wwPDB EM Validation Summary Report

Jun 17, 2025 – 06:07 PM JST

PDB ID	:	8XKU / pdb_00008xku
EMDB ID	:	EMD-38425
Title	:	Cryo-EM structure of the Ycf2-FtsHi motor complex from Arabidopsis in ATP-bound state
Authors	:	Liang, K.; Zhan, X.; Xu, Q.; Wu, J.; Yan, Z.
Deposited on	:	2023-12-24
Resolution	:	3.20 Å(reported)

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

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

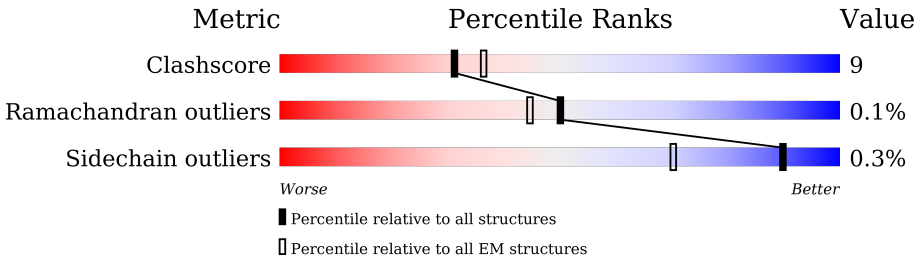
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	855	23% 66% 19% 15%
2	B	1008	13% 67% 17% 16%
3	C	1320	42% 56% 14% 30%
4	D	2294	10% 28% 7% 65%
5	E	946	29% 46% 7% 47%
6	F	876	31% 43% 12% 45%
7	G	396	8% 56% 15% 28%
8	H	348	12% 84%

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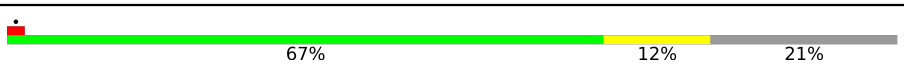
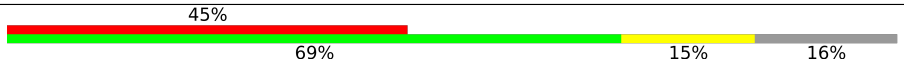
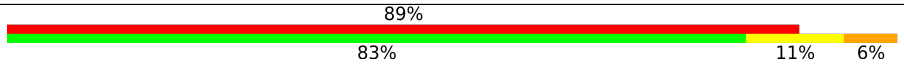
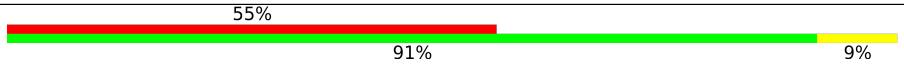
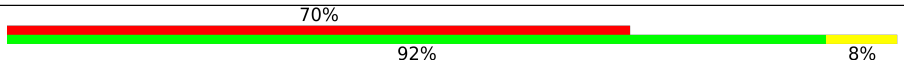
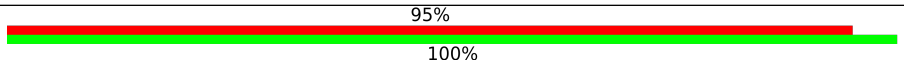
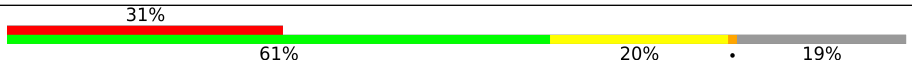
Mol	Chain	Length	Quality of chain
9	I	403	
9	J	403	
10	K	80	
11	L	18	
12	M	11	
13	N	37	
14	O	17	
15	P	19	
16	R	328	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	ATP	A	902	-	-	X	-
18	ATP	B	1103	-	-	X	-
20	PX2	B	1104	-	-	X	-

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 45544 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 Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	730	5841	3718	1000	1103	20	0	0

- Molecule 2 is a protein called ATP-dependent zinc metalloprotease FTSH 12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	845	6879	4404	1195	1251	29	0	0

- Molecule 3 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	921	7494	4775	1299	1386	34	0	0

- Molecule 4 is a protein called Protein Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	805	6659	4314	1145	1173	27	0	0

- Molecule 5 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	498	3881	2451	690	729	11	0	0

- Molecule 6 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	478	Total	C	N	O	S	0	0
			3744	2356	667	701	20		

- Molecule 7 is a protein called AtTam46.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	285	Total	C	N	O	S	0	0
			2375	1615	370	379	11		

- Molecule 8 is a protein called At4g28210.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	54	Total	C	N	O	S	0	0
			459	310	76	72	1		

- Molecule 9 is a protein called Malate dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		
9	J	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		

- Molecule 10 is a protein called Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	67	Total	C	N	O	S	0	0
			555	359	98	97	1		

- Molecule 11 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	18	Total	C	N	O	S	0	0
			131	89	21	20	1		

- Molecule 12 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	11	Total	C	N	O	0	0
			84	59	13	12		

- Molecule 13 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	37	Total	C	N	O	S	0	0
			246	159	45	41	1		

- Molecule 14 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	17	Total	C	N	O	0	0
			132	89	25	18		

- Molecule 15 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	19	Total	C	N	O	0	0
			95	57	19	19		

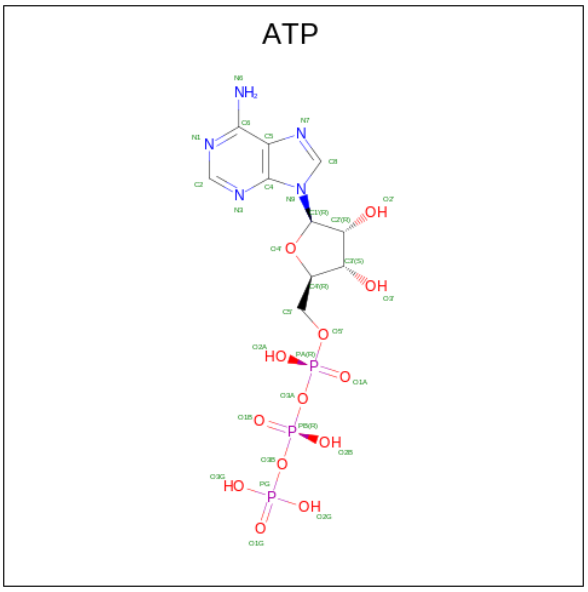
- Molecule 16 is a protein called Embryo defective 2737.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	267	Total	C	N	O	S	0	0
			2151	1371	367	397	16		

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	Mg	0
			1	1	
17	B	1	Total	Mg	0
			1	1	

- Molecule 18 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

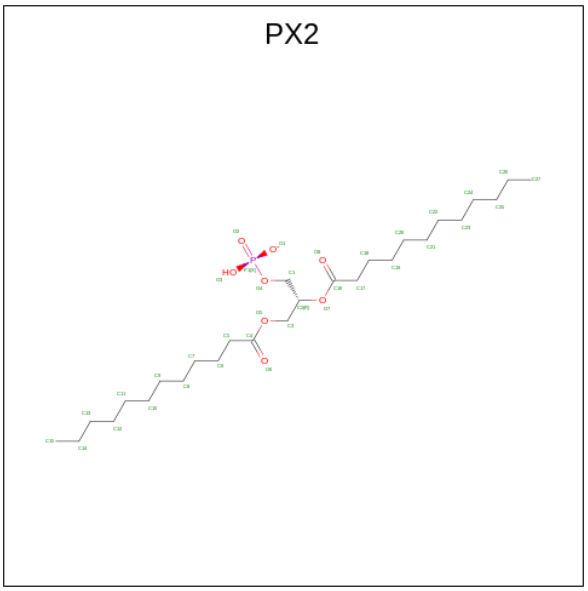


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Zn	0
			1	1	
19	R	2	Total	Zn	0
			2	2	

- Molecule 20 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (CCD ID: PX2) (formula: $C_{27}H_{52}O_8P$).



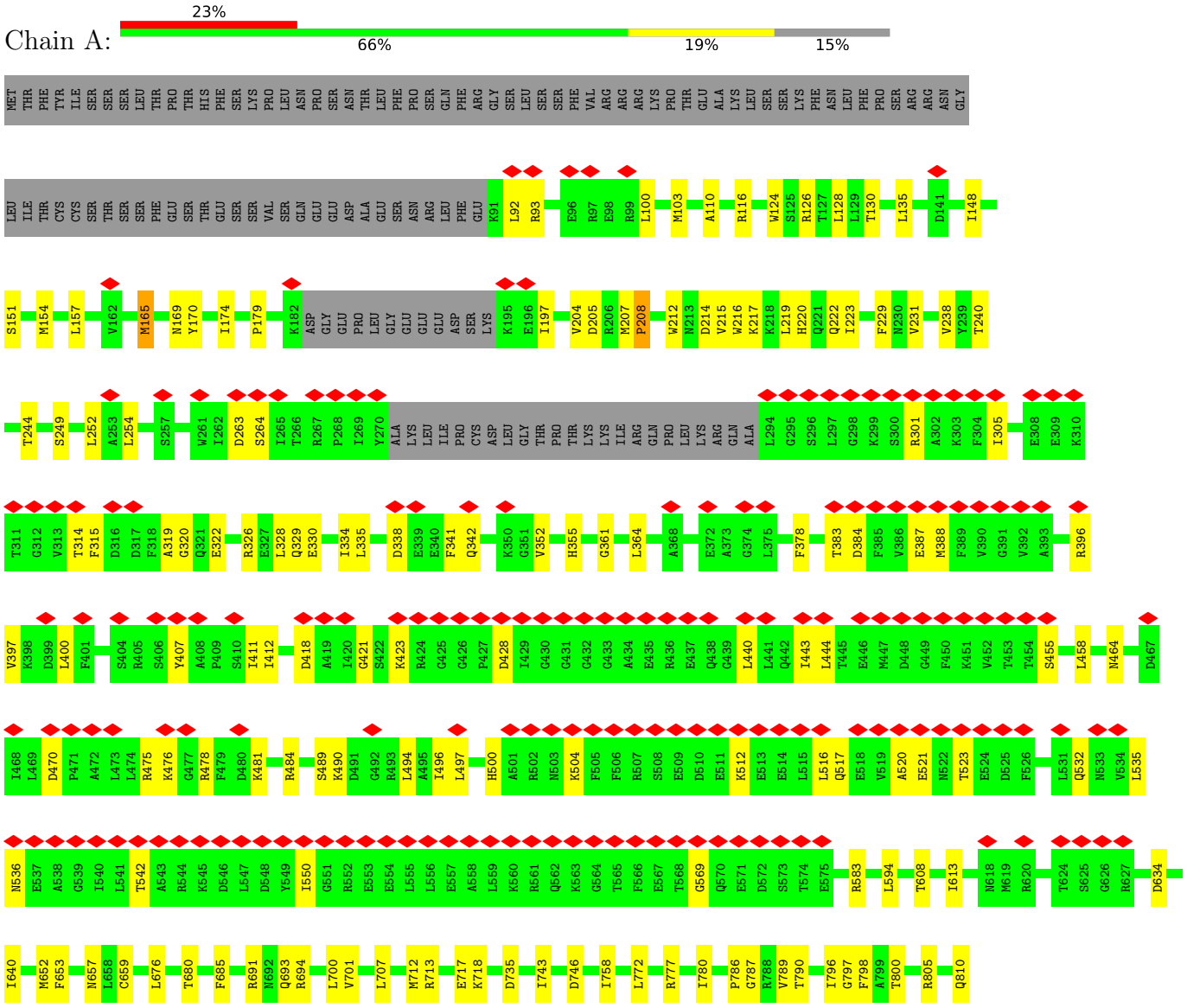
Mol	Chain	Residues	Atoms				AltConf
20	B	1	Total	C	O	P	0
			25	16	8	1	

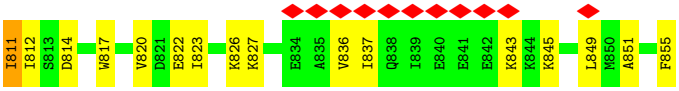
3 Residue-property plots (i)

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.

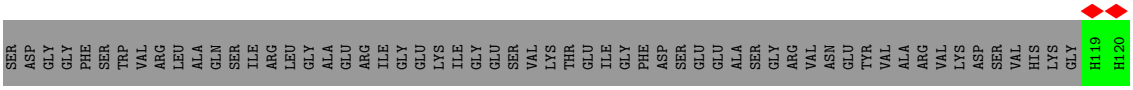
• Molecule 1: Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic

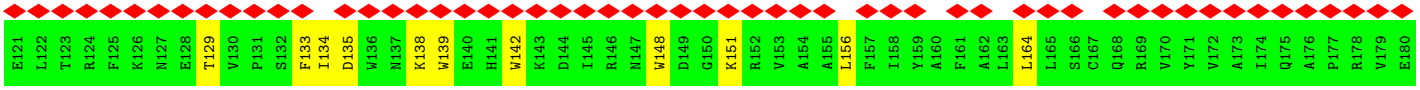
Chain A:

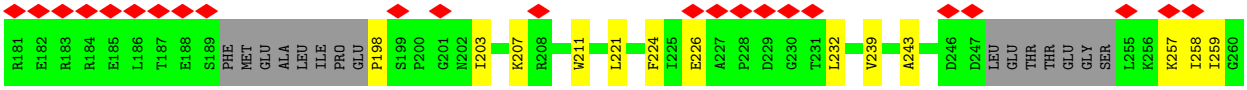


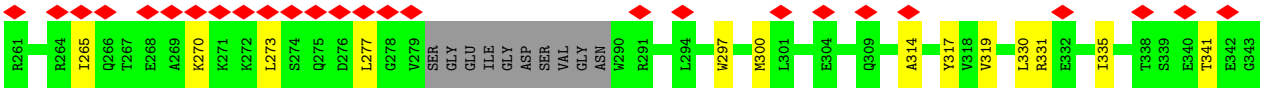


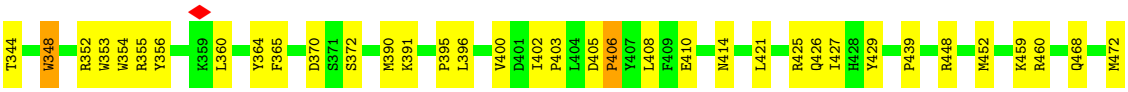
• Molecule 2: ATP-dependent zinc metalloprotease FTSH 12, chloroplastic

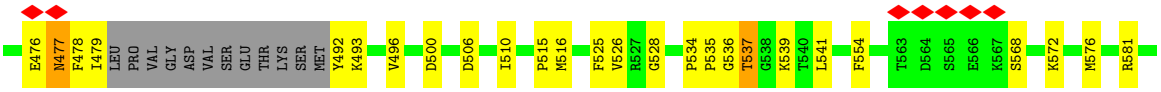


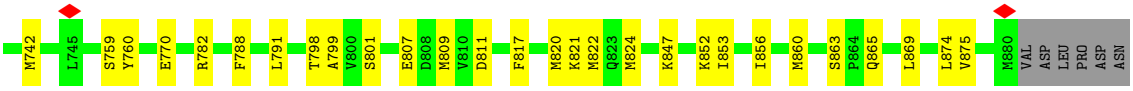




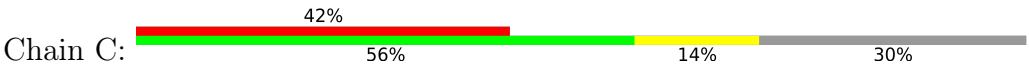


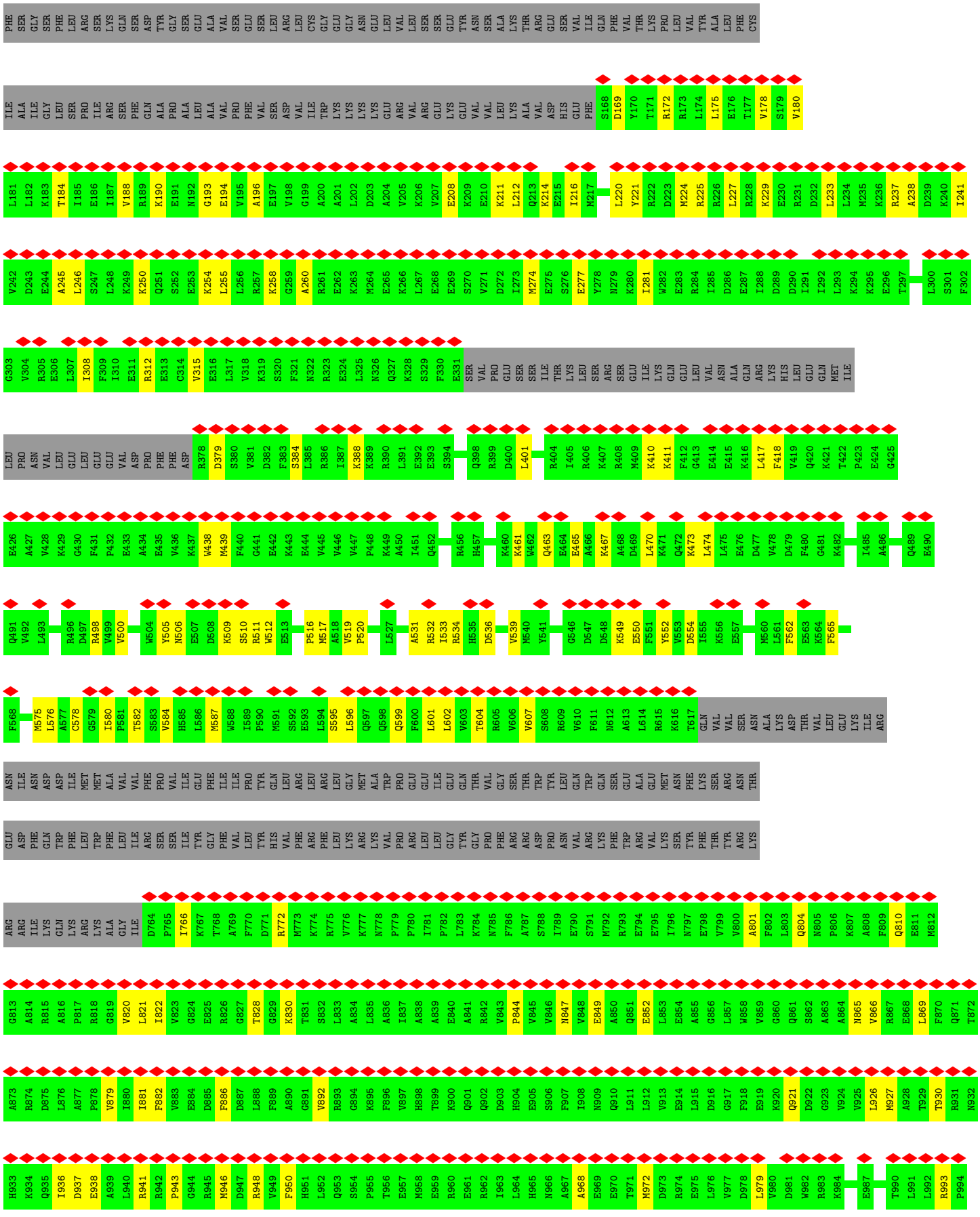


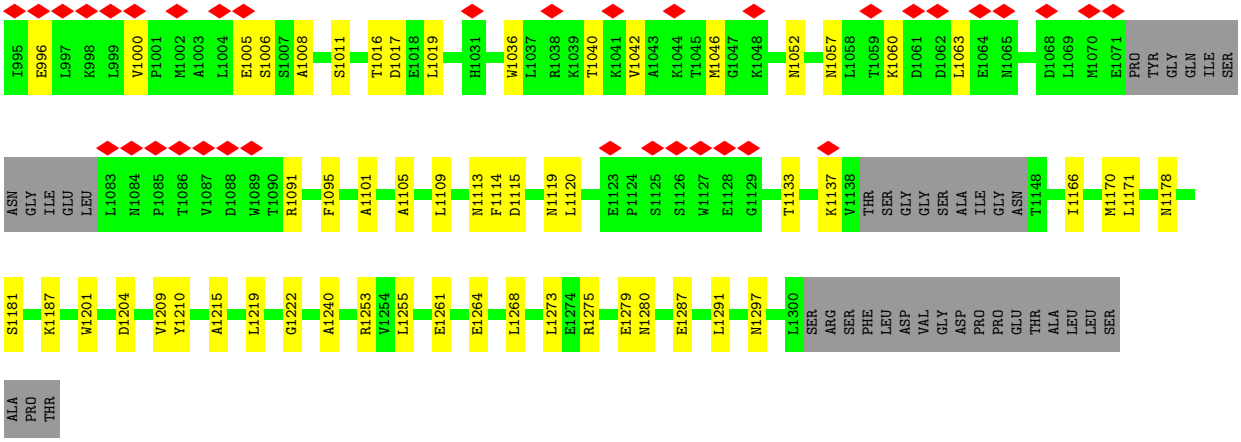




• Molecule 3: Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic

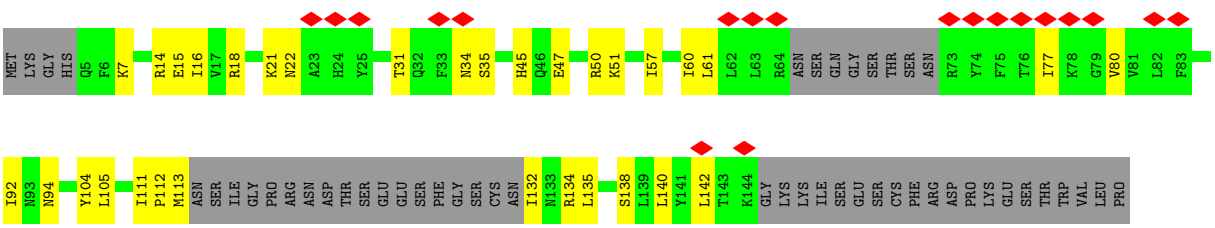


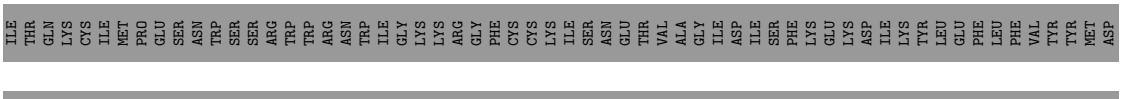

PHE SER GLY SER PHE LEU ARG SER LYS GLN SER ASP TYR GLY SER GLU ALA VAL SER GLU SER LEU ARG LEU CYS GLY GLU GLY ASN GLU LEU VAL LEU SER SER GLU TYR ASN SER ALA LYS THR ARG GLU SER VAL ILE GLN PHE VAL THR LYS PRO LEU VAL TYR ALA LEU PHE CYS
ILE ALA ILE GLY LEU SER PRO ILE ARG SER PHE GLN ALA PRO ALA LEU ALA VAL PRO PHE VAL SER ASP VAL ILE TRP LYS LYS LYS GLU ARG VAL ARG GLU LYS GLU VAL VAL LEU LYS ALA VAL ASP HIS GLU PHE S168 D169 Y170 T171 R172 R173 L174 L175 E176 T177 V178 S179 V180
L181 L182 K183 T184 I185 E186 I187 V188 R189 K190 E191 N192 G193 E194 V195 A196 E197 V198 G199 A200 A201 L202 D203 A204 V205 K206 V207 E208 K209 E210 K211 L212 Q213 K214 E215 I216 M217 L220 Y221 R222 D223 M224 R225 R226 L227 R228 K229 E230 R231 D232 L233 L234 M235 K236 R237 A238 D239 K240 I241
V242 D243 E244 A245 L246 S247 L248 K249 K250 Q251 S252 E253 K254 L255 L256 R257 K258 G259 A260 R261 E262 K263 M264 E265 K266 L267 E268 E269 S270 V271 D272 I273 M274 E275 S276 E277 Y278 N279 K280 I281 W282 E283 R284 I285 D286 E287 I288 D289 D290 I291 I292 L293 K294 K295 E296 T297 L300 S301 F302
G303 V304 R305 E306 L307 I308 F309 I310 E311 R312 E313 C314 V315 E316 L317 V318 K319 S320 F321 N322 R323 E324 L325 N326 Q327 K328 S329 F330 E331 SER VAL PRO GLU SER SER ILE THR LYS LEU SER ARG SER GLU ILE LYS GLN GLU LEU VAL ASN ALA GLN ARG LYS HIS LEU LEU GLU GLN MET ILE
LEU PRO ASN VAL LEU GLU LEU GLU GLU VAL ASP PRO PHE PHE ASP R378 D379 S380 V381 D382 F383 S384 L385 R386 I387 K388 K389 R390 L391 E392 E393 S394 Q398 R399 D400 L401 R404 I405 R406 K407 R408 M409 K410 K411 F412 G413 E414 E415 K416 L417 F418 V419 Q420 K421 T422 P423 E424 G425
E426 A427 V428 K429 G430 F431 P432 E433 A434 E435 V436 K437 W438 M439 F440 G441 E442 K443 E444 V445 V446 V447 P448 K449 A450 I451 Q452 R456 H457 K460 K461 W462 Q463 E464 E465 A466 K467 A468 D469 L470 K471 Q472 K473 L474 L475 E476 D477 V478 D479 F480 G481 K482 I485 A486 Q489 E490
Q491 V492 L493 R496 D497 R498 V499 V500 W504 Y505 N506 E507 D508 K509 S510 R511 W512 E513 P516 M517 A518 V519 P520 L527 A531 R532 I533 R534 H535 D536 V539 M540 Y541 G546 D547 D548 K549 E550 F551 Y552 V553 D554 I555 K556 E557 M560 L561 F562 E563 K564 F565
F568 M575 L576 A577 C578 G579 I580 P581 T582 S583 V584 H585 L586 M587 W588 I589 P590 M591 S592 E593 L594 S595 L596 Q597 Q598 Q599 F600 L601 L602 V603 T604 R605 V606 V607 S608 R609 V610 F611 N612 A613 L614 R615 K616 T617 GLN VAL VAL SER ASN ALA LYS ASP THR VAL LEU GLU LYS ILE ARG
ASN ILE ASN ASP ASP ILE MET MET ALA VAL VAL PHE PRO VAL ILE GLU PHE ILE ILE PRO TYR GLN LEU ARG LEU ARG LEU GLY MET ALA TRP PRO GLU GLU ILE LEU GLU GLN THR VAL GLY SER THR TRP TYR LEU GLN TRP GLN SER GLU ALA GLU MET ASN PHE LYS SER ARG ASN THR
GLU ASP PHE GLN TRP PHE LEU TRP PHE LEU ILE ARG SER SER ILE TYR GLY PHE VAL LEU TYR HIS VAL PHE ARG PHE LEU LYS ARG LYS VAL PRO ARG LEU LEU LEU GLY TYR GLY PRO PHE ARG ARG ASP PRO ASN VAL ARG LYS PHE TRP ARG VAL LYS SER TYR PHE THR TYR ARG LYS
ARG ARG ILE LYS GLN LYS ARG LYS ALA GLY ILE D764 P765 I766 K767 T768 A769 F770 D771 R772 M773 K774 R775 V776 K777 N778 P779 P780 I781 P782 L783 K784 N785 F786 A787 S788 I789 E790 S791 M792 R793 E794 E795 I796 N797 E798 V799 V800 A801 F802 L803 Q804 N805 P806 K807 A808 F809 Q810 E811 M812
G813 A814 R815 A816 P817 R818 G819 V820 L821 I822 V823 G824 E825 R826 G827 T828 G829 K830 T831 S832 L833 A834 L835 A836 I837 A838 A839 E840 A841 R842 V843 P844 V845 V846 N847 V848 E849 A850 Q851 E852 L853 E854 A855 G856 L857 W858 V859 G860 Q861 S862 A863 A864 N865 V866 R867 E868 L869 F870 Q871 T872
A873 R874 D875 L876 A877 P878 V879 I880 I881 F882 V883 E884 D885 F886 D887 L888 F889 A890 G891 V892 R893 G894 K895 F896 V897 H898 T899 K900 Q901 Q902 D903 H904 E905 S906 F907 I908 N909 Q910 L911 L912 V913 E914 L915 D916 G917 F918 E919 K920 Q921 D922 G923 V924 V925 L926 M927 A928 T929 T930 R931 N932
H933 K934 Q935 I936 D937 E938 A939 L940 R941 R942 P943 G944 R945 M946 D947 R948 V949 F950 H951 L952 Q953 S954 P955 T956 E957 M958 E959 R960 E961 R962 I963 L964 H965 N966 A967 A968 E969 E970 T971 M972 D973 R974 E975 L976 V977 D978 L979 V980 D981 W982 R983 K984 E987 T990 L991 L992 R993 P994

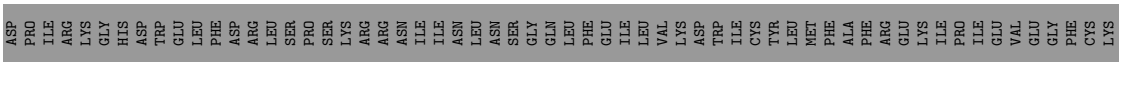


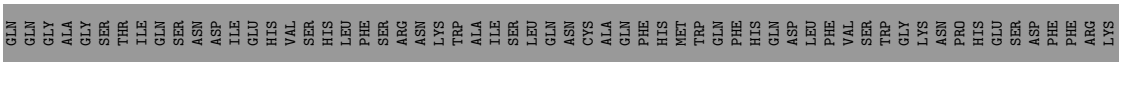
• Molecule 4: Protein Ycf2

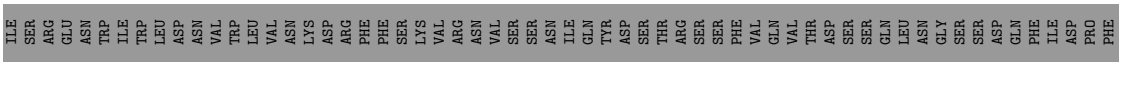
Chain D:

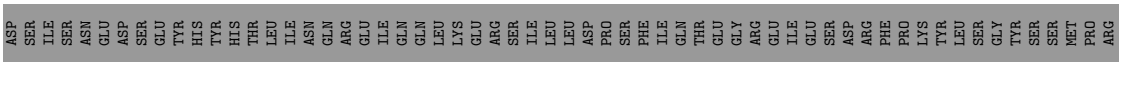


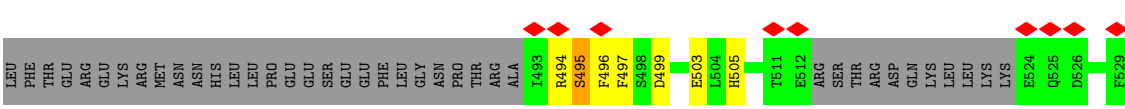


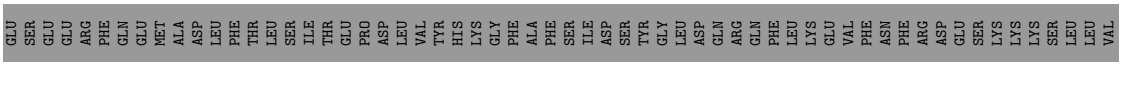


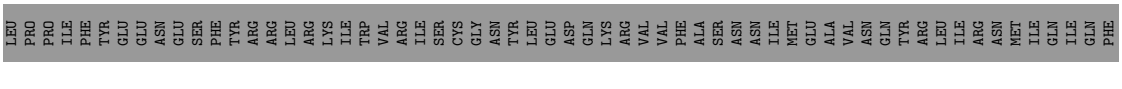


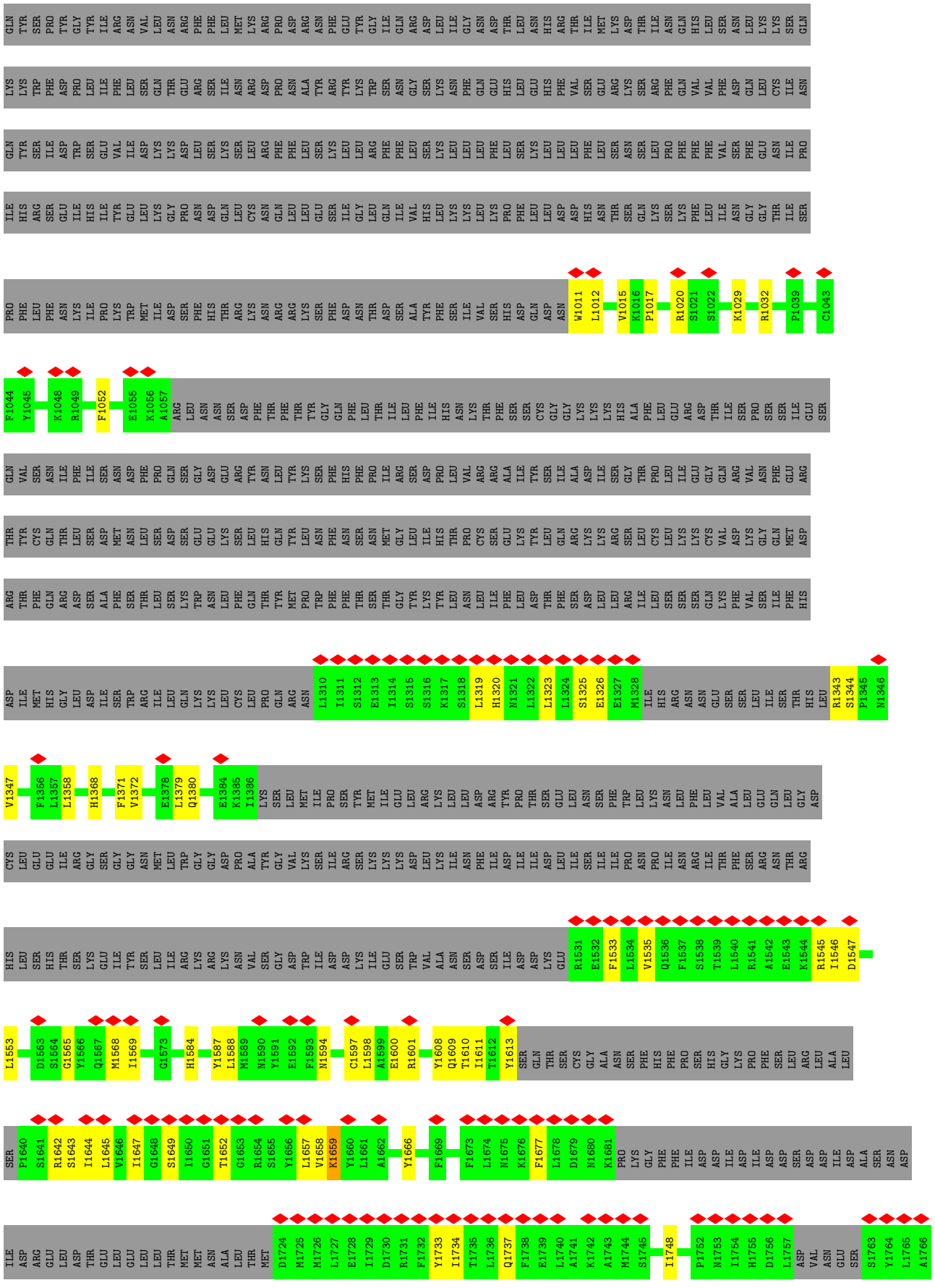


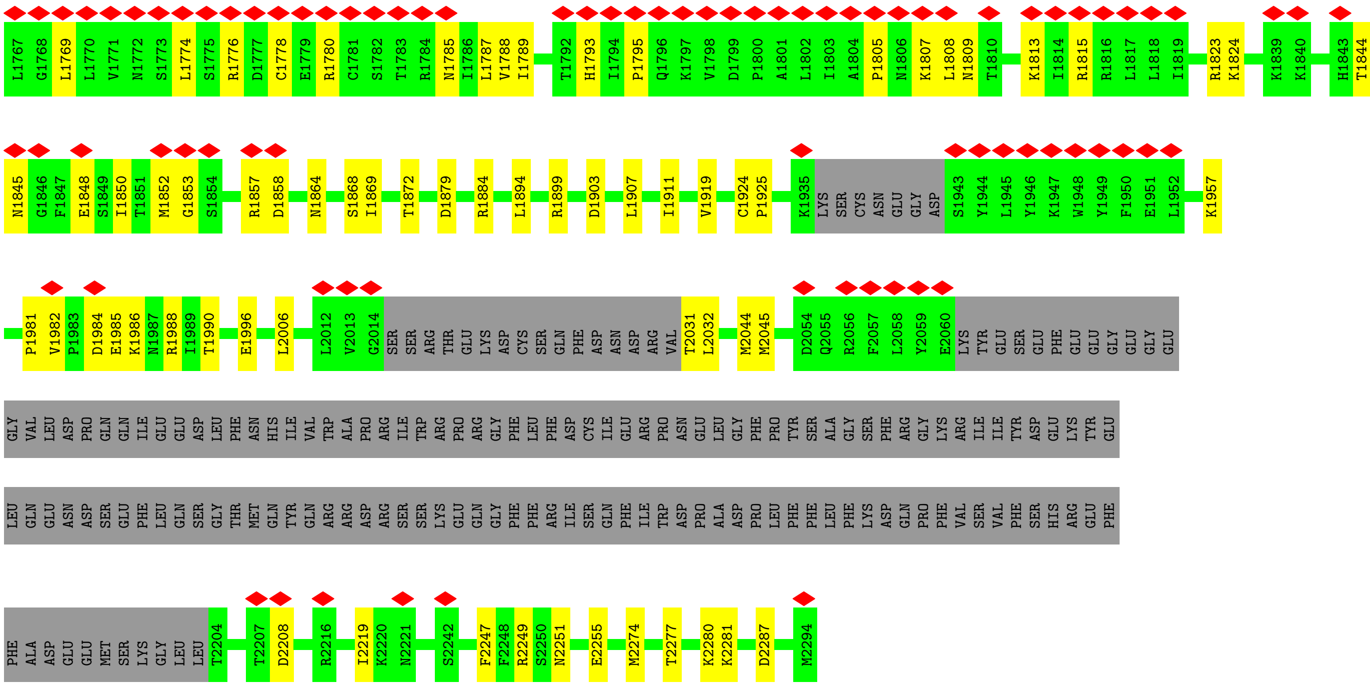




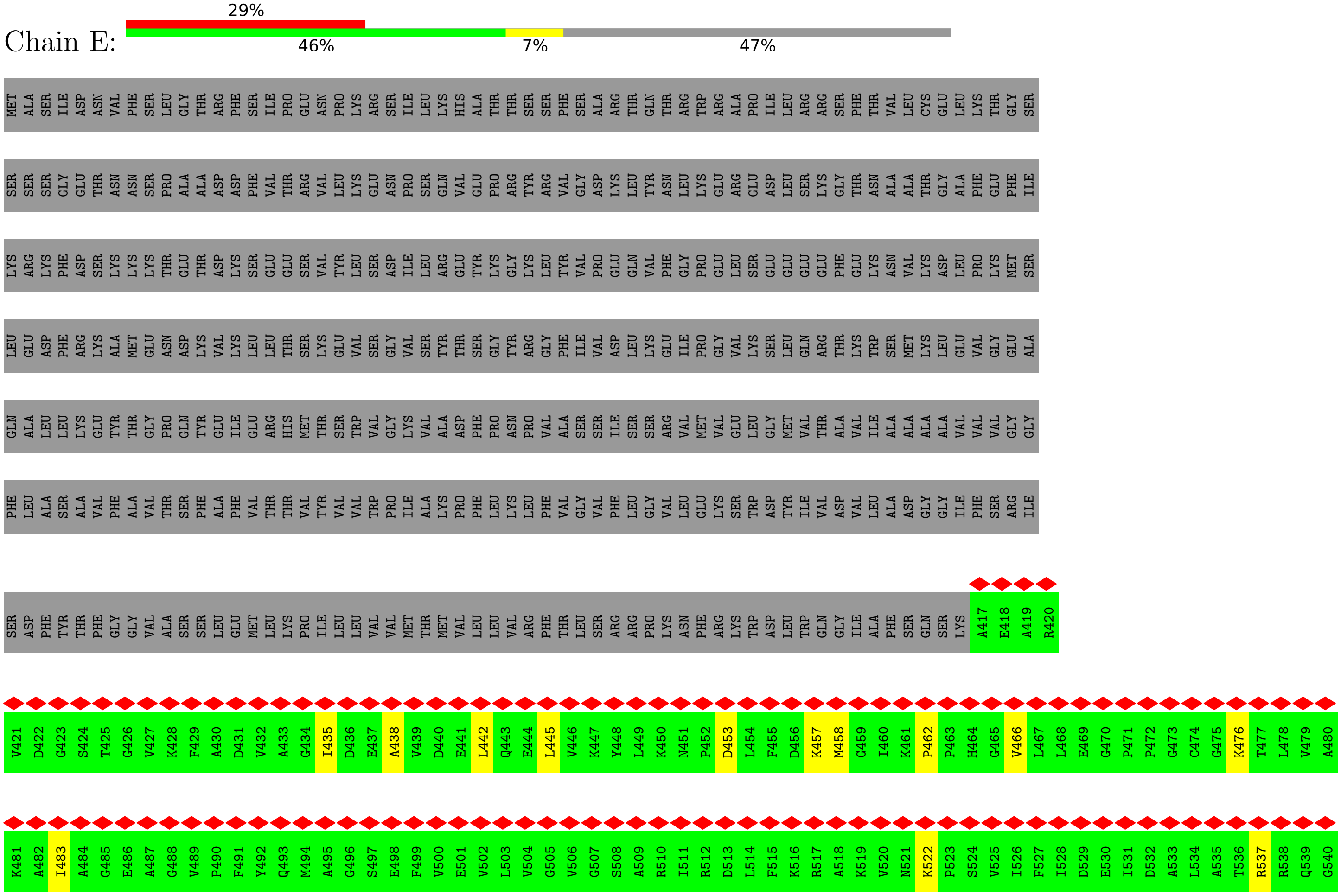


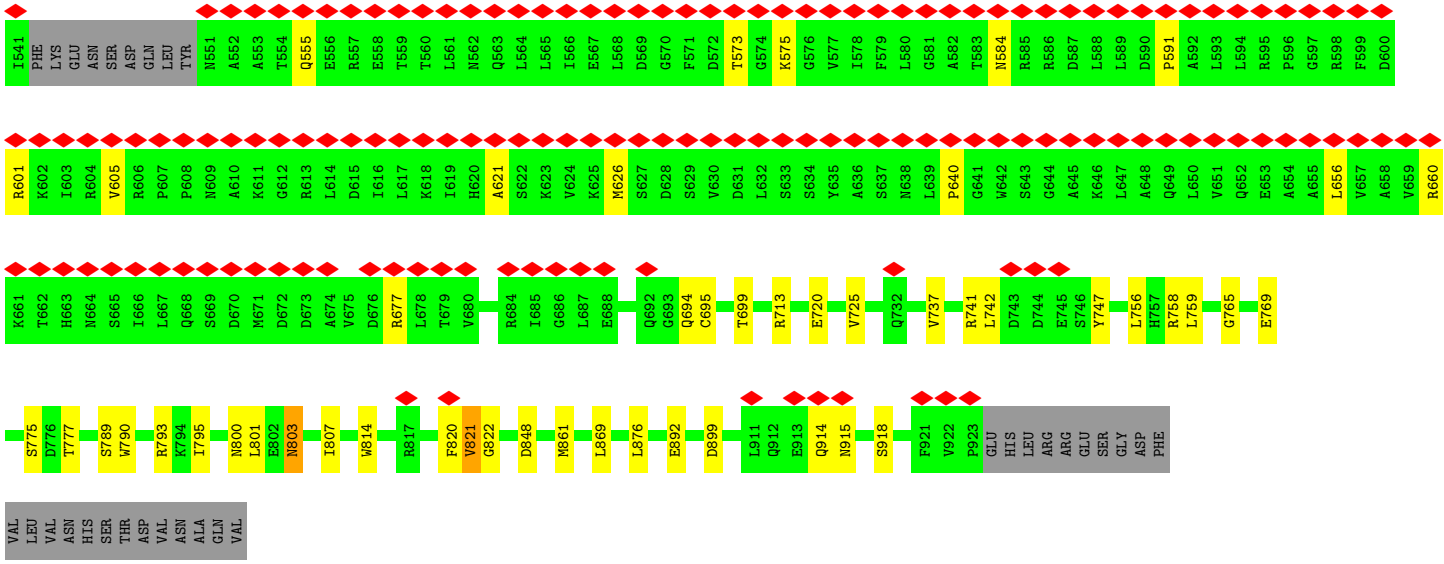


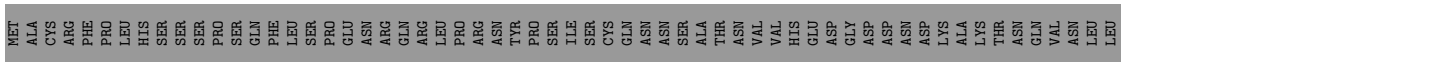

GLN TYR SER PRO TYR GLY TYR ILE ARG ASN VAL LEU ASN ARG PHE PHE LEU MET LYS ARG PRO ASP ARG ASN PHE GLU TYR GLY ILE GLN ARG ASP LEU ILE GLY ASN ASP THR LEU ASN HIS ARG THR ILE MET LYS ASP THR ILE ASN GLN HIS LEU LEU SER ASN LEU LYS LYS SER GLN
LYS LYS TRP PHE ASP PRO LEU ILE PHE LEU SER GLN THR GLU ARG SER ILE ASN ARG ASP PRO ASN ALA TYR ARG TYR LYS TRP SER ASN GLY SER LYS SER ARG PHE GLN VAL VAL PHE ASP GLN LEU CYS ILE ASN
GLN TYR SER ILE ASP TRP SER GLU VAL ILE ASP LYS LYS ASP LEU ARG PHE PHE LEU SER LYS LEU LEU LEU PHE LEU SER LYS LEU LEU LEU LEU PRO
ILE HIS ARG SER GLU ILE HIS ILE TYR GLU LEU LYS GLY PRO ASN ASP GLN LEU CYS ASN GLN LEU LEU GLU SER ILE GLY LEU GLN ILE VAL HIS LEU LYS LYS LEU LYS PRO PHE LEU LEU ASP HIS ASN THR SER GLN LYS SER GLY LYS SER PHE LEU ILE ASN GLY GLY THR ILE SER
PRO PHE LEU PHE ASN LYS ILE PRO LYS TRP MET ILE ASP SER PHE HIS THR ARG LYS ASN ARG ARG LYS SER PHE ASP ASN THR ASP SER ALA TYR PHE SER ILE VAL SER HIS ASP GLN ASN W1011 L1012 V1015 K1016 P1017 R1020 S1021 S1022 K1029 R1032 P1039 C1043
F1044 Y1045 K1048 R1049 F1052 E1055 K1056 A1057 ARG LEU ASN ASN SER ASP PHE THR PHE THR TYR GLY GLN PHE LEU THR ILE LEU PHE ILE HIS ASN LYS THR PHE SER SER CYS GLY GLY LYS LYS LYS HIS ALA PHE LEU GLU ARG ASP THR ILE SER PRO SER SER ILE GLU GLU SER
GLN VAL SER ASN ILE PHE ILE SER ASN ASP PHE PRO GLN SER GLY ASP GLU ARG TYR ASN LEU TYR LYS SER PHE HIS PHE PRO ILE ARG SER ASP PRO LEU VAL ARG ARG ALA ILE TYR SER ILE ALA ASP ILE SER LYS GLY THR PRO LEU ILE GLU GLY GLN ARG VAL ASN PHE GLU ARG
THR TYR CYS GLN THR LEU SER ASP MET ASN LEU SER ASP SER GLU GLU LYS SER LEU HIS GLN TYR LEU ASN PHE ASN SER ASN MET GLY LEU ILE HIS THR PRO CYS SER GLU LYS TYR LEU GLN ARG LYS LYS ARG SER LEU CYS LEU LYS LYS CYS VAL ASP LYS GLY ILE HIS MET ASP
ARG THR PHE GLN ARG ASP SER ALA PHE SER THR LEU SER LYS TRP ASN LEU PHE GLN THR TYR MET PRO TRP PHE PHE THR SER TRP LYS TYR LYS GLY PHE THR PHE SER ASP LEU LEU ARG ILE LEU SER SER SER GLN LYS PHE VAL SER ILE PHE HIS
ASP ILE MET HIS GLY LEU ASP ILE SER TRP ARG ILE LEU GLN LYS LYS LEU CYS LEU PRO GLN ARG ASN L1310 I1311 S1312 E1313 I1314 S1315 S1316 K1317 S1318 L1319 H1320 N1321 L1322 L1323 L1324 S1325 E1326 E1327 M1328 ILE HIS ARG ASN ASN GLU SER SER LEU ILE SER THR HIS LEU R1343 S1344 P1345 N1346
V1347 F1356 L1357 L1358 H1368 F1371 V1372 E1378 L1379 Q1380 E1384 K1385 I1386 LYS SER LEU MET ILE PRO SER TYR MET ILE GLU LEU ARG LYS LEU LEU ASP ARG TYR PRO THR SER GLU LEU ASN SER PHE TRP LEU LYS ASN LEU PHE LEU VAL ALA LEU GLU GLN LEU GLY ASP
CYS LEU GLU GLU ILE ARG GLY GLY SER GLY GLY ASN MET LEU TRP GLY GLY ASP PRO ALA TYR GLY VAL LYS SER ILE ARG SER LYS LYS LYS ASP LEU LYS ILE ASN PHE ILE ASP ILE ILE ASP LEU ILE SER ILE ILE PRO ASN PRO ILE ASN ARG ILE THR PHE SER ARG ASN THR ARG
HIS LEU SER HIS THR SER LYS GLU ILE TYR SER LEU ILE ARG LYS ARG LYS ASN VAL SER GLY ASP TRP ILE ASP ASP LYS ILE GLU GLU SER TRP VAL ALA ASN SER ASP SER ILE ASP ASP LYS GLU R1531 E1532 F1533 L1534 V1535 Q1536 F1537 S1538 T1539 L1540 R1541 A1542 E1543 K1544 R1545 I1546 D1547
L1553 D1563 S1564 G1565 Y1566 Q1567 M1568 I1569 G1573 H1584 Y1587 L1588 M1589 N1590 Y1591 E1592 F1593 N1594 C1597 L1598 A1599 E1600 R1601 Y1608 Q1609 T1610 I1611 T1612 Y1613 SER GLN THR SER CYS GLY ALA ASN SER PHE HIS PHE PRO SER HIS GLY LYS PRO PHE SER LEU ARG LEU ALA LEU
SER P1640 S1641 R1642 S1643 I1644 L1645 V1646 I1647 G1648 S1649 I1650 G1651 T1652 G1653 R1654 S1655 Y1656 L1657 V1658 K1659 Y1660 L1661 A1662 Y1666 F1669 F1673 L1674 N1675 K1676 F1677 L1678 D1679 N1680 K1681 PRO LYS GLY PHE PHE ILE ASP ASP ILE ASP ILE ASP ASP ASP ASP ILE ASP ASP ALA SER ASN ASP
ILE ASP ARG GLU LEU ASP THR GLU LEU GLU LEU LEU THR MET MET ASN ALA LEU THR MET D1724 M1725 M1726 L1727 E1728 I1729 D1730 R1731 F1732 Y1733 I1734 T1735 L1736 Q1737 F1738 E1739 L1740 A1741 K1742 A1743 M1744 S1745 I1748 P1752 N1753 I1754 H1755 D1756 L1757 ASP VAL ASN GLU SER S1763 Y1764 L1765 A1766



• Molecule 5: Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic

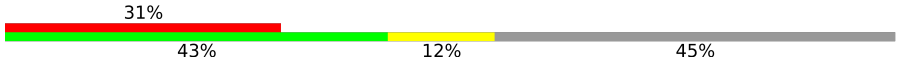


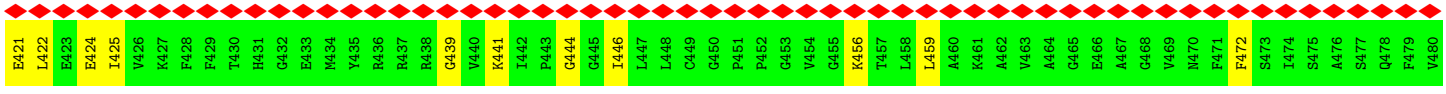


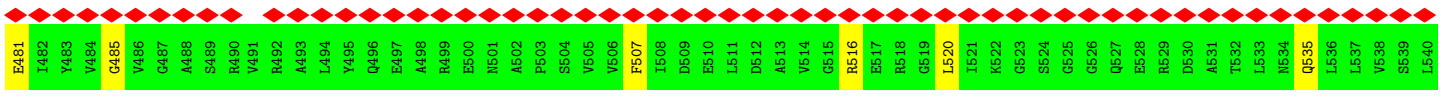


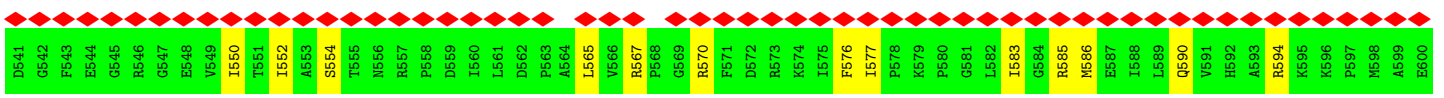
• Molecule 6: Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic

Chain F:

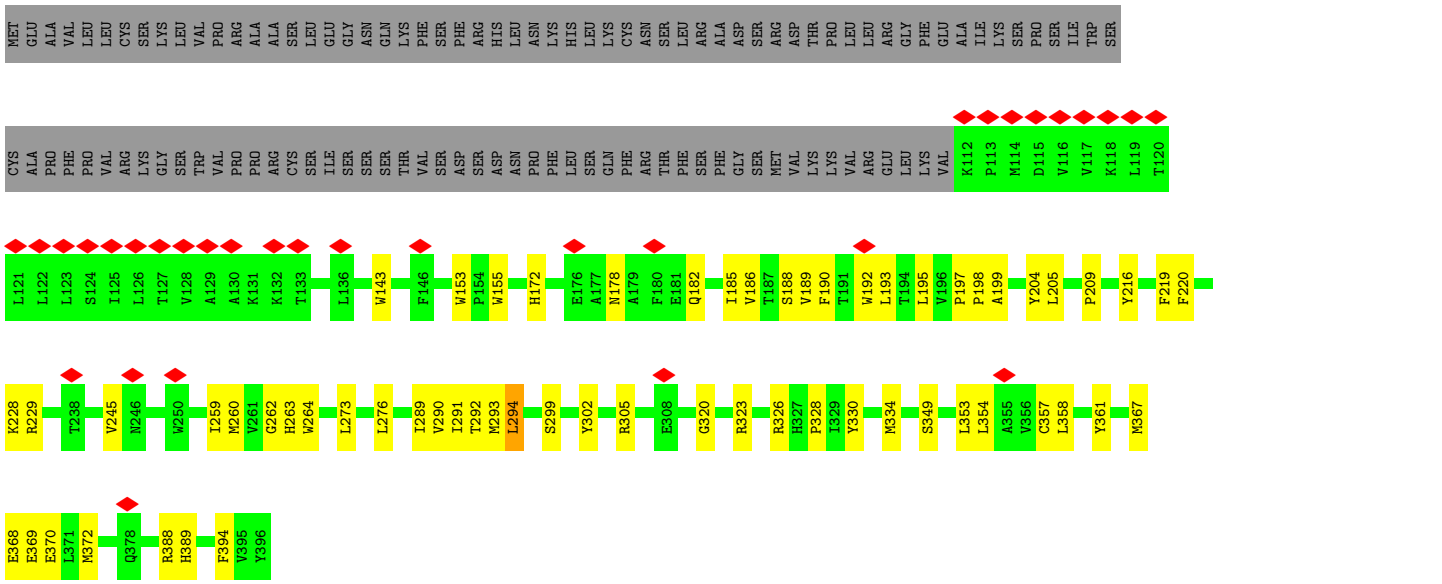




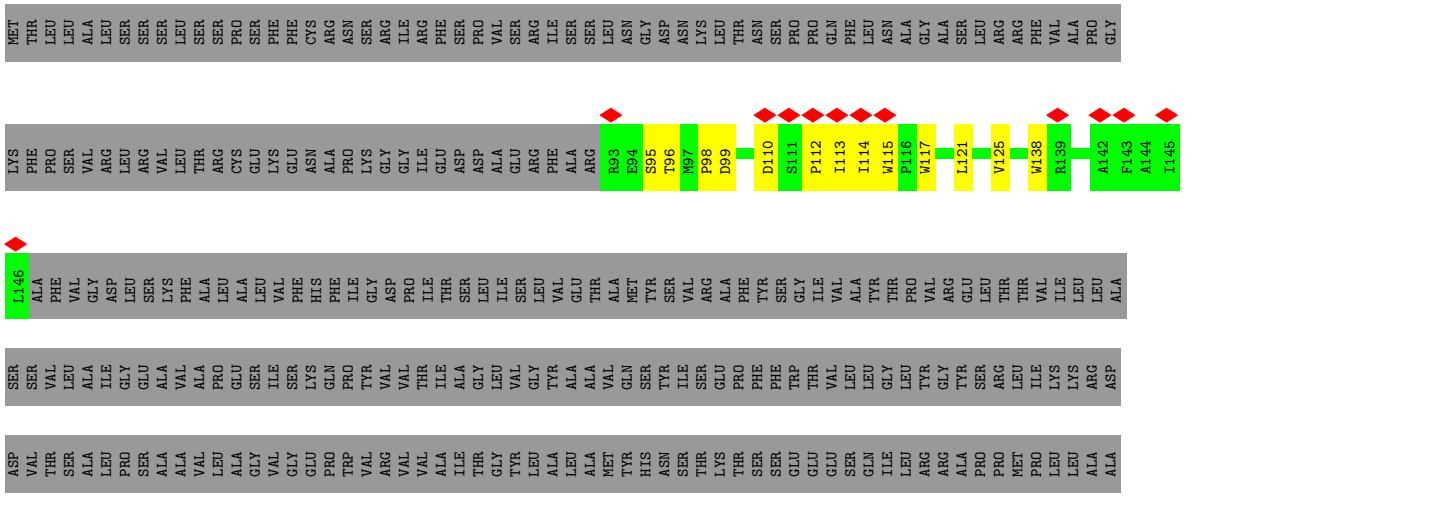




• Molecule 7: AtTam46

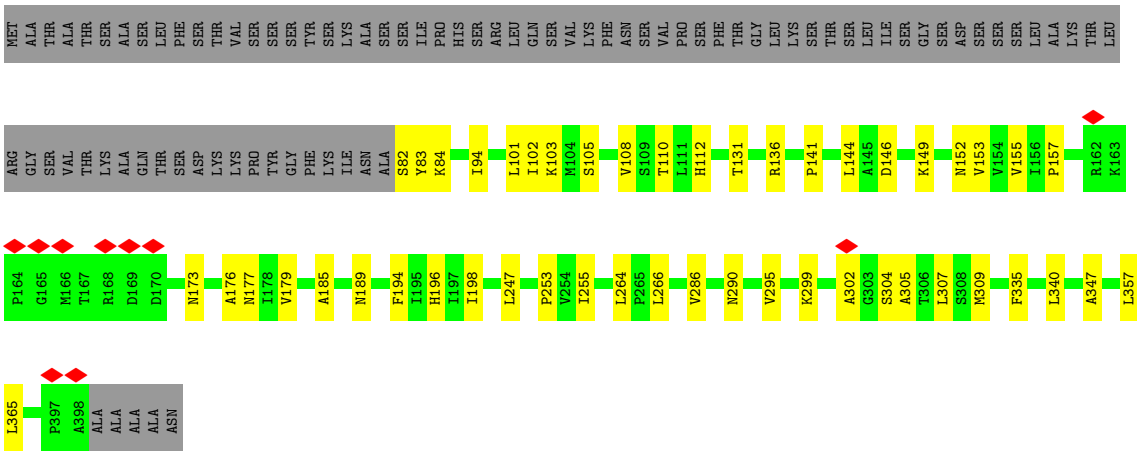


• Molecule 8: At4g28210



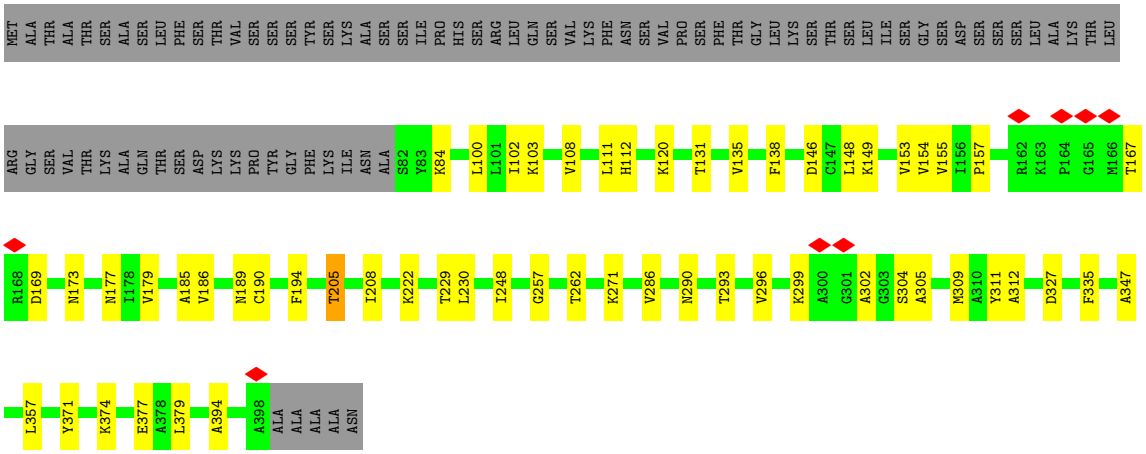
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain I:



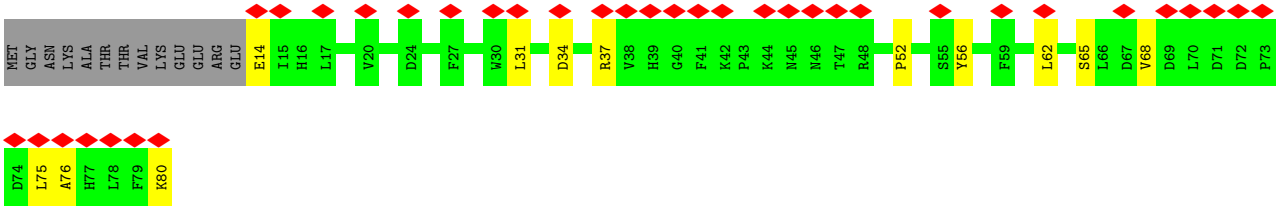
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain J:



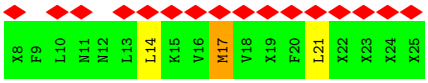
• Molecule 10: Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B

Chain K:



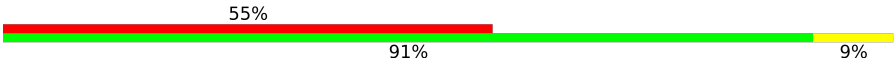
• Molecule 11: UNK

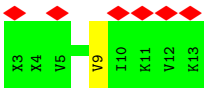
Chain L:



• Molecule 12: UNK

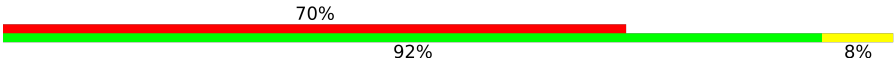
Chain M:

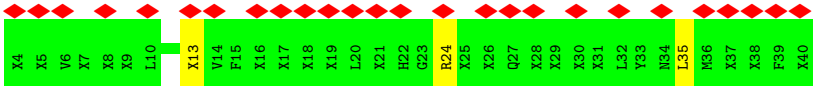




• Molecule 13: UNK

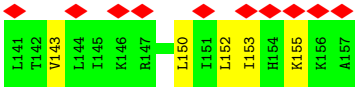
Chain N:





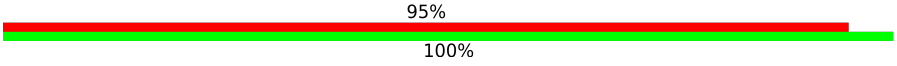
• Molecule 14: UNK

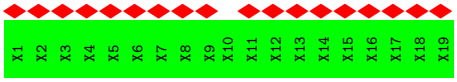
Chain O:



• Molecule 15: UNK

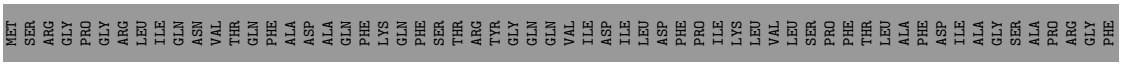
Chain P:

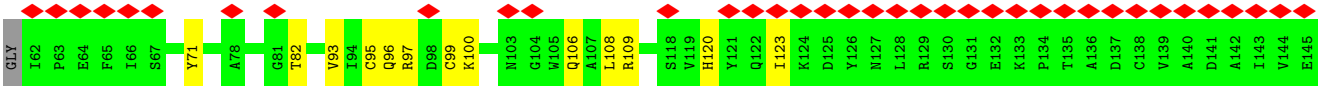


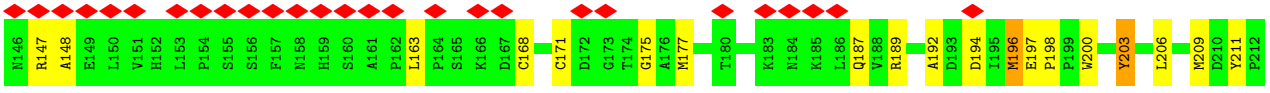


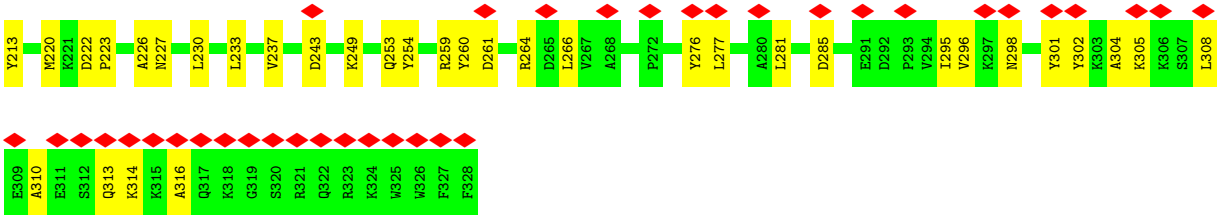
• Molecule 16: Embryo defective 2737

Chain R:








Y213
M220
K221
D222
P223
A226
N227
L230
L233
V237
D243
K249
Q253
Y254
R259
Y260
D261
R264
D265
L266
V267
A268
P272
Y276
L277
A280
L281
D285
E291
D292
P293
V294
I295
V296
K297
N298
Y301
Y302
K303
A304
K305
K306
S307
L308
E309
A310
E311
S312
Q313
K314
K315
A316
Q317
K318
G319
S320
R321
Q322
R323
K324
W325
W326
F327
F328

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	738896	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.115	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PX2, MG, ATP, ZN

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	0.17	0/5952	0.47	0/8038
2	B	0.23	1/7022 (0.0%)	0.55	5/9460 (0.1%)
3	C	0.16	0/7627	0.46	0/10262
4	D	0.18	0/6804	0.49	1/9177 (0.0%)
5	E	0.14	0/3953	0.38	0/5357
6	F	0.16	0/3798	0.44	1/5115 (0.0%)
7	G	0.23	0/2470	0.58	2/3375 (0.1%)
8	H	0.17	0/477	0.41	0/651
9	I	0.15	0/2399	0.41	0/3261
9	J	0.15	0/2399	0.42	2/3261 (0.1%)
10	K	0.21	0/570	0.47	0/772
11	L	0.28	0/101	0.95	1/133 (0.8%)
12	M	0.23	0/74	0.72	0/99
13	N	0.15	0/142	0.52	0/179
14	O	0.22	0/132	0.59	0/175
16	R	0.19	0/2206	0.49	0/2986
All	All	0.18	1/46126 (0.0%)	0.48	12/62301 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
4	D	0	2
5	E	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	406	PRO	CG-CD	-9.93	1.17	1.50

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	406	PRO	CA-N-CD	-12.98	93.82	112.00
2	B	406	PRO	N-CD-CG	-11.01	86.69	103.20
11	L	17	MET	CB-CG-SD	7.94	136.51	112.70
2	B	406	PRO	CA-CB-CG	-6.63	91.91	104.50
7	G	293	MET	CA-CB-CG	6.01	126.13	114.10

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	ILE	Peptide
2	B	476	GLU	Peptide
2	B	477	ASN	Peptide
2	B	990	LYS	Peptide
4	D	495	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5841	0	5858	153	0
2	B	6879	0	6912	176	0
3	C	7494	0	7625	129	0
4	D	6659	0	6763	139	0
5	E	3881	0	3926	44	0
6	F	3744	0	3823	74	0
7	G	2375	0	2353	52	0
8	H	459	0	455	10	0
9	I	2363	0	2437	29	0
9	J	2363	0	2437	35	0
10	K	555	0	561	12	0
11	L	131	0	123	4	0
12	M	84	0	97	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	N	246	0	175	5	0
14	O	132	0	161	5	0
15	P	95	0	21	0	0
16	R	2151	0	2123	55	0
17	A	1	0	0	0	0
17	B	1	0	0	0	0
18	A	31	0	12	33	0
18	B	31	0	12	19	0
19	B	1	0	0	0	0
19	R	2	0	0	0	0
20	B	25	0	23	32	0
All	All	45544	0	45897	790	0

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

The worst 5 of 790 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TRP:CZ2	20:B:1104:PX2:H33	1.28	1.65
2:B:354:TRP:CE2	20:B:1104:PX2:H33	1.11	1.59
2:B:354:TRP:CH2	20:B:1104:PX2:C16	1.89	1.53
2:B:354:TRP:CZ2	20:B:1104:PX2:C18	1.94	1.48
2:B:354:TRP:CE2	20:B:1104:PX2:C18	1.98	1.46

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	724/855 (85%)	691 (95%)	31 (4%)	2 (0%)	37 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	833/1008 (83%)	798 (96%)	33 (4%)	2 (0%)	44 75
3	C	911/1320 (69%)	890 (98%)	21 (2%)	0	100 100
4	D	775/2294 (34%)	719 (93%)	56 (7%)	0	100 100
5	E	494/946 (52%)	478 (97%)	15 (3%)	1 (0%)	44 75
6	F	476/876 (54%)	460 (97%)	16 (3%)	0	100 100
7	G	283/396 (72%)	272 (96%)	11 (4%)	0	100 100
8	H	52/348 (15%)	51 (98%)	1 (2%)	0	100 100
9	I	315/403 (78%)	310 (98%)	5 (2%)	0	100 100
9	J	315/403 (78%)	309 (98%)	6 (2%)	0	100 100
10	K	65/80 (81%)	59 (91%)	6 (9%)	0	100 100
11	L	12/18 (67%)	11 (92%)	1 (8%)	0	100 100
12	M	8/11 (73%)	5 (62%)	3 (38%)	0	100 100
13	N	17/37 (46%)	13 (76%)	4 (24%)	0	100 100
14	O	15/17 (88%)	11 (73%)	4 (27%)	0	100 100
16	R	265/328 (81%)	252 (95%)	13 (5%)	0	100 100
All	All	5560/9340 (60%)	5329 (96%)	226 (4%)	5 (0%)	50 80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	478	PHE
5	E	821	VAL
1	A	208	PRO
2	B	477	ASN
1	A	812	ILE

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	628/744 (84%)	626 (100%)	2 (0%)	91 96
2	B	734/872 (84%)	730 (100%)	4 (0%)	86 93
3	C	817/1177 (69%)	816 (100%)	1 (0%)	92 98
4	D	753/2151 (35%)	752 (100%)	1 (0%)	92 98
5	E	422/817 (52%)	422 (100%)	0	100 100
6	F	399/757 (53%)	397 (100%)	2 (0%)	86 93
7	G	246/347 (71%)	245 (100%)	1 (0%)	89 94
8	H	46/287 (16%)	46 (100%)	0	100 100
9	I	261/332 (79%)	261 (100%)	0	100 100
9	J	261/332 (79%)	260 (100%)	1 (0%)	89 94
10	K	62/73 (85%)	62 (100%)	0	100 100
11	L	12/12 (100%)	12 (100%)	0	100 100
12	M	9/9 (100%)	9 (100%)	0	100 100
13	N	16/16 (100%)	16 (100%)	0	100 100
14	O	14/15 (93%)	13 (93%)	1 (7%)	12 42
16	R	236/286 (82%)	234 (99%)	2 (1%)	79 90
All	All	4916/8227 (60%)	4901 (100%)	15 (0%)	90 96

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	1666	TYR
16	R	196	MET
6	F	577	ILE
16	R	203	TYR
9	J	120	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	1555	HIS
5	E	555	GLN
16	R	278	GLN
16	R	96	GLN
4	D	1558	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ATP	A	902	17	26,33,33	0.88	0	31,52,52	1.85	5 (16%)
18	ATP	B	1103	17	26,33,33	0.89	0	31,52,52	1.85	6 (19%)
20	PX2	B	1104	-	24,24,35	1.98	7 (29%)	28,29,40	2.65	14 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ATP	A	902	17	-	3/18/38/38	0/3/3/3
18	ATP	B	1103	17	-	3/18/38/38	0/3/3/3
20	PX2	B	1104	-	-	9/26/26/37	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	1104	PX2	O5-C4	4.57	1.46	1.33
20	B	1104	PX2	O7-C2	-4.23	1.36	1.46
20	B	1104	PX2	O8-C16	-4.11	1.10	1.22
20	B	1104	PX2	P1-O3	-3.09	1.43	1.54
20	B	1104	PX2	O6-C4	-2.76	1.14	1.22

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	B	1104	PX2	O7-C16-C17	4.69	121.61	111.50
20	B	1104	PX2	C19-C18-C17	-4.62	96.59	113.19
20	B	1104	PX2	O5-C4-C5	4.57	126.24	111.91
18	A	902	ATP	PB-O3B-PG	-4.41	117.69	132.83
18	B	1103	ATP	PB-O3B-PG	-4.40	117.73	132.83

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	902	ATP	C5'-O5'-PA-O1A
18	B	1103	ATP	C5'-O5'-PA-O1A
20	B	1104	PX2	C1-O4-P1-O1
20	B	1104	PX2	C1-O4-P1-O2
20	B	1104	PX2	C1-O4-P1-O3

There are no ring outliers.

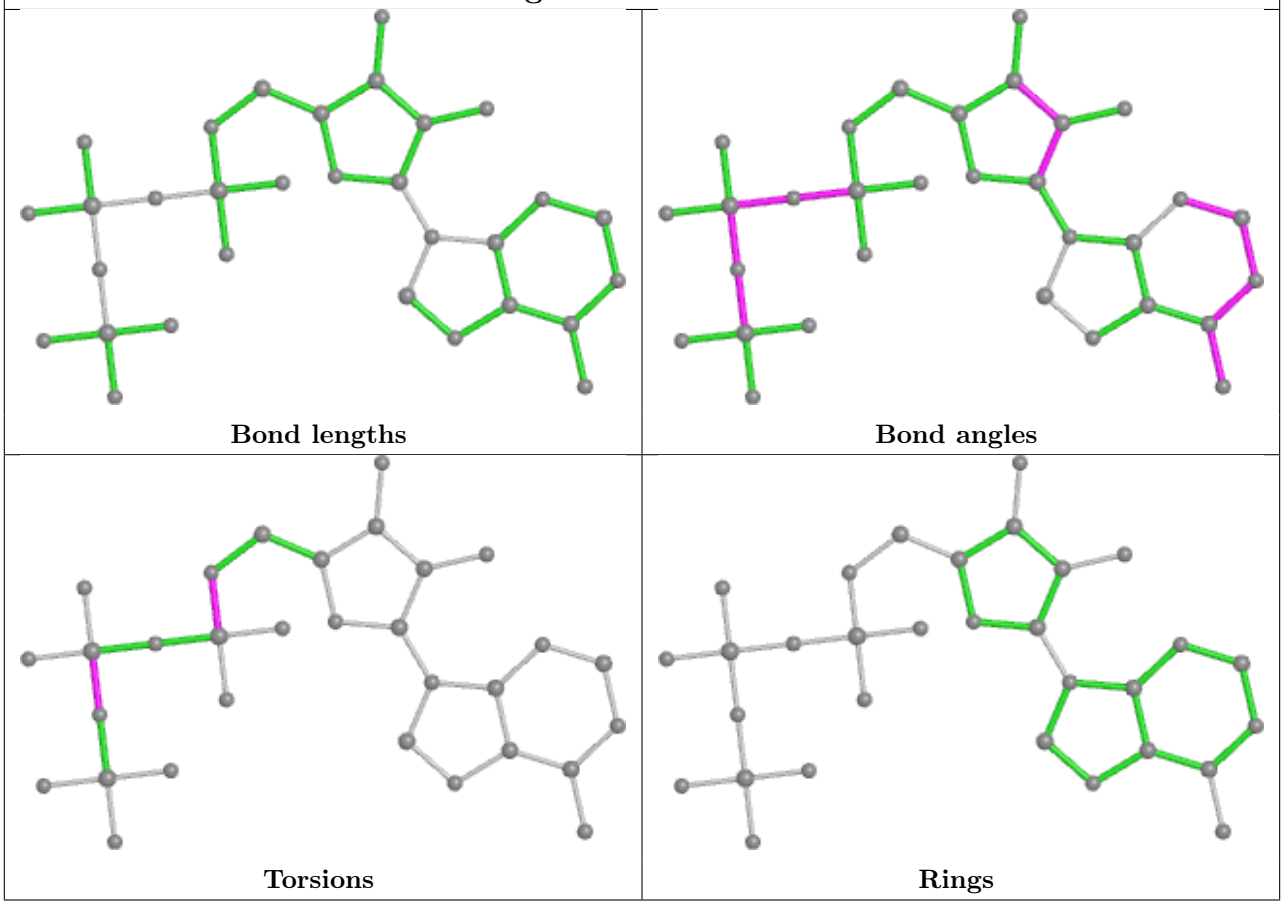
3 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	902	ATP	33	0
18	B	1103	ATP	19	0
20	B	1104	PX2	32	0

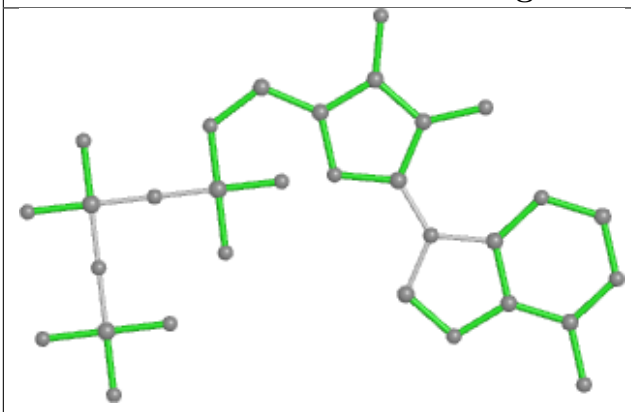
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

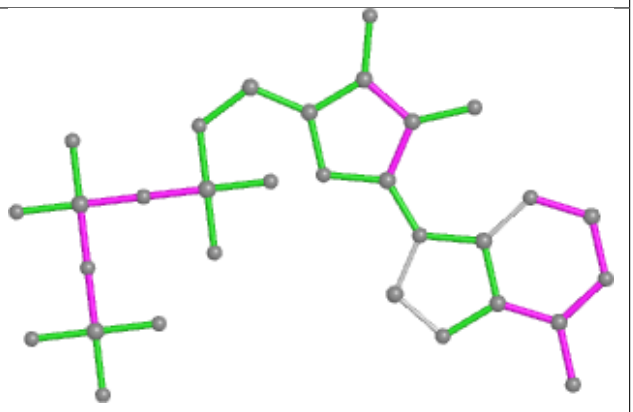
Ligand ATP A 902



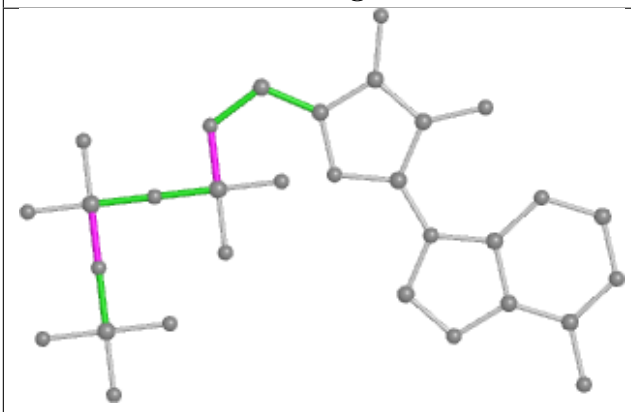
Ligand ATP B 1103



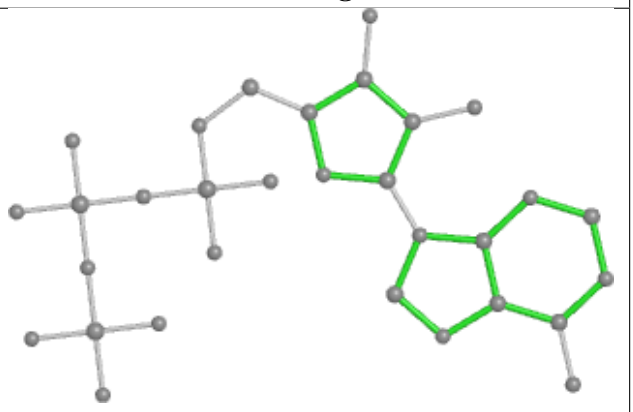
Bond lengths



Bond angles

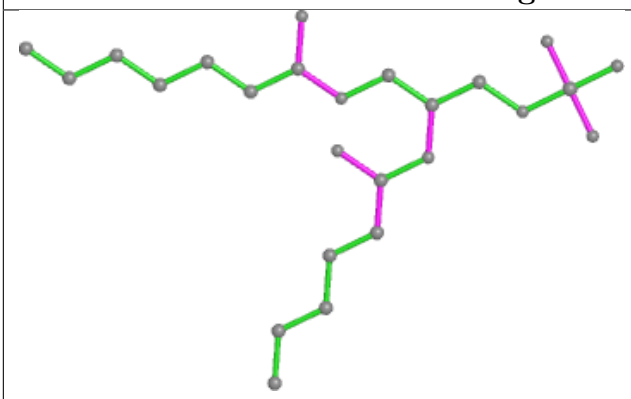


Torsions

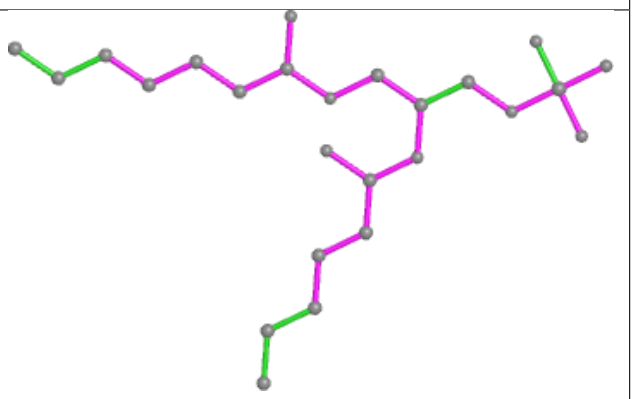


Rings

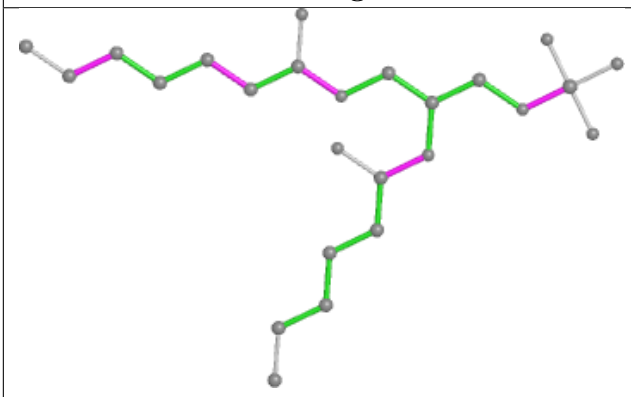
Ligand PX2 B 1104



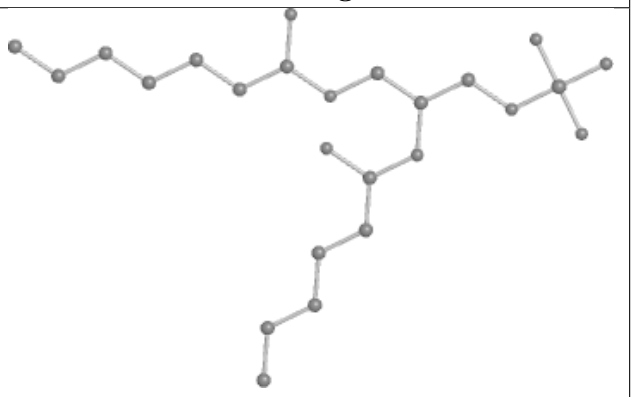
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

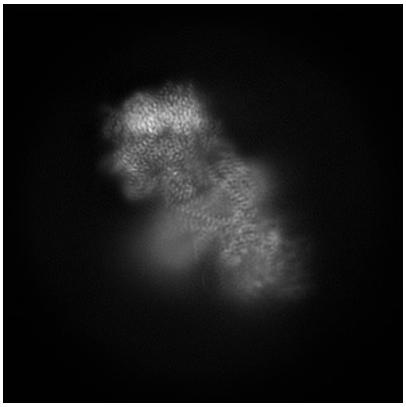
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38425. These allow visual inspection of the internal detail of the map and identification of artifacts.

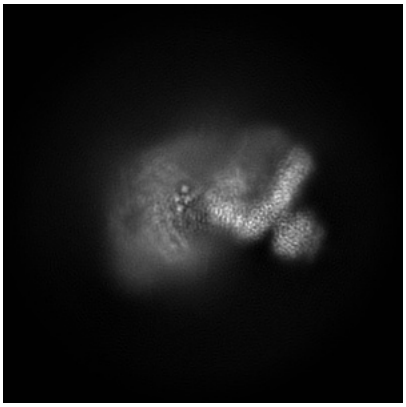
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

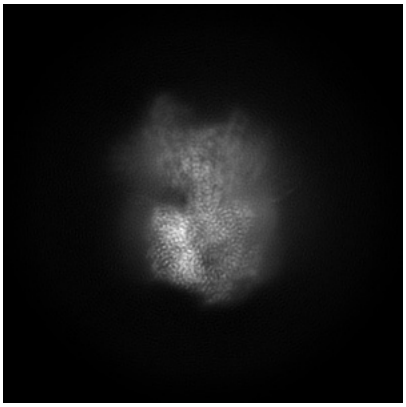
6.1.1 Primary map



X



Y

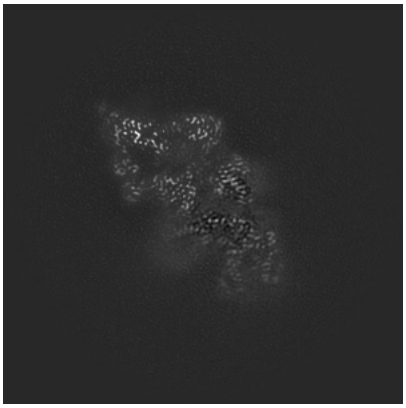


Z

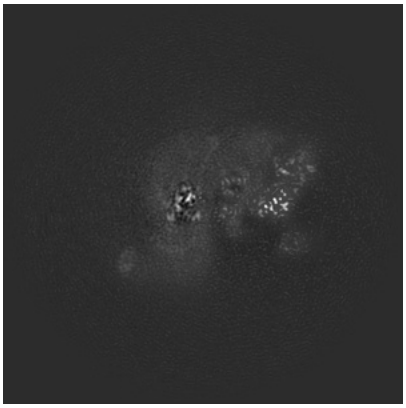
The images above show the map projected in three orthogonal directions.

6.2 Central slices

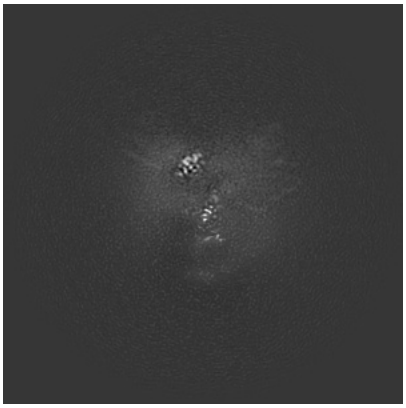
6.2.1 Primary map



X Index: 180



Y Index: 180

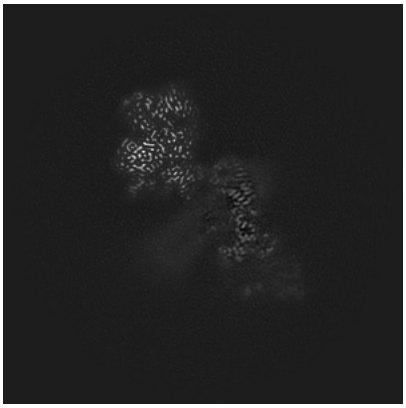


Z Index: 180

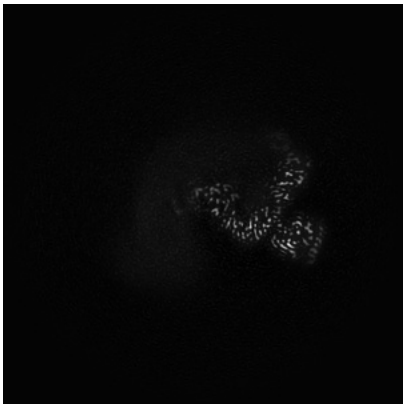
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

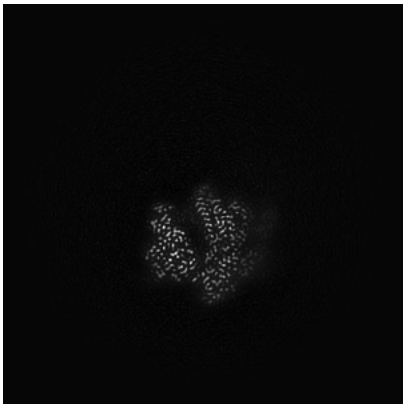
6.3.1 Primary map



X Index: 163



Y Index: 156

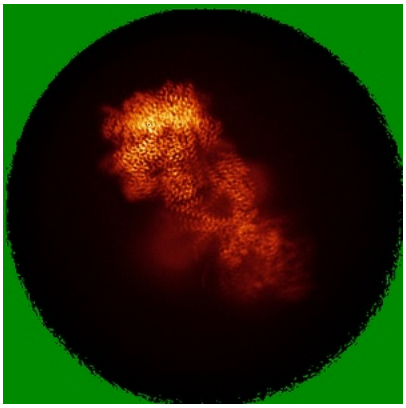


Z Index: 254

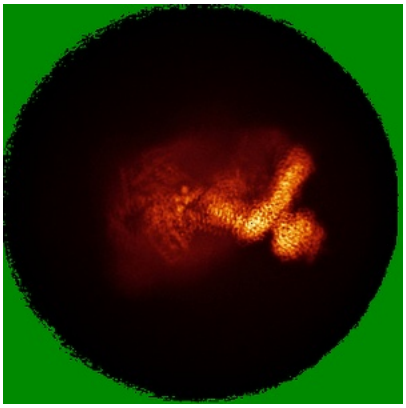
The images above show the largest variance slices of the map in three orthogonal directions.

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

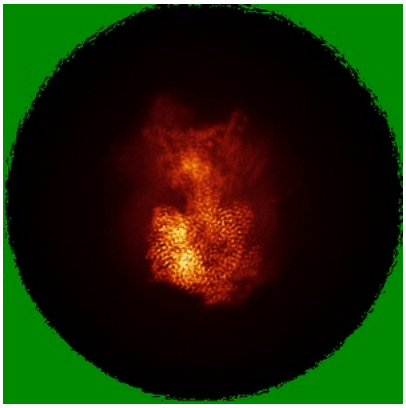
6.4.1 Primary map



X



Y



Z

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 0.009. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

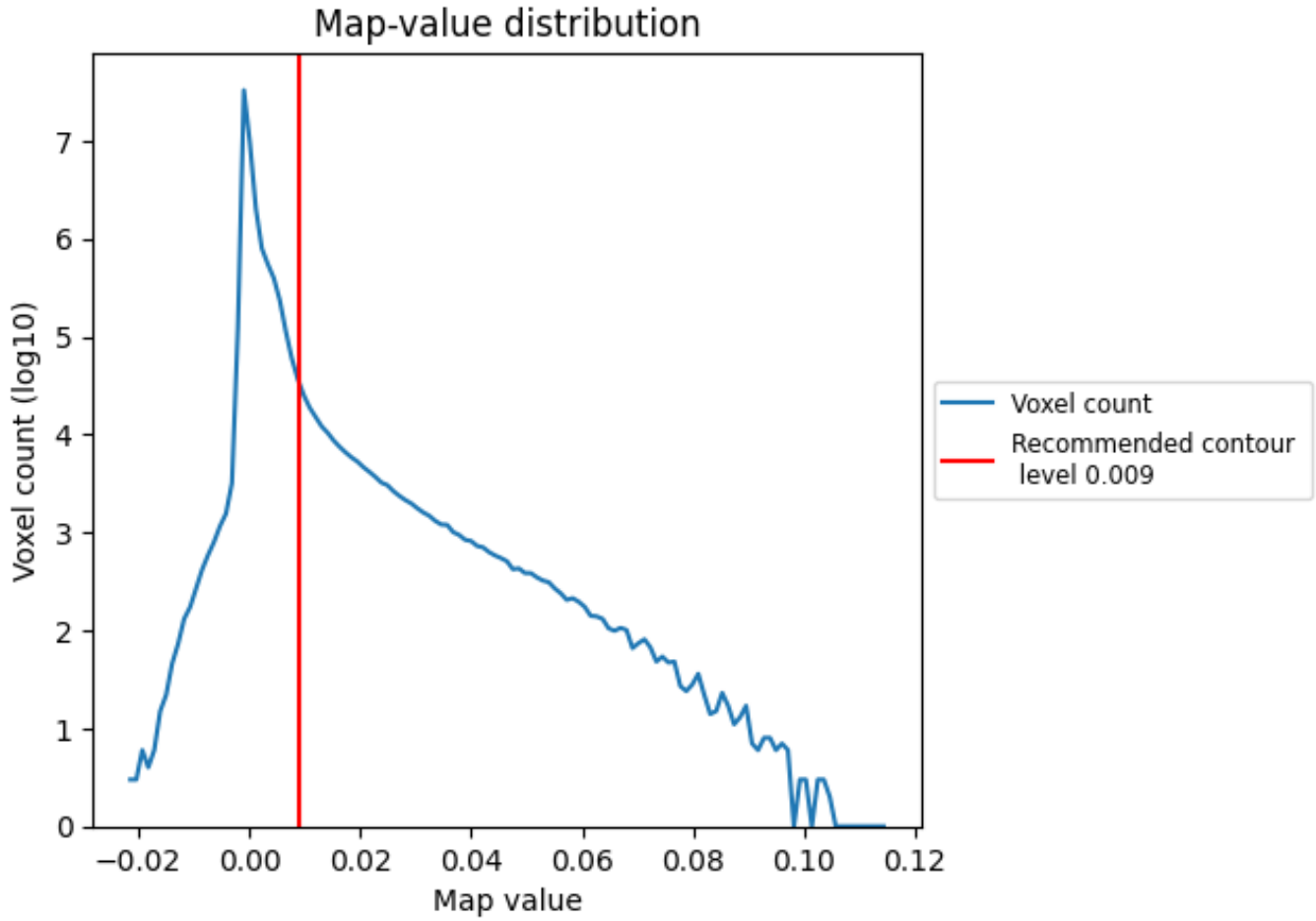
6.6 Mask visualisation (i)

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

7 Map analysis

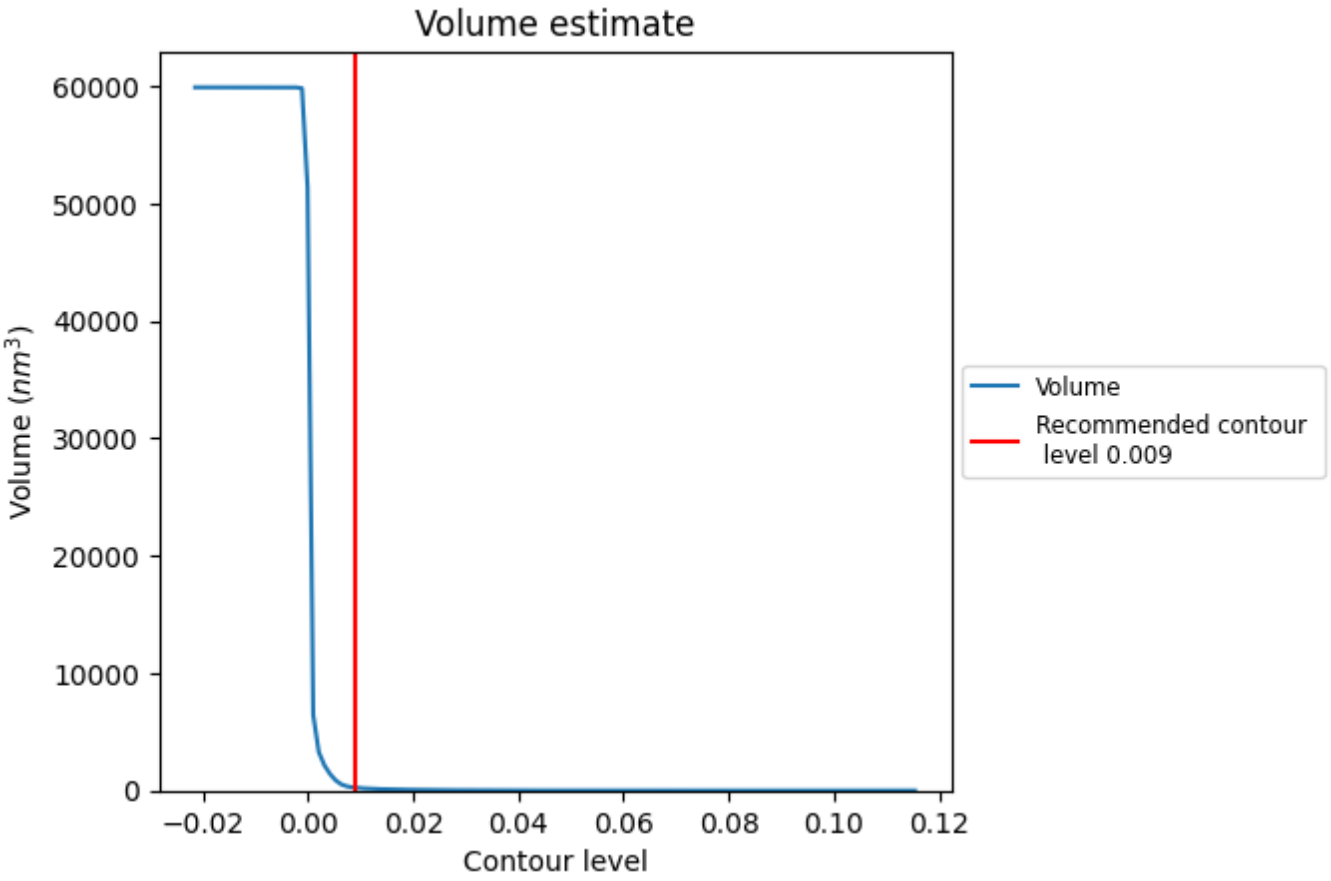
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

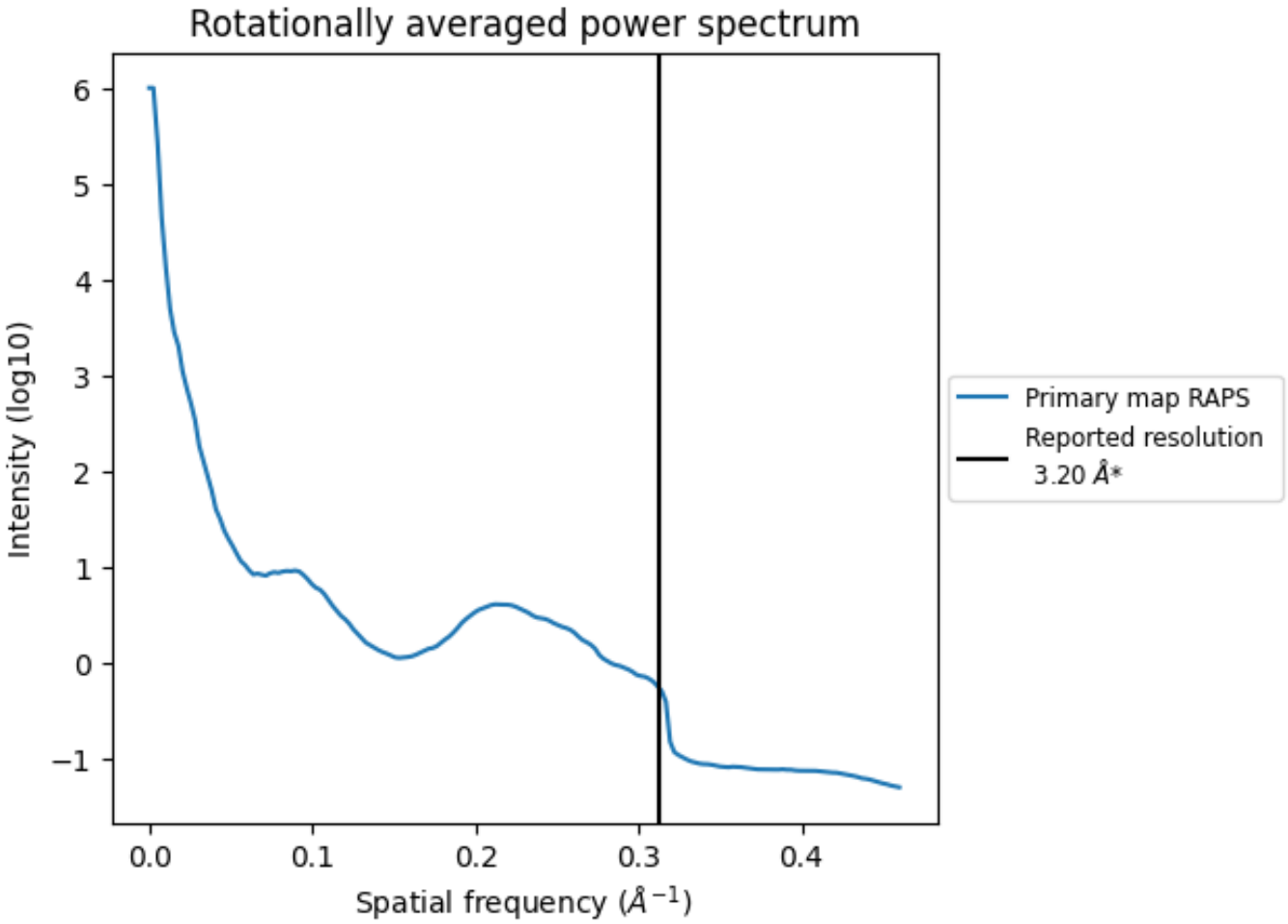
7.2 Volume estimate (i)



The volume at the recommended contour level is 249 nm^3; this corresponds to an approximate mass of 225 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 0.312 $Å^{-1}$

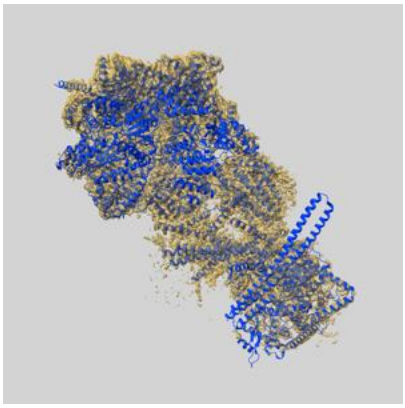
8 Fourier-Shell correlation (i)

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

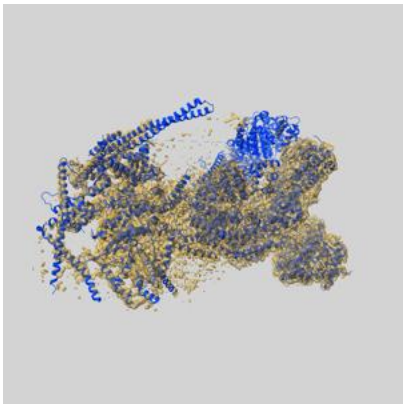
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38425 and PDB model 8XKU. Per-residue inclusion information can be found in section 3 on page 9.

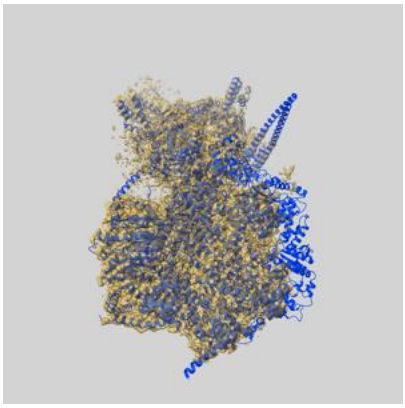
9.1 Map-model overlay



X



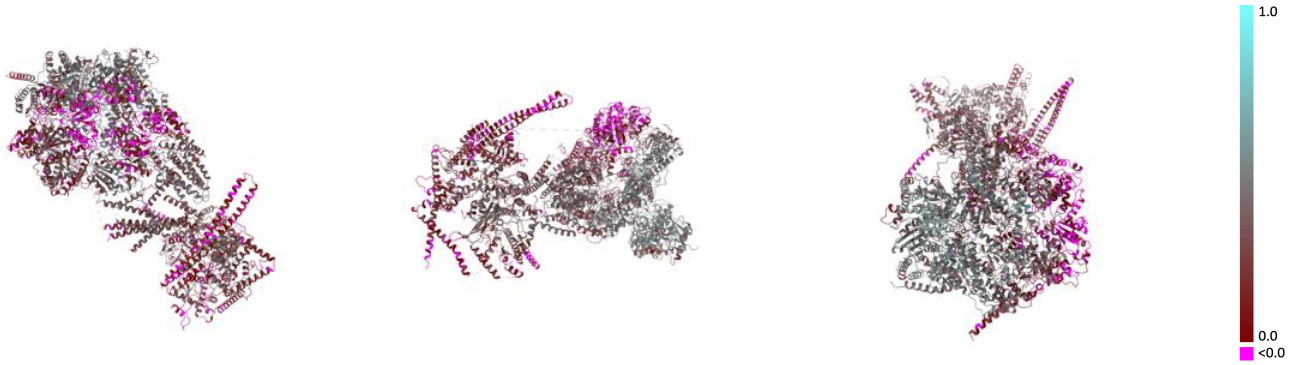
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.009 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.

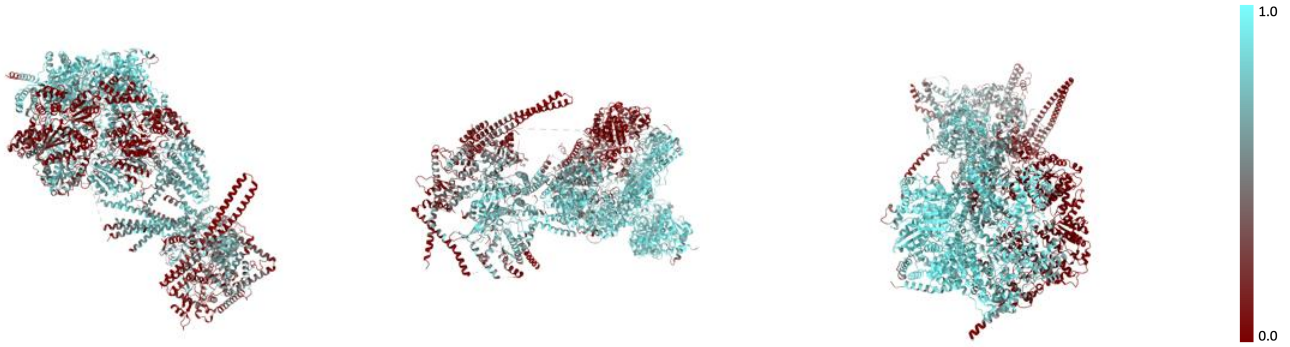
9.2 Q-score mapped to coordinate model (i)



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.

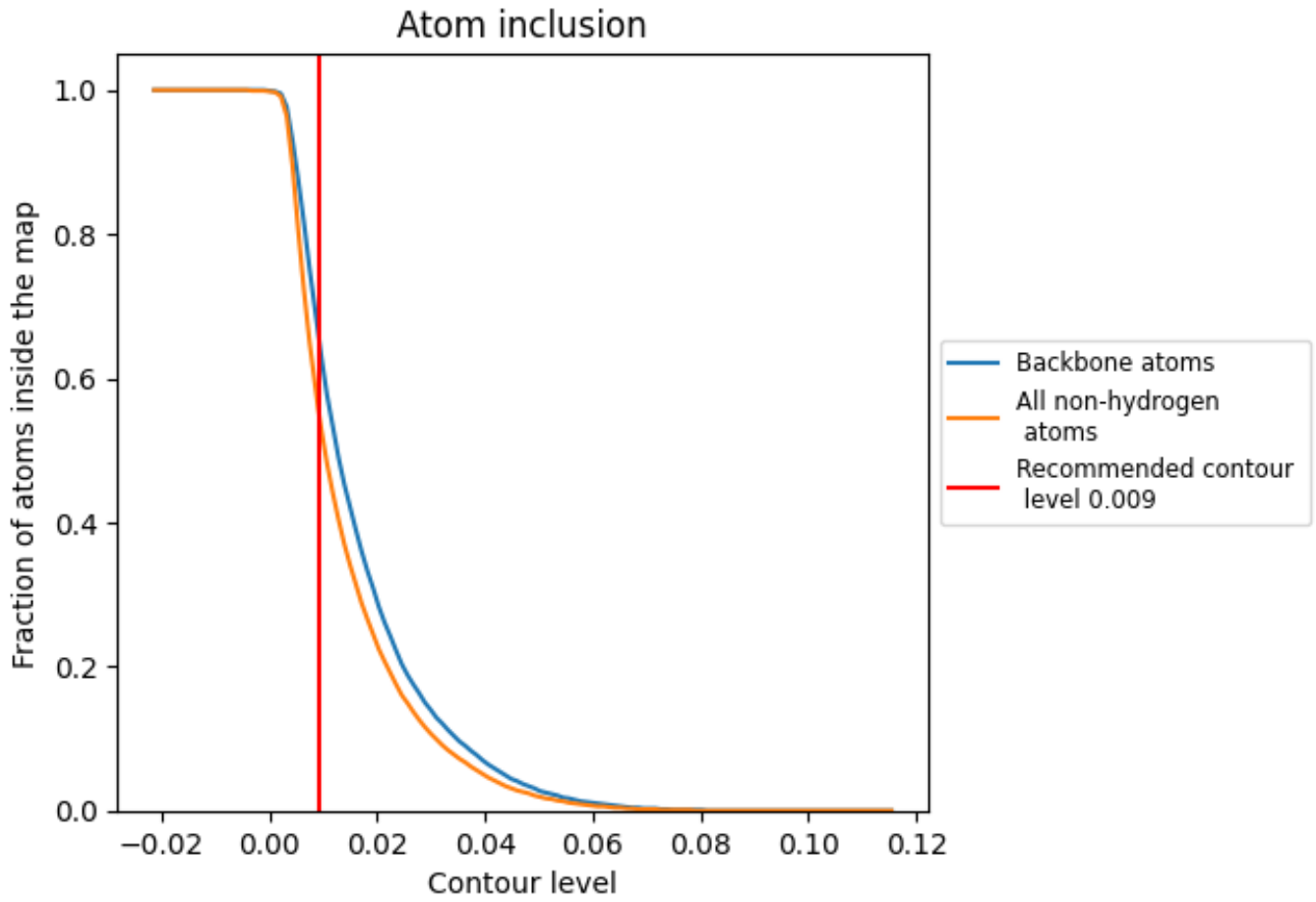
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.009).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 56% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5580	0.3040
A	0.6090	0.3260
B	0.7080	0.3600
C	0.3380	0.2030
D	0.5830	0.3230
E	0.4010	0.2060
F	0.3870	0.2610
G	0.7150	0.3440
H	0.6660	0.3500
I	0.8660	0.4610
J	0.8700	0.4660
K	0.3460	0.2390
L	0.1680	0.1950
M	0.3610	0.2750
N	0.2880	0.2530
O	0.3540	0.3120
P	0.1160	0.1110
R	0.4750	0.2460