HA	1:C:579:LYS:NZ	2.36	0.40
1:C:1609:PHE:CZ	1:C:1613:LEU:HD13	2.56	0.40
1:C:1711:PHE:HE2	1:C:1713:LYS:HB3	1.86	0.40
1:C:1800:TRP:CZ2	1:C:1802:PRO:HG3	2.56	0.40
1:D:2097:ASP:OD1	1:D:2098:SER:N	2.54	0.40
1:E:2018:ARG:N	1:E:2467:GLY:O	2.52	0.40
1:E:2097:ASP:OD1	1:E:2098:SER:N	2.54	0.40
1:E:2448:LEU:HB2	1:E:2458:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:HD22	1:A:749:GLN:NE2	2.36	0.40
1:A:2369:GLY:HA3	1:A:2374:ASN:HA	2.03	0.40
1:B:461:VAL:HA	1:B:474:VAL:HG21	2.03	0.40
1:B:733:TRP:NE1	1:B:748:THR:HB	2.36	0.40
1:B:2168:SER:HA	1:B:2171:VAL:HG12	2.04	0.40
1:C:663:LEU:HD22	1:C:749:GLN:NE2	2.36	0.40
1:C:1048:THR:HG23	1:C:1061:LEU:HD11	2.04	0.40
1:D:1042:GLU:HA	1:D:1045:ILE:HD12	2.03	0.40
1:D:1711:PHE:HE2	1:D:1713:LYS:HB3	1.87	0.40
1:D:2124:LEU:O	1:D:2128:VAL:HG12	2.22	0.40
1:E:971:LEU:O	1:E:973:ILE:HG12	2.21	0.40
1:A:487:ARG:HE	1:A:635:ASN:HD21	1.70	0.40
1:A:1975:SER:OG	1:A:1977:ASP:OD1	2.33	0.40
1:B:371:LYS:HA	1:B:377:GLU:HA	2.04	0.40
1:B:661:LYS:HB2	1:B:750:GLU:HB2	2.04	0.40
1:B:1607:THR:HG21	1:B:1768:PHE:CZ	2.52	0.40
1:B:2097:ASP:OD1	1:B:2098:SER:N	2.54	0.40
1:C:2328:ALA:HB2	1:C:2516:LYS:HB3	2.03	0.40
1:D:540:SER:OG	1:D:560:VAL:HA	2.21	0.40
1:D:1607:THR:HG22	1:D:1609:PHE:H	1.86	0.40
1:D:1609:PHE:CZ	1:D:1613:LEU:HD13	2.57	0.40
1:D:2216:ARG:NH2	1:E:2077:GLU:OE2	2.53	0.40
1:D:2277:GLU:OE2	1:D:2291:PHE:HB2	2.21	0.40
1:D:2328:ALA:HB2	1:D:2516:LYS:HB3	2.03	0.40
1:E:116:ALA:O	1:E:120:THR:HG23	2.20	0.40
1:E:538:LEU:HD12	1:E:566:LEU:HD22	2.04	0.40
1:A:540:SER:OG	1:A:560:VAL:HA	2.22	0.40
1:A:733:TRP:NE1	1:A:748:THR:HB	2.36	0.40
1:A:2328:ALA:HB2	1:A:2516:LYS:HB3	2.04	0.40
1:B:1166:ARG:HB2	1:C:1614:VAL:HG11	2.04	0.40
1:B:1711:PHE:HE2	1:B:1713:LYS:HB3	1.87	0.40
1:B:2124:LEU:O	1:B:2128:VAL:HG12	2.22	0.40
1:B:2328:ALA:HB2	1:B:2516:LYS:HB3	2.04	0.40
1:B:2388:GLN:HA	1:B:2485:SER:HA	2.04	0.40
1:C:124:ARG:HG2	1:C:1911:ALA:HB1	2.03	0.40
1:C:456:ILE:O	1:C:460:ILE:HG13	2.21	0.40
1:C:676:HIS:CD2	1:E:2295:GLY:HA3	2.56	0.40
1:C:1094:ILE:HD11	1:C:1113:LEU:HB2	2.04	0.40
1:C:1120:GLU:HB3	1:C:1146:LYS:HE2	2.02	0.40
1:D:149:ALA:O	1:D:154:ASN:ND2	2.49	0.40
1:E:1676:ILE:HD12	1:E:1690:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2412:ILE:HD11	1:E:2477:ILE:HG12	2.02	0.40
1:A:458:GLU:HA	1:A:461:VAL:HG12	2.04	0.40
1:A:478:VAL:O	1:A:481:THR:HG22	2.21	0.40
1:B:456:ILE:O	1:B:460:ILE:HG13	2.22	0.40
1:B:569:THR:HG21	1:B:587:ASN:HB3	2.02	0.40
1:B:1050:ARG:O	1:B:1053:GLN:HB2	2.22	0.40
1:B:2295:GLY:HA3	1:E:676:HIS:CD2	2.56	0.40
1:C:500:ASN:HB2	1:C:627:LEU:HD13	2.04	0.40
1:E:283:LYS:HB2	1:E:293:LEU:HD22	2.04	0.40
1:E:1782:ARG:HE	1:E:1782:ARG:HB3	1.76	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	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	B	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	C	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
1	D	2114/2535 (83%)	2065 (98%)	49 (2%)	0	100	100
1	E	2114/2535 (83%)	2066 (98%)	48 (2%)	0	100	100
All	All	10570/12675 (83%)	10329 (98%)	241 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1816/2173 (84%)	1811 (100%)	5 (0%)	92 98
1	B	1816/2173 (84%)	1811 (100%)	5 (0%)	92 98
1	C	1816/2173 (84%)	1811 (100%)	5 (0%)	92 98
1	D	1816/2173 (84%)	1811 (100%)	5 (0%)	92 98
1	E	1816/2173 (84%)	1811 (100%)	5 (0%)	92 98
All	All	9080/10865 (84%)	9055 (100%)	25 (0%)	92 98

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1049	MET
1	A	1868	TYR
1	A	1965	GLN
1	A	2399	ARG
1	A	2430	GLN
1	B	1049	MET
1	B	1868	TYR
1	B	1965	GLN
1	B	2399	ARG
1	B	2430	GLN
1	C	1049	MET
1	C	1868	TYR
1	C	1965	GLN
1	C	2399	ARG
1	C	2430	GLN
1	D	1049	MET
1	D	1868	TYR
1	D	1965	GLN
1	D	2399	ARG
1	D	2430	GLN
1	E	1049	MET
1	E	1868	TYR
1	E	1965	GLN
1	E	2399	ARG
1	E	2430	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	969	GLN
1	A	2057	GLN
1	B	852	GLN
1	B	892	GLN
1	B	969	GLN
1	B	2057	GLN
1	C	852	GLN
1	C	892	GLN
1	C	969	GLN
1	C	2057	GLN
1	D	852	GLN
1	D	892	GLN
1	D	969	GLN
1	E	852	GLN
1	E	892	GLN
1	E	969	GLN

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.

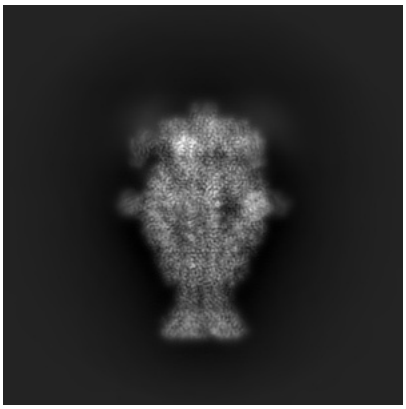
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16791. These allow visual inspection of the internal detail of the map and identification of artifacts.

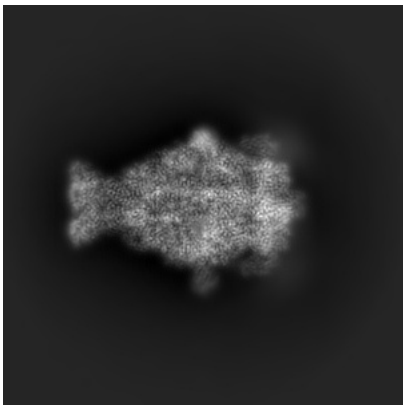
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

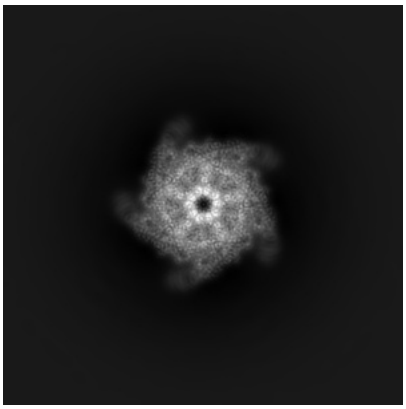
6.1.1 Primary map



X

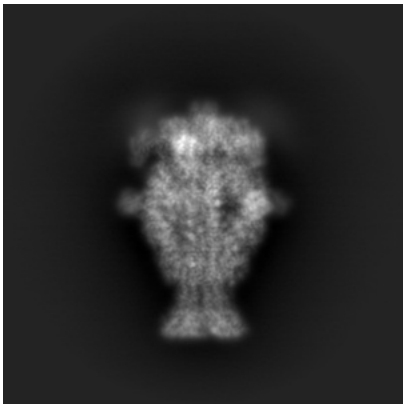


Y

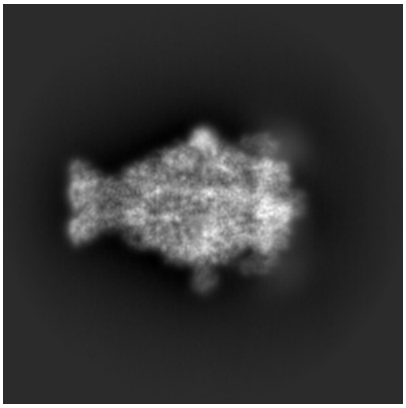


Z

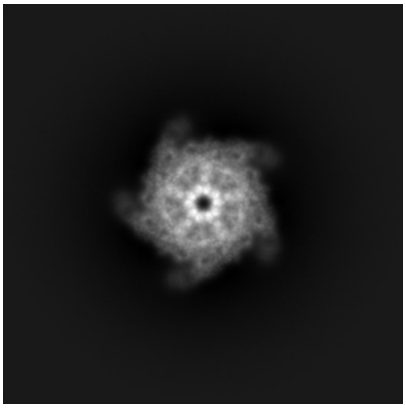
6.1.2 Raw map



X



Y



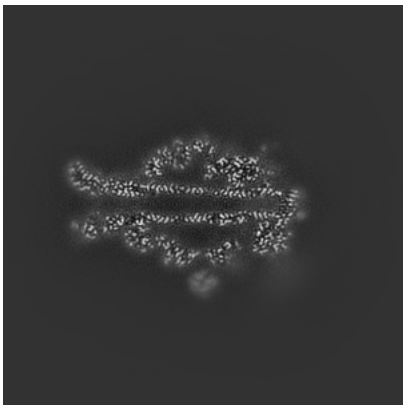
Z

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

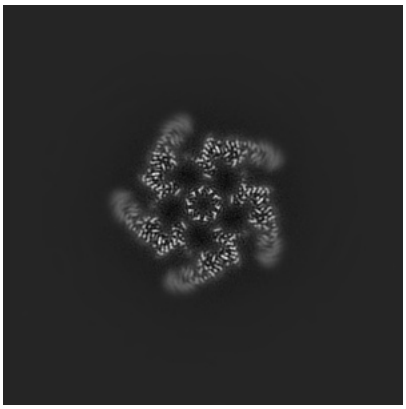
6.2 Central slices (i)

6.2.1 Primary map

X Index: 176

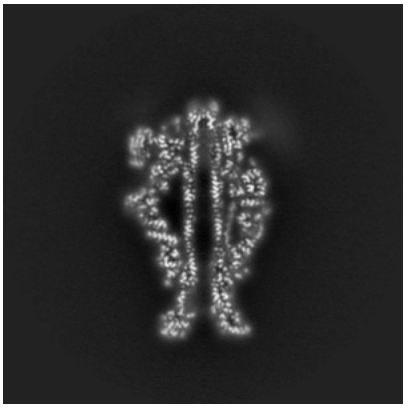


Y Index: 176

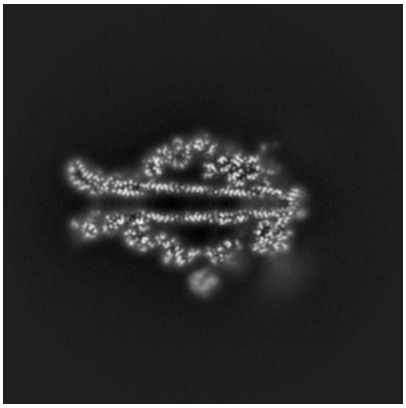


Z Index: 176

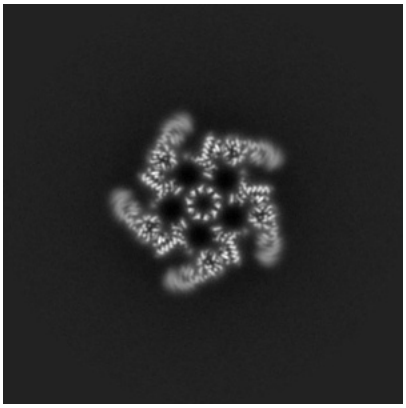
6.2.2 Raw map



X Index: 176



Y Index: 176



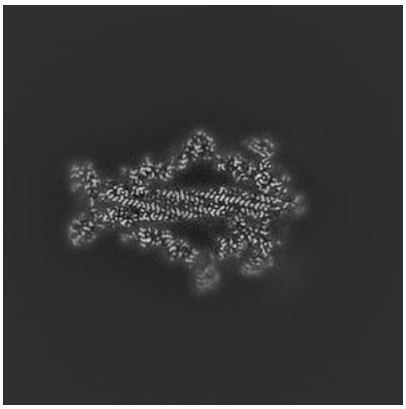
Z Index: 176

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

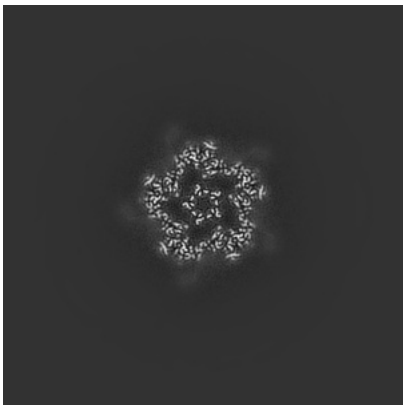
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 187

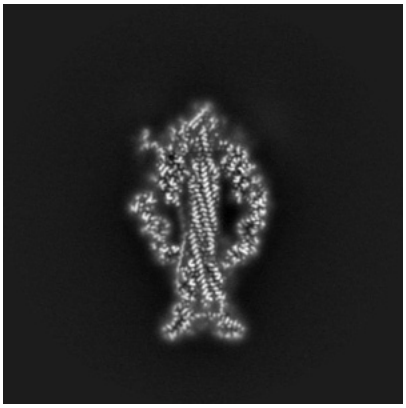


Y Index: 166

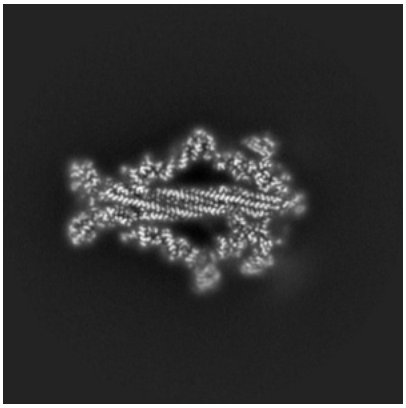


Z Index: 192

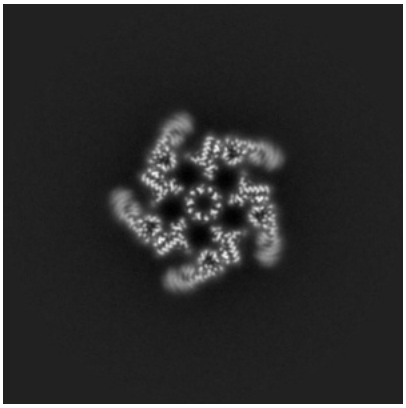
6.3.2 Raw map



X Index: 187



Y Index: 166

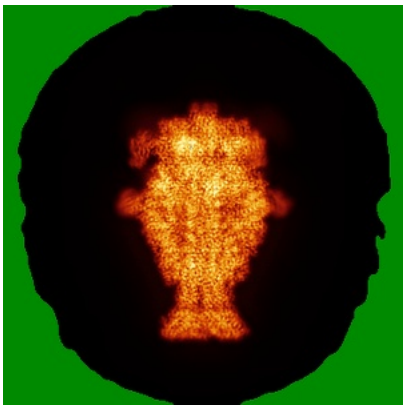


Z Index: 177

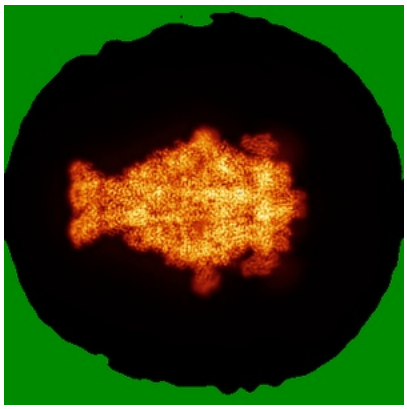
The images above show the largest variance slices of the map in three orthogonal directions.

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

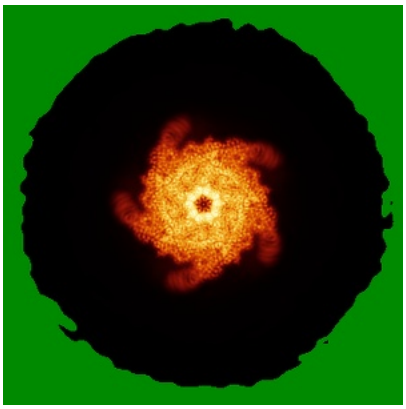
6.4.1 Primary map



X



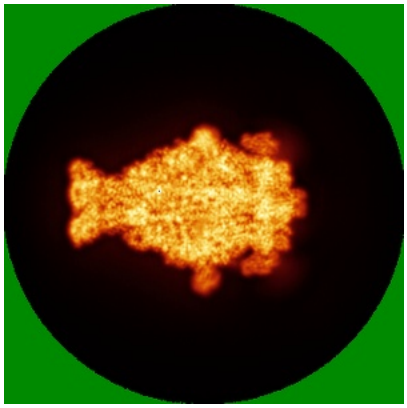
Y



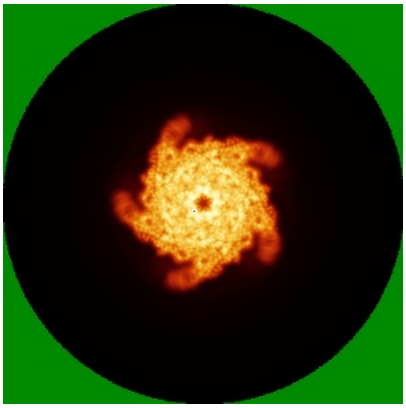
Z

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 0.07. 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.

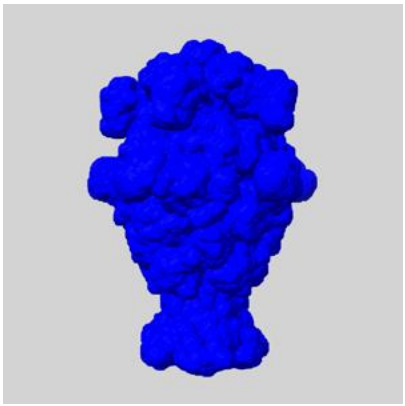
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

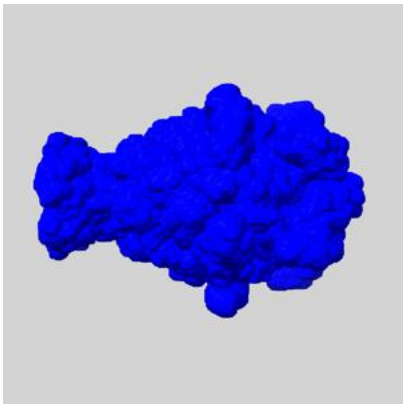
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

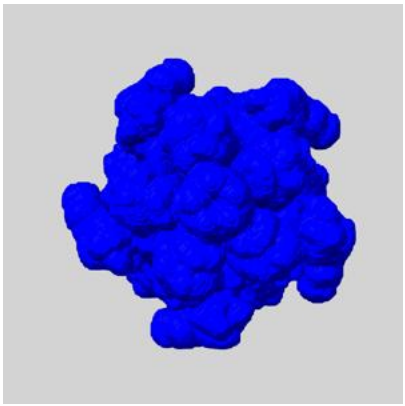
6.6.1 emd_16791_msk_1.map



X



Y

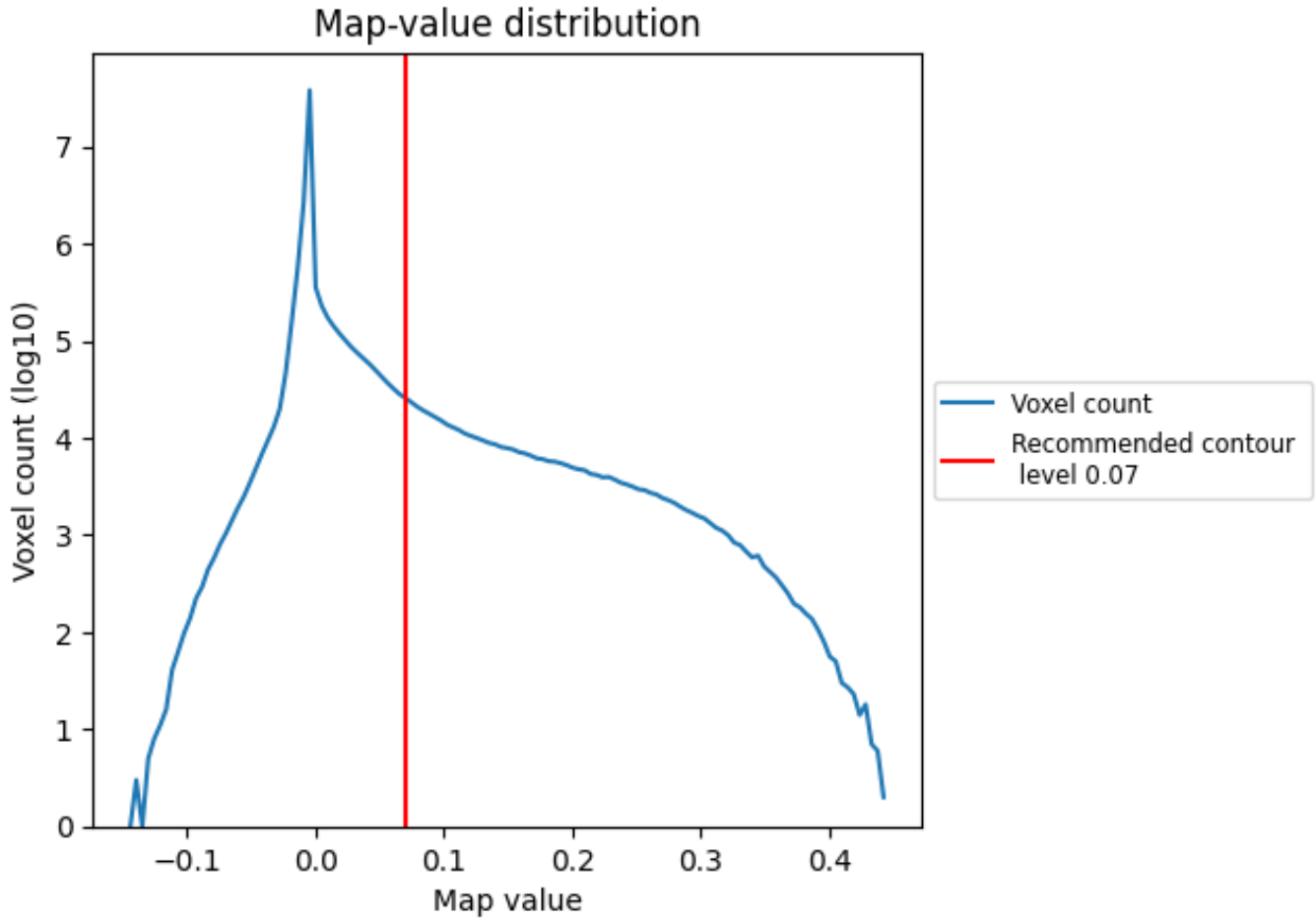


Z

7 Map analysis

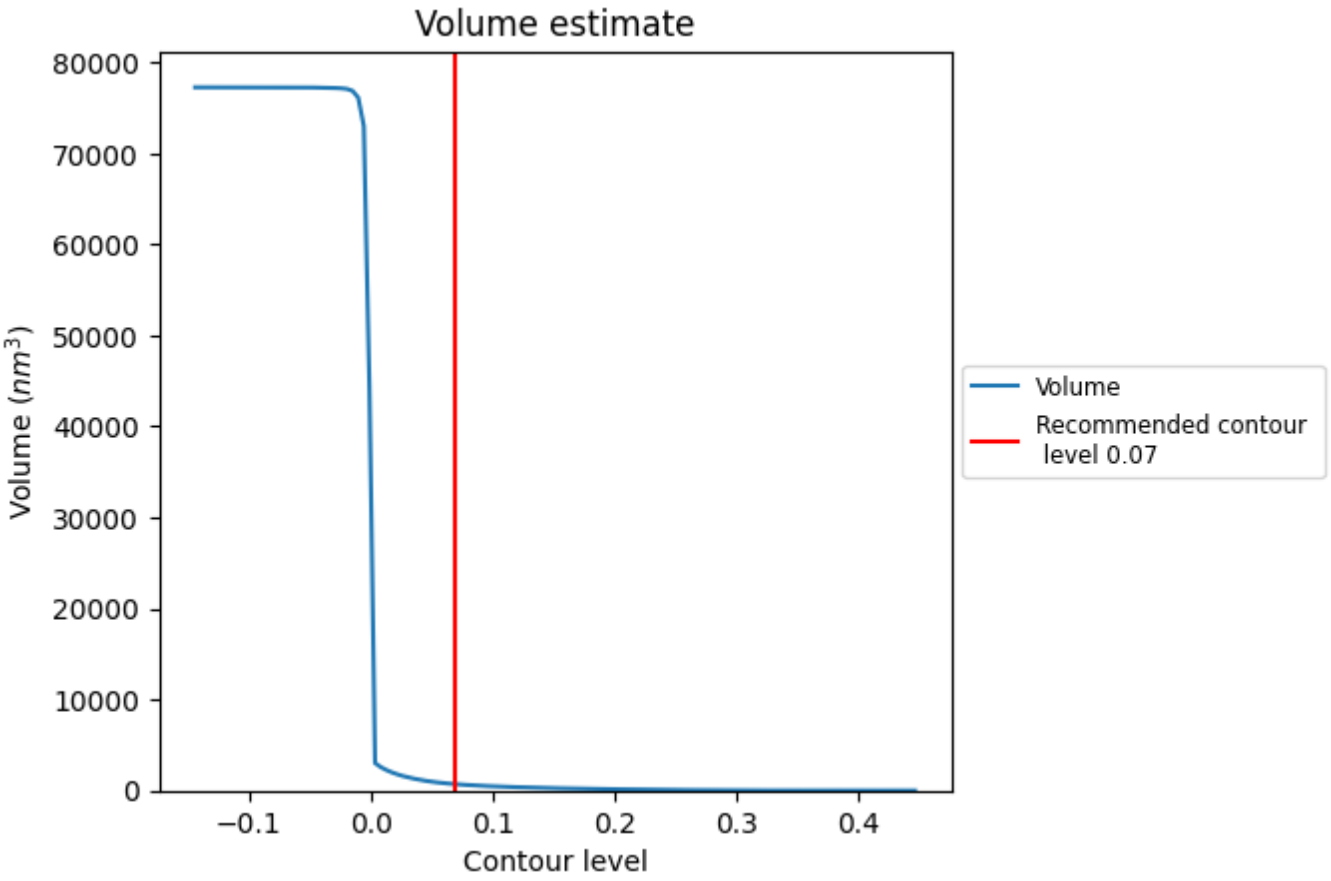
This section contains the results of statistical analysis of the map.

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.

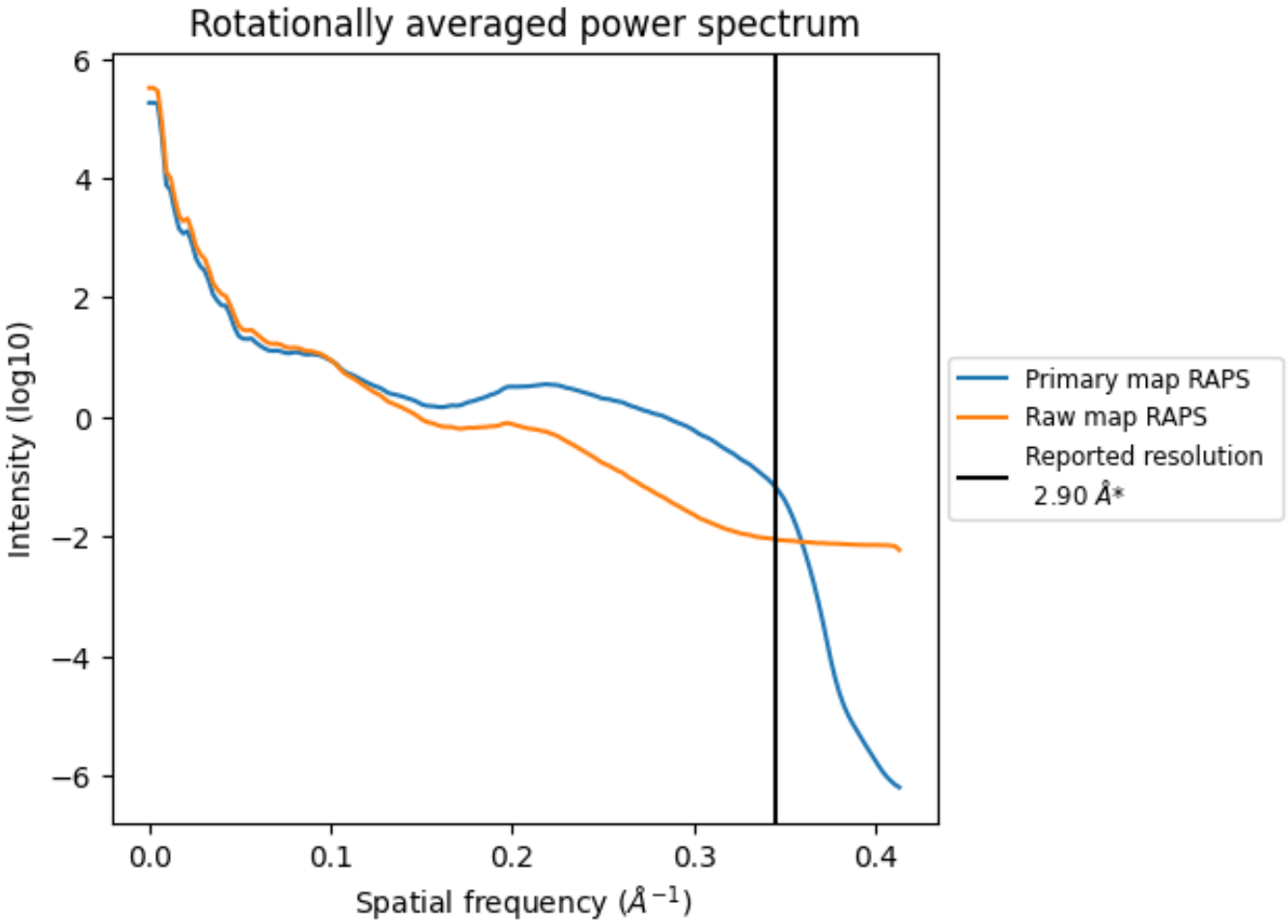
7.2 Volume estimate



The volume at the recommended contour level is 702 nm^3; this corresponds to an approximate mass of 634 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)

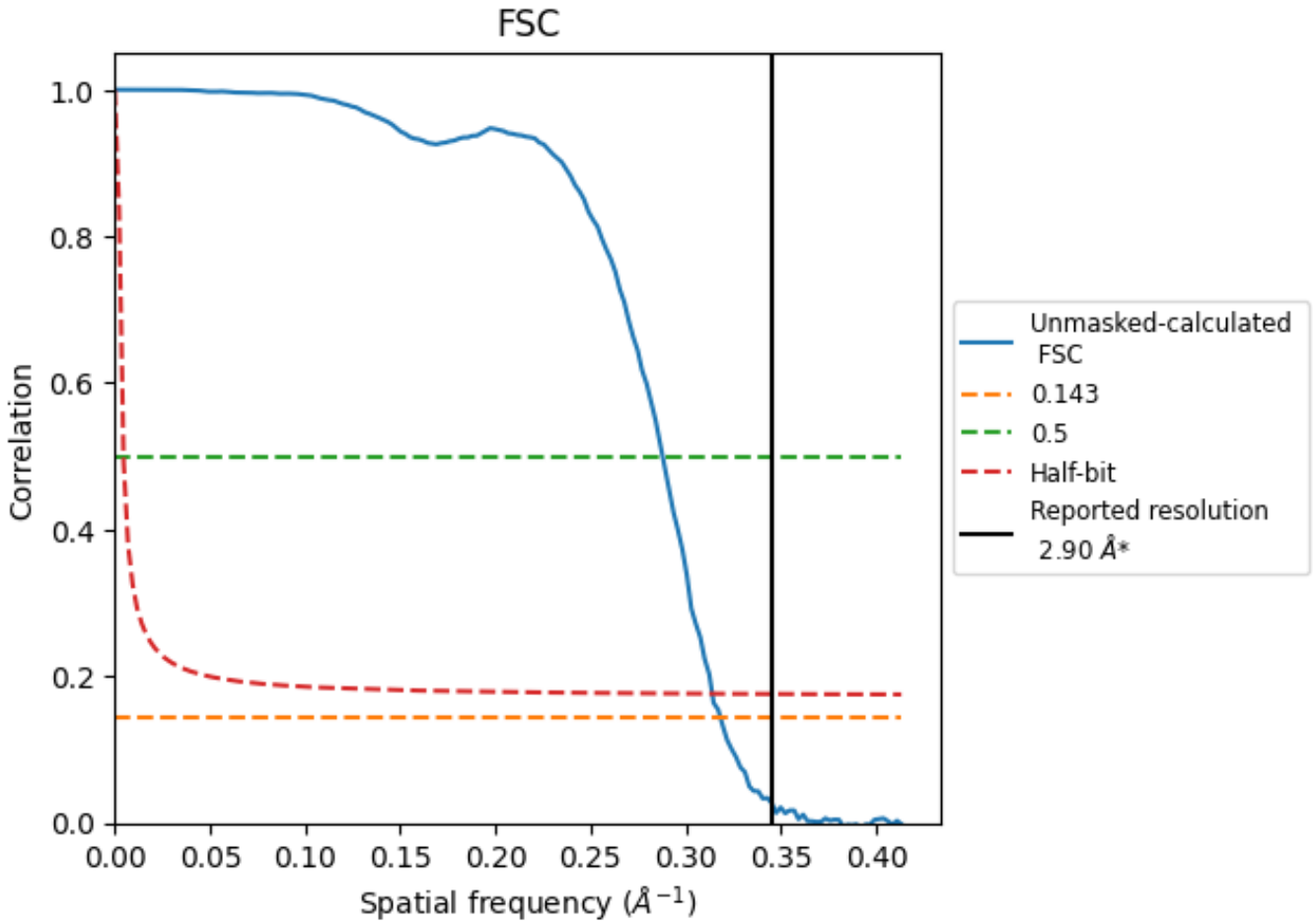


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

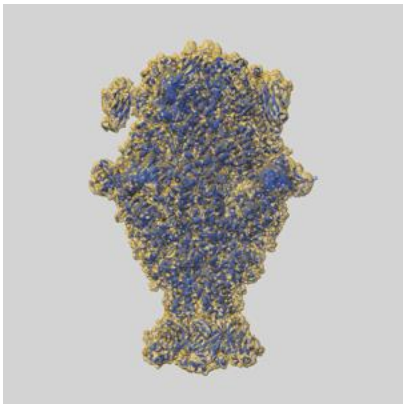
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.14	3.47	3.19

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

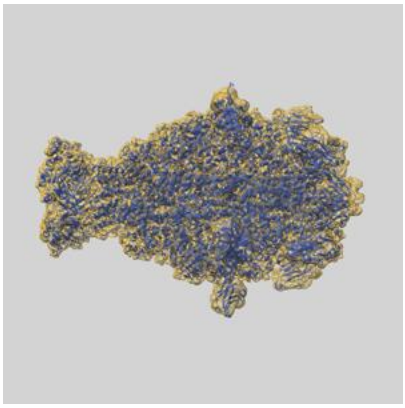
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16791 and PDB model 8CPZ. Per-residue inclusion information can be found in section 3 on page 6.

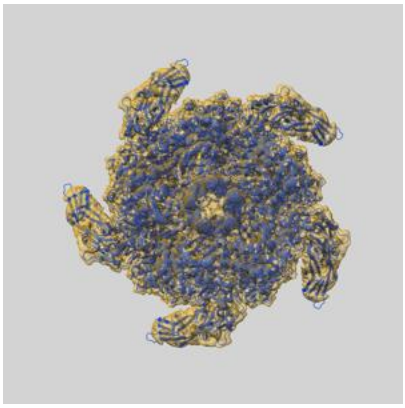
9.1 Map-model overlay



X



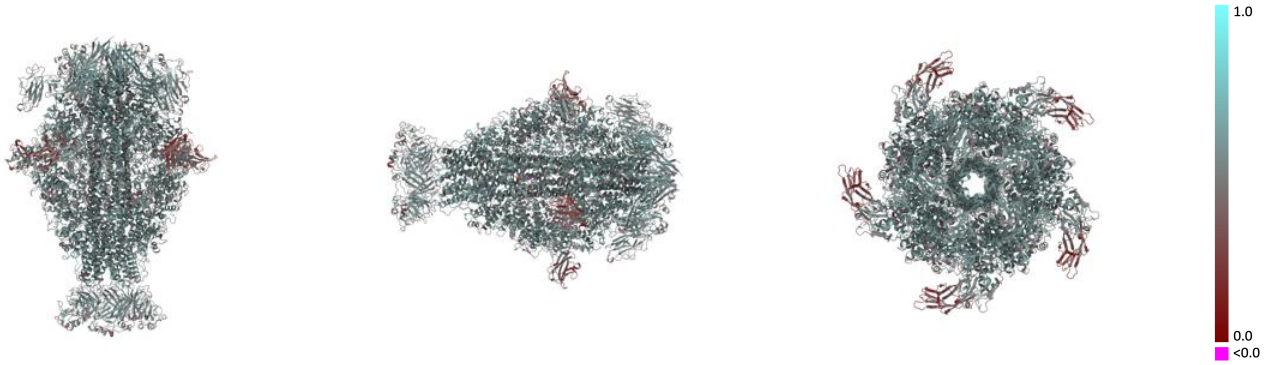
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

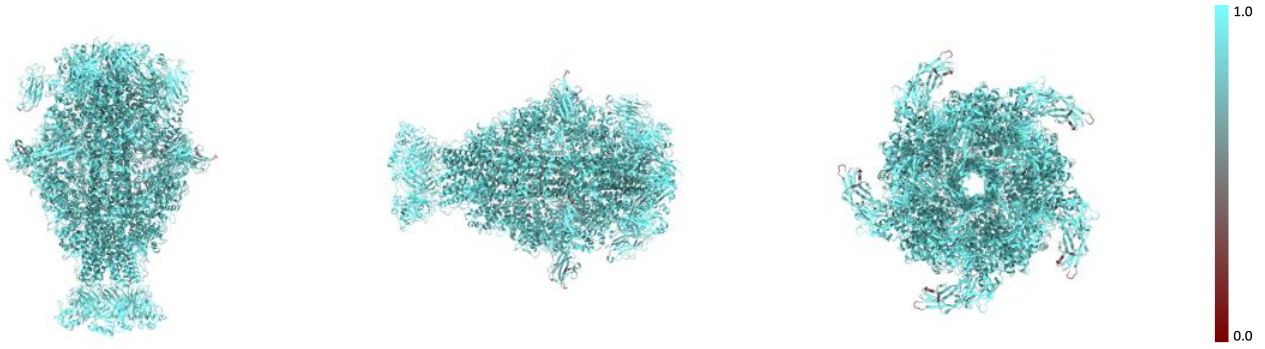
9.2 Q-score mapped to coordinate model (i)



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.

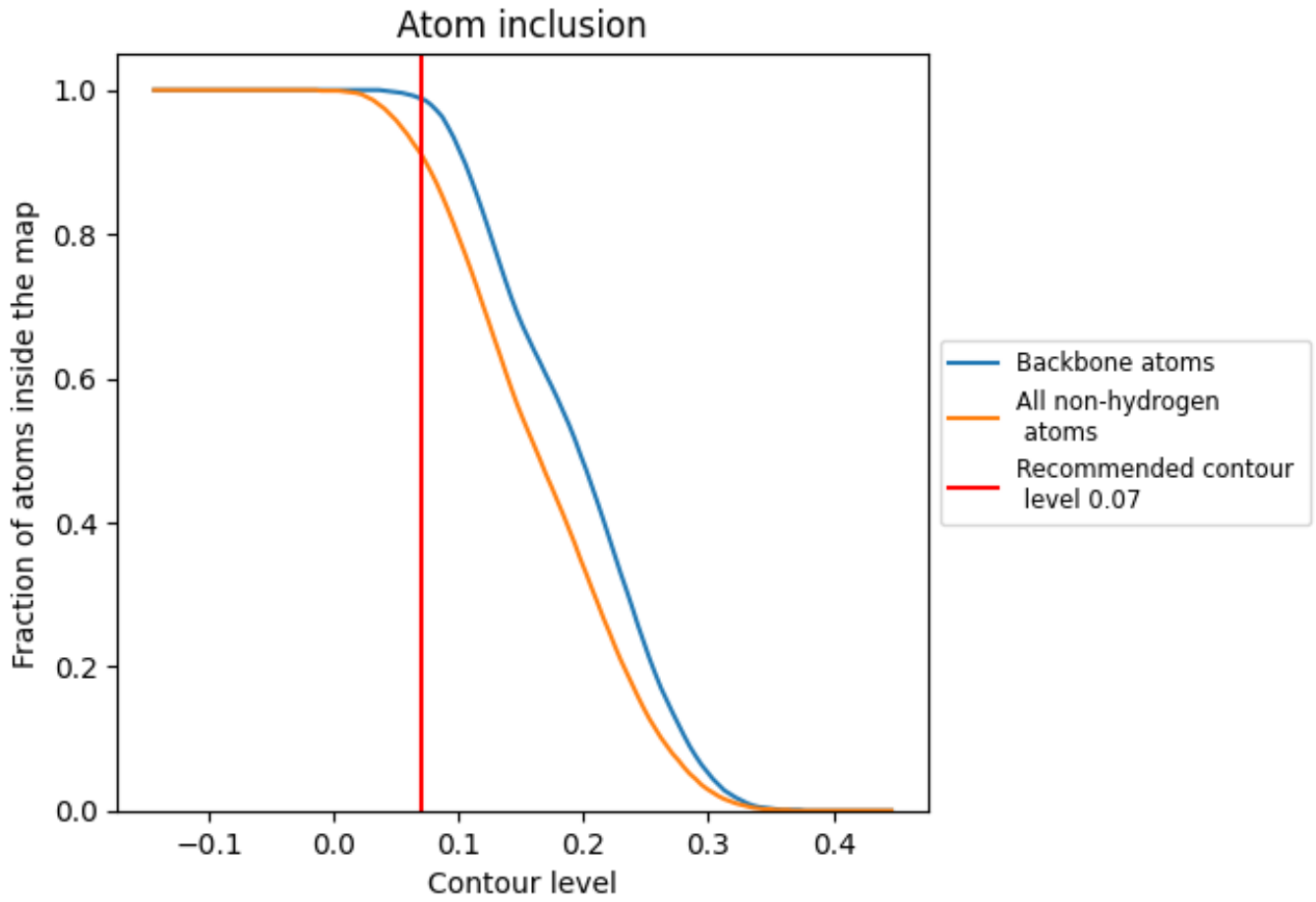
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 91% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9110	0.5260
A	0.9100	0.5260
B	0.9110	0.5270
C	0.9100	0.5270
D	0.9110	0.5260
E	0.9110	0.5260