Full wwPDB EM Validation Report ⓘ

Jun 17, 2025 – 06:08 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 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:

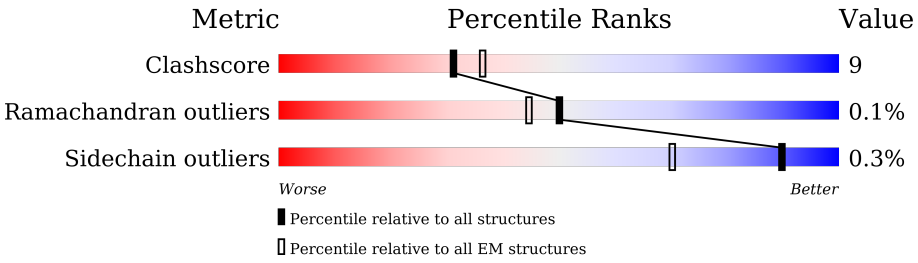
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
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	67% 12% 21%
9	J	403	65% 14% 21%
10	K	80	45% 69% 15% 16%
11	L	18	89% 83% 11% 6%
12	M	11	55% 91% 9%
13	N	37	70% 92% 8%
14	O	17	59% 71% 29%
15	P	19	95% 100%
16	R	328	31% 61% 20% 19%

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

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		

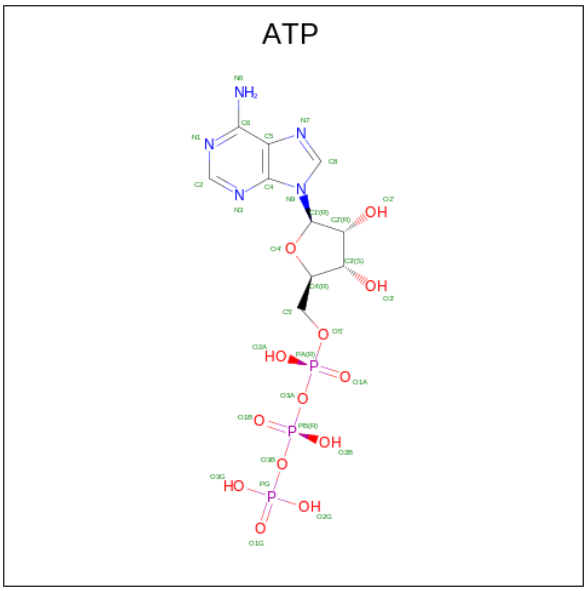
- Molecule 16 is a protein called Embryo defective 2737.

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: $C_{10}H_{16}N_5O_{13}P_3$).

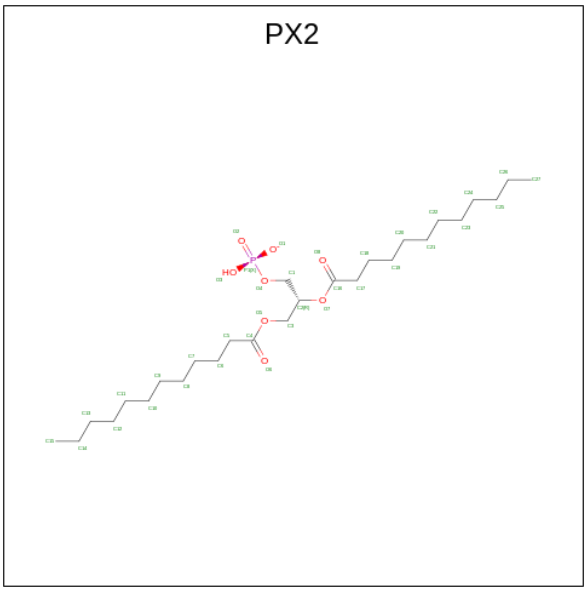


Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
18	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- 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: $C_{27}H_{52}O_8P$).



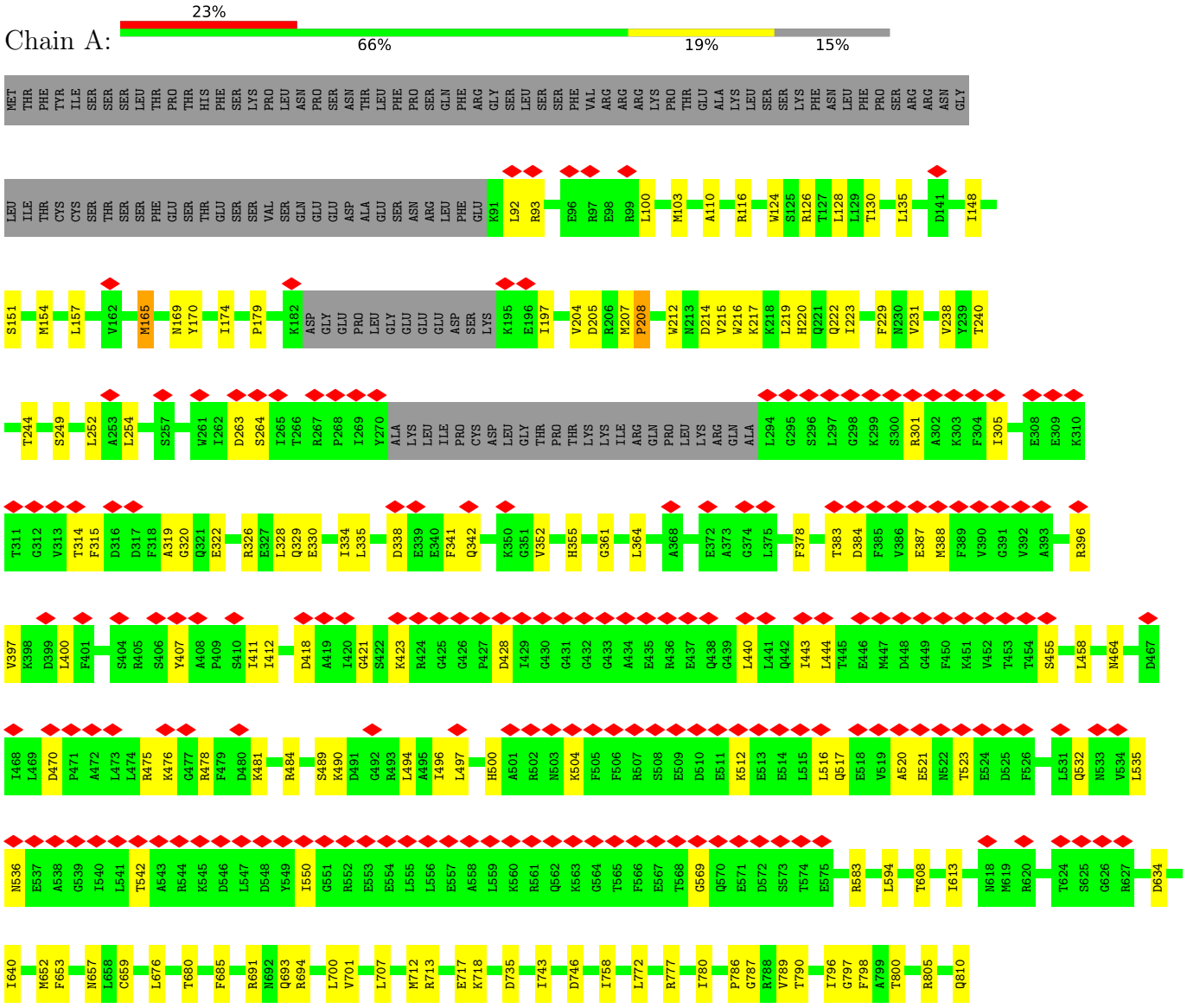
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
20	B	1	25	16	8	1	0

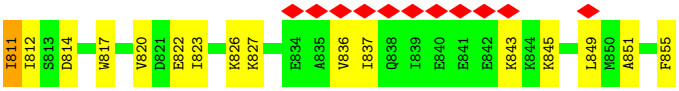
3 Residue-property plots (i)

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

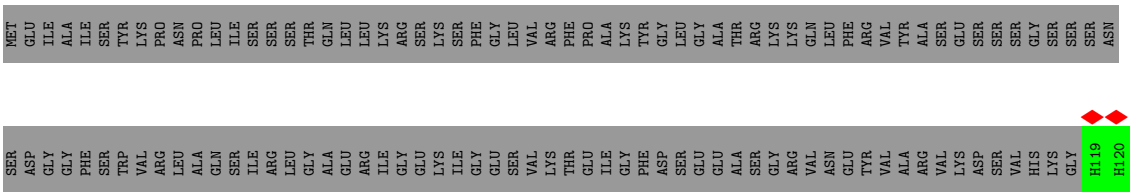
Chain A:

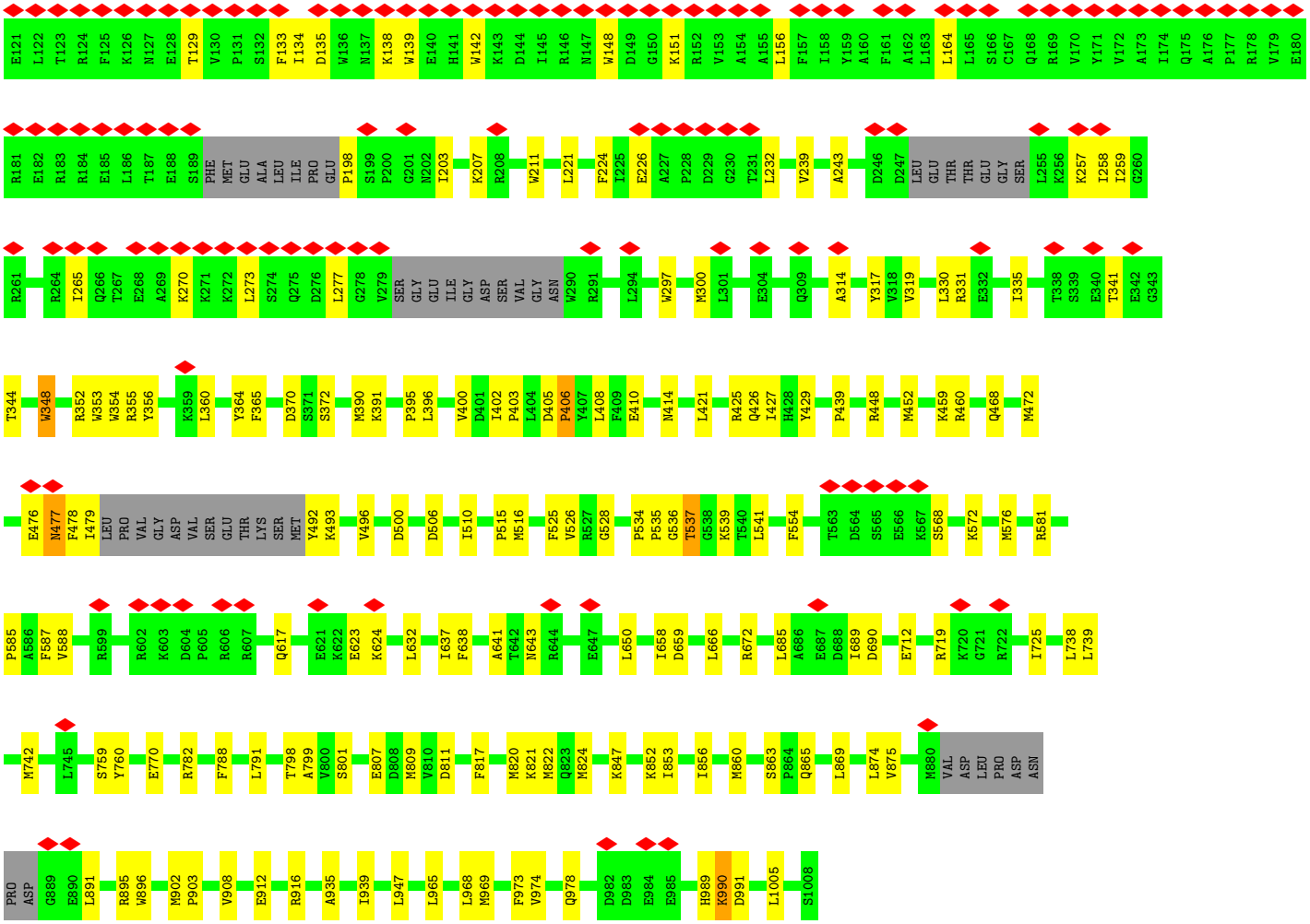




• Molecule 2: ATP-dependent zinc metalloprotease FTSH 12, chloroplastic

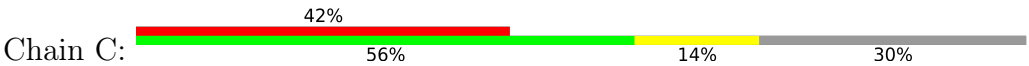
Chain B:

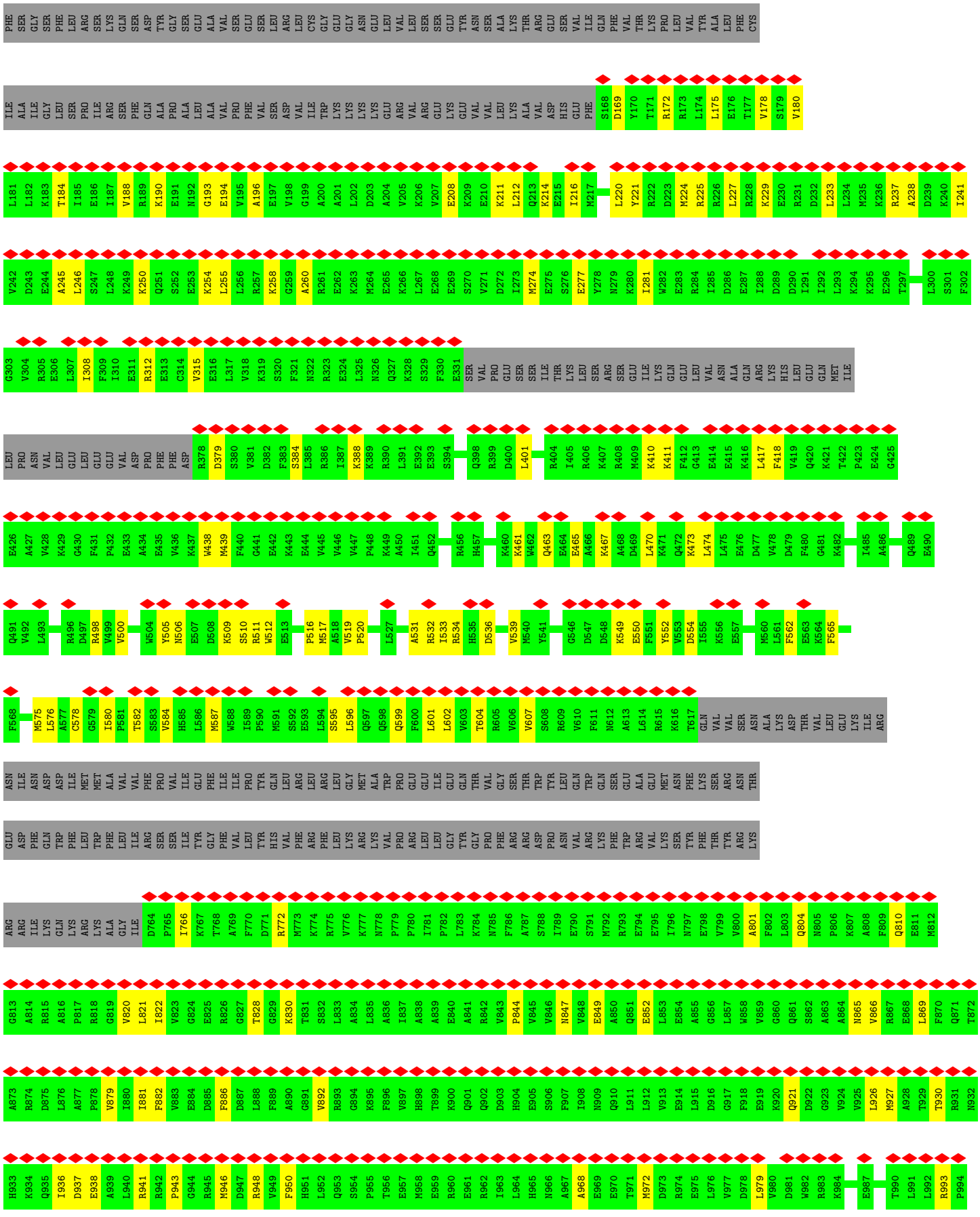


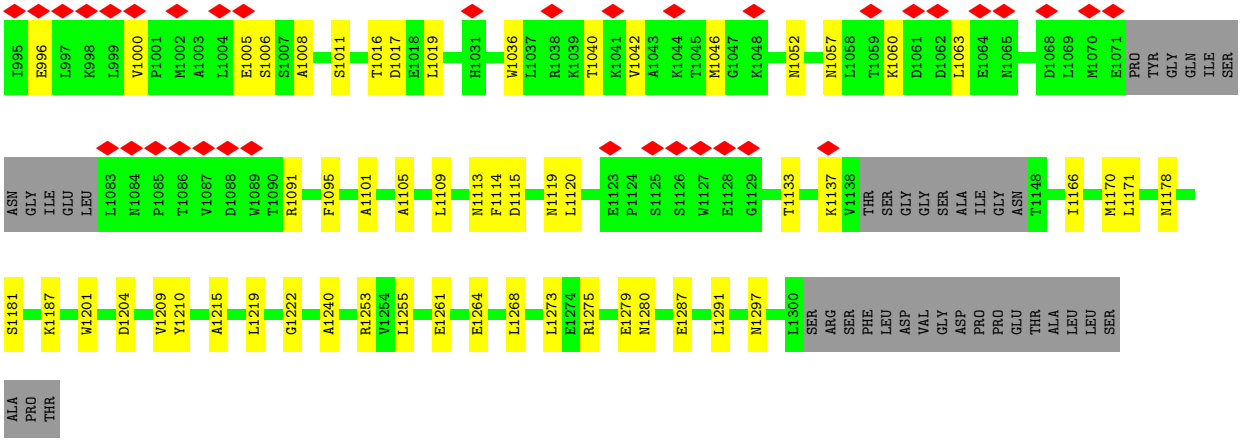


• Molecule 3: Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic

Chain C:

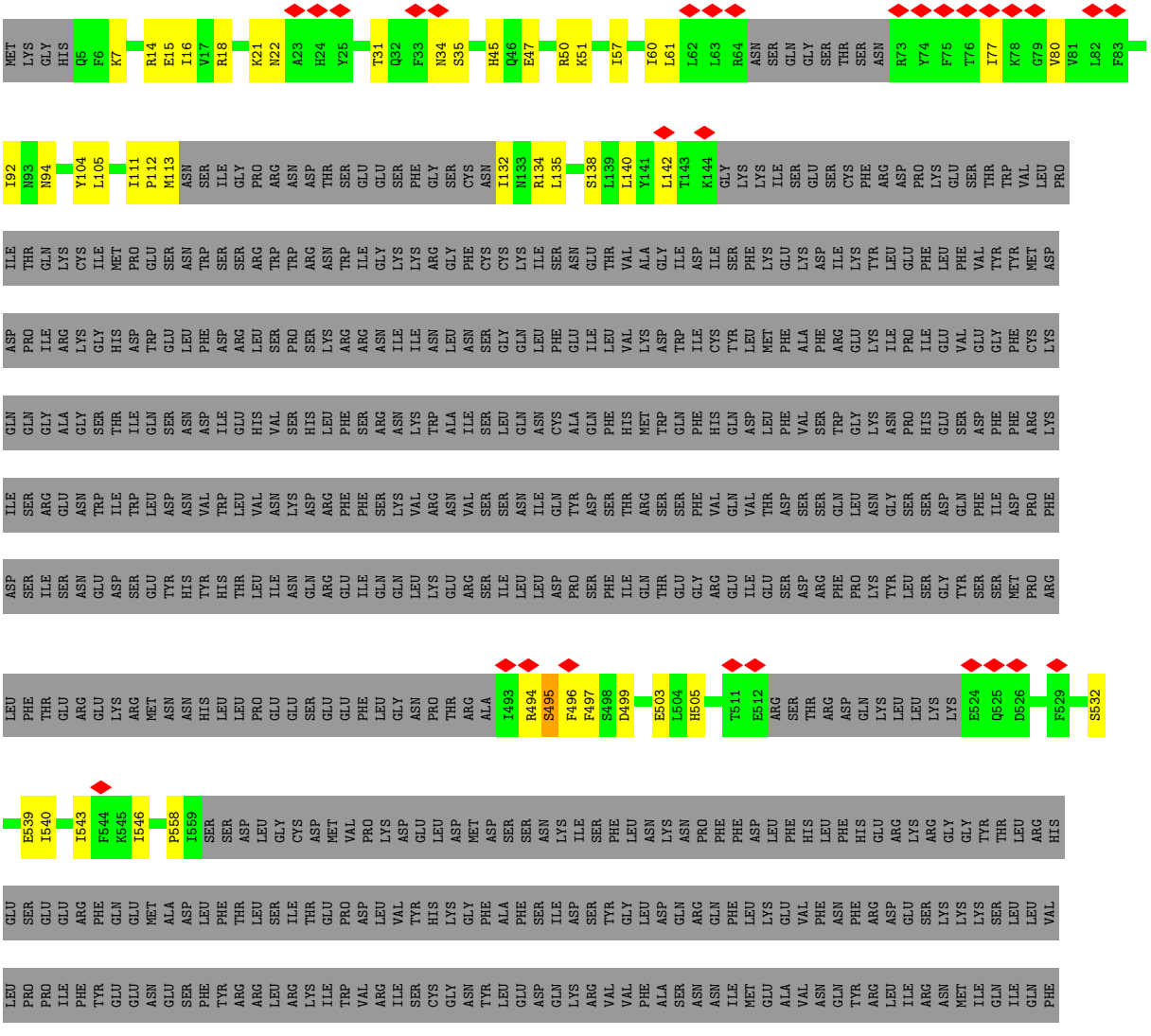


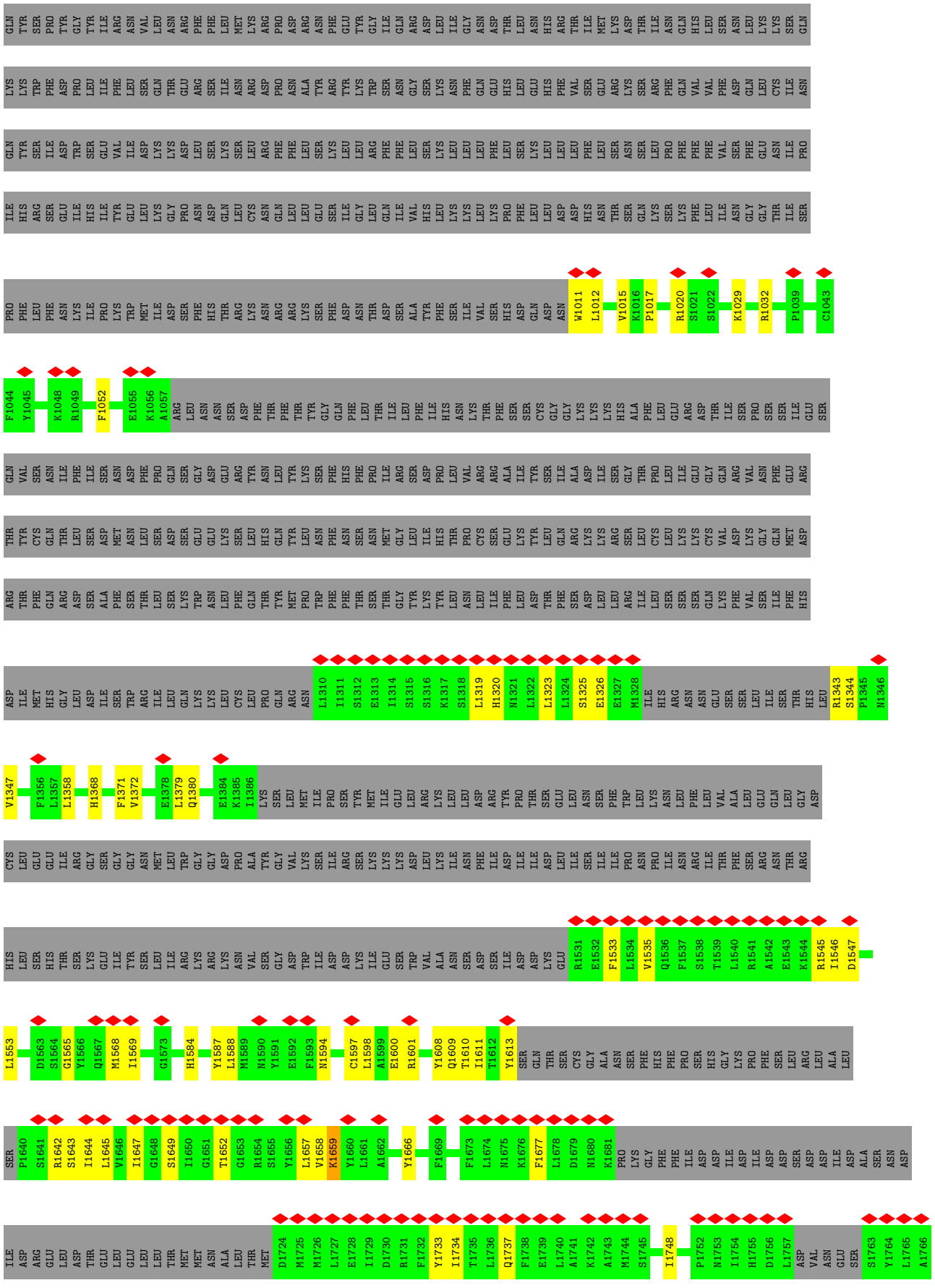


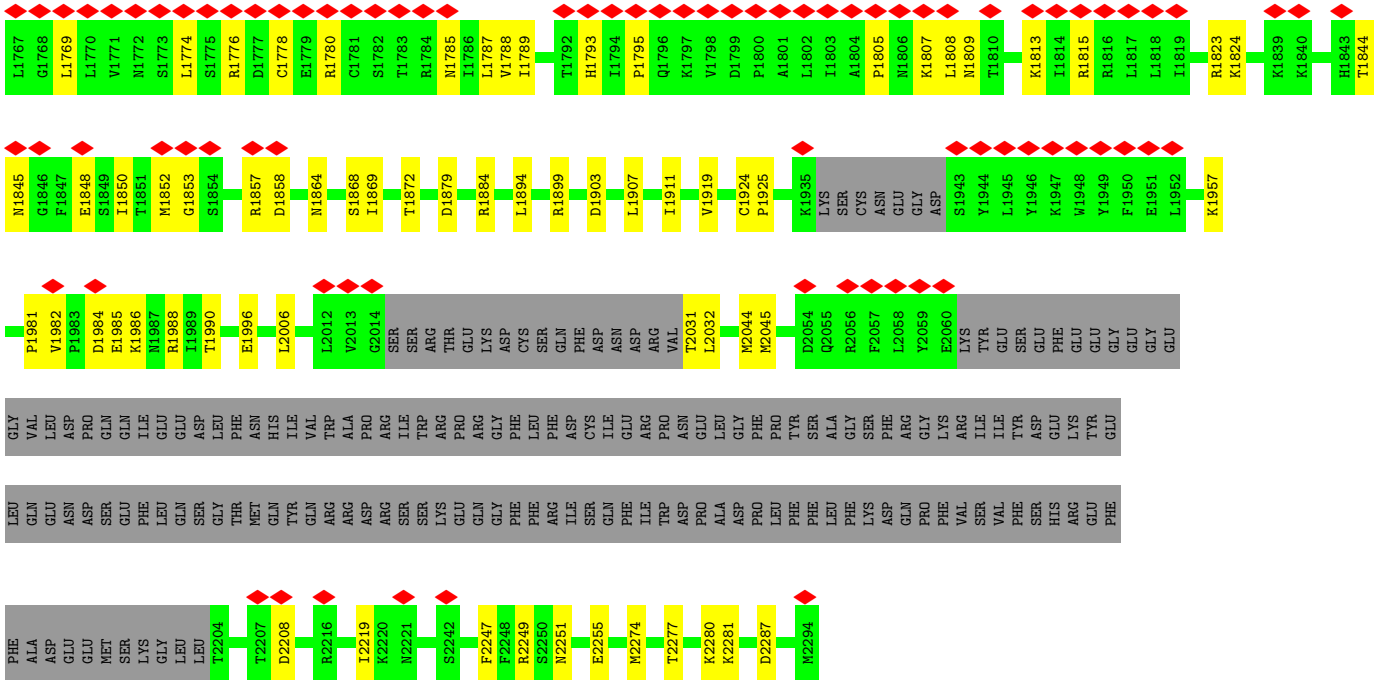


• Molecule 4: Protein Ycf2

Chain D:

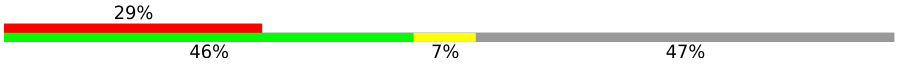


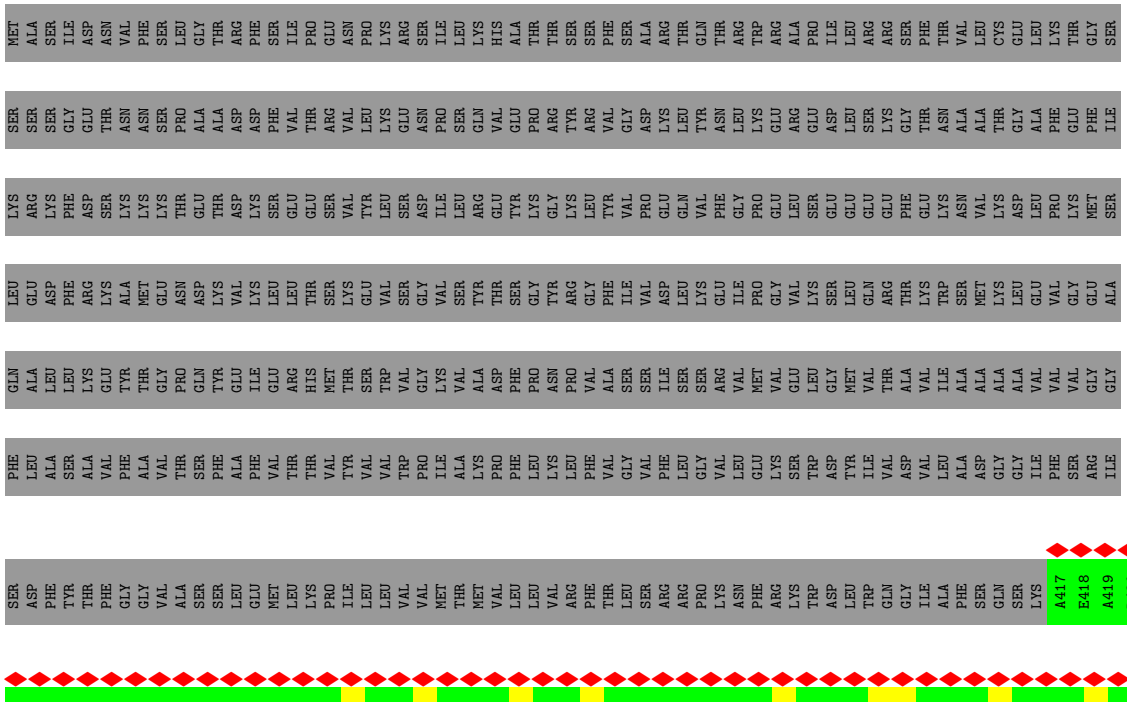

GLN TYR SER PRO TYR GLY TYR ILE ARG ASN VAL LEU ASN ARG PHE PHE LEU MET LYS ARG PRO ASP ARG ASN PHE GLU TYR GLY ILE GLN ARG ASP LEU ILE GLY ASN ASP THR LEU ASN HIS ARG THR ILE ASN GLN HIS LEU LEU SER ASN LEU LYS LYS SER GLN
LYS LYS TRP PHE ASP PRO LEU ILE PHE LEU SER GLN THR GLU ARG SER ILE ASN ARG ASP PRO ASN ALA TYR ARG TYR LYS TRP SER ASN GLY SER LYS SER ASN PHE GLU ARG 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 SER LYS LEU LEU LEU PHE LEU SER LYS LEU LEU LEU LEU PRO PHE PHE PHE PHE VAL SER PHE GLN GLU LEU ASN ILE 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 LEU LYS PRO PHE LEU LEU ASP ASP HIS ASN THR SER GLN LYS SER 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 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 LEU PHE GLN THR THR TYR MET PRO TRP PHE PHE THR SER TRP LYS TYR LYS GLY THR GLY TYR LYS TYR LEU ASN LEU ILE PHE LEU ASP 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 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 SER 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 ILE ASP ALA SER ASN ASP
ILE ASP ARG GLU LEU ASP THR GLU LEU 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

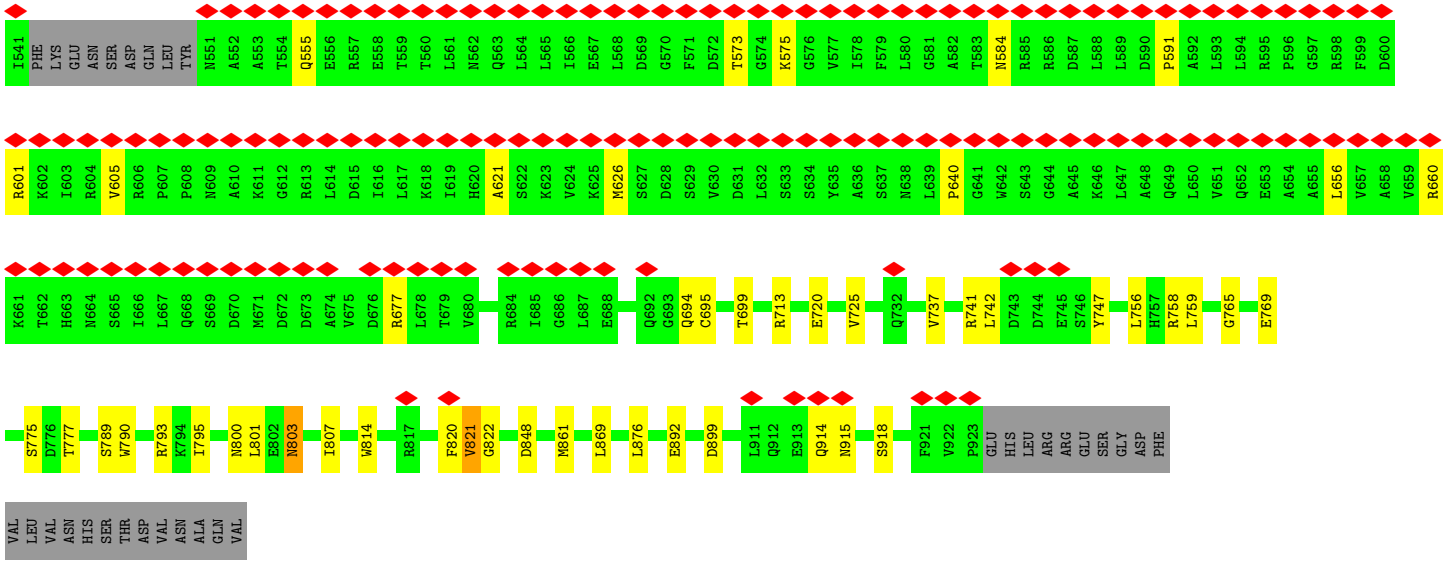


• Molecule 5: Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic

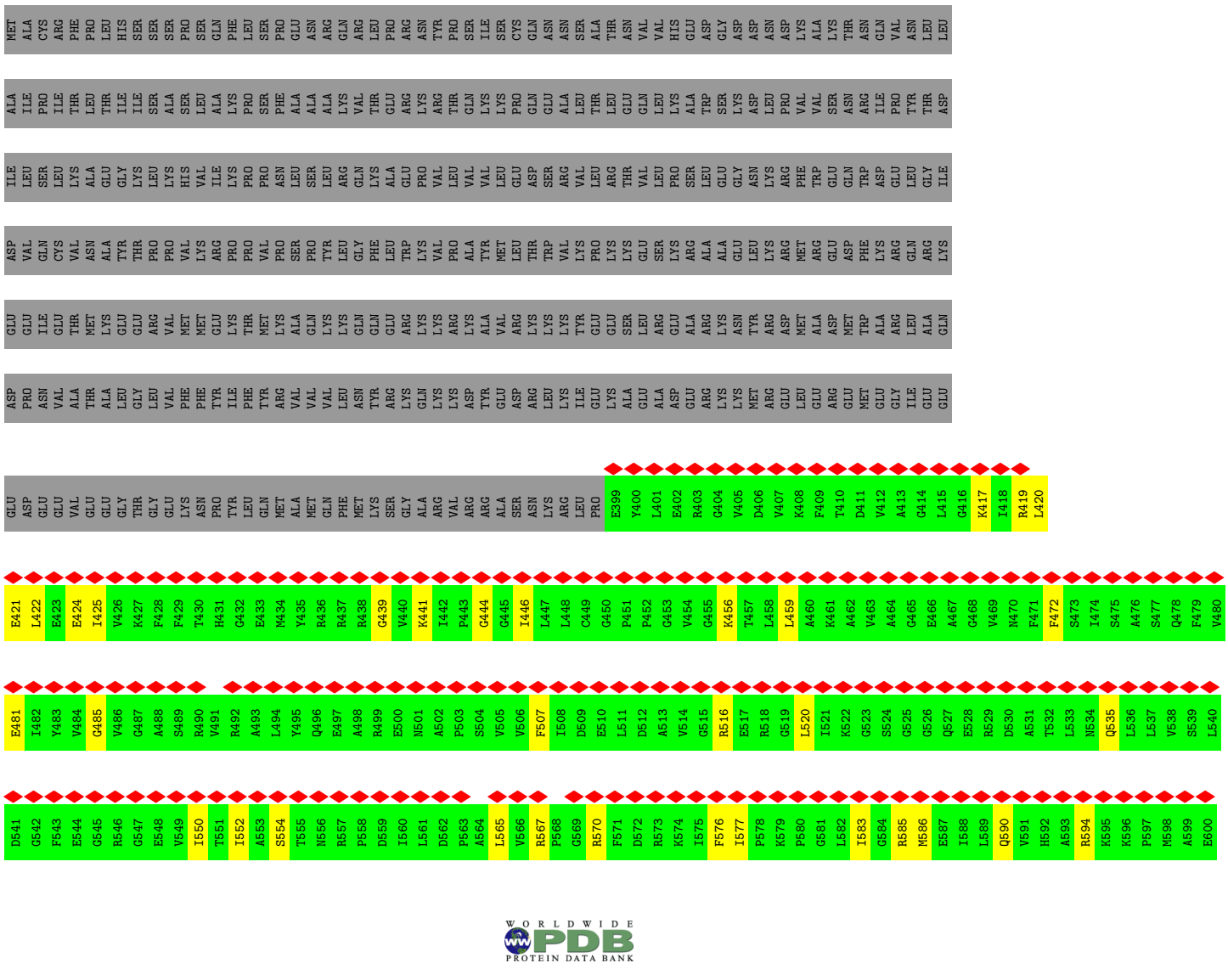
Chain E:



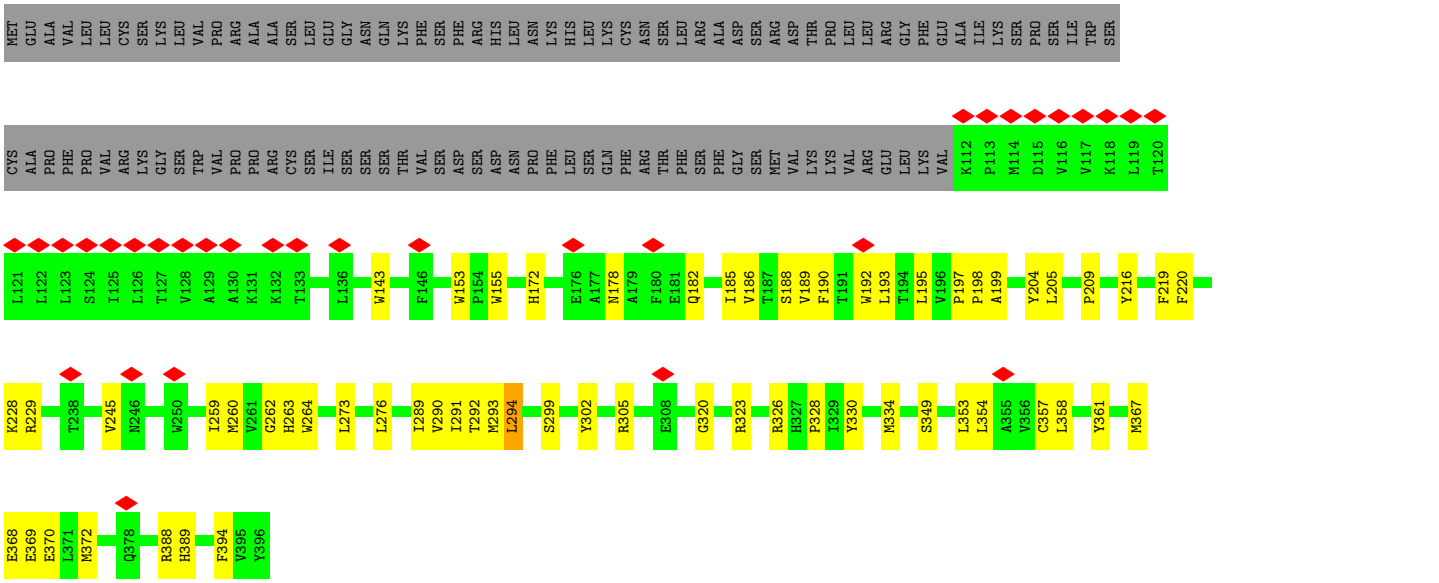




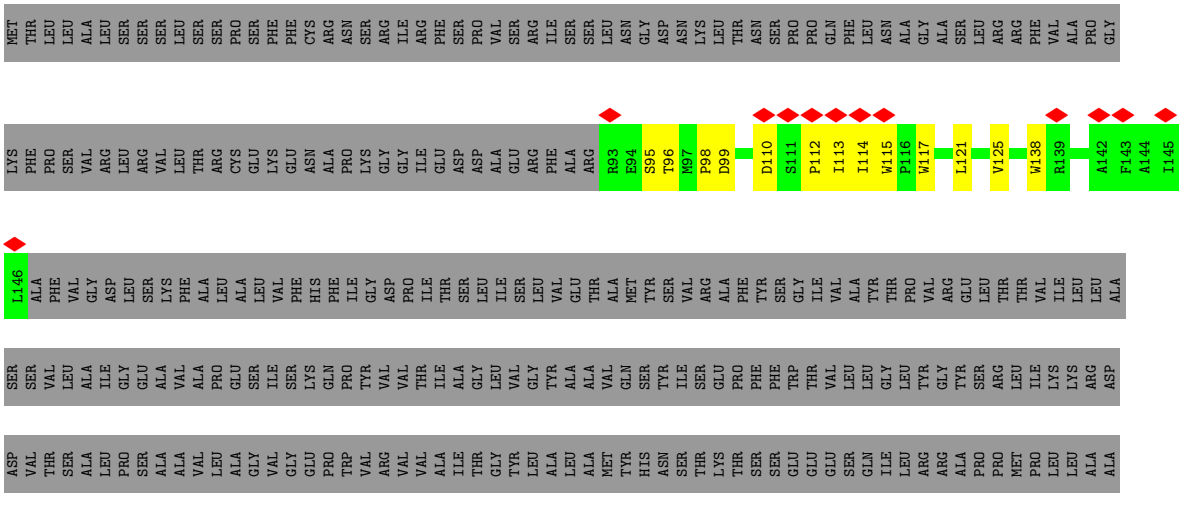
• Molecule 6: Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic



• Molecule 7: AtTam46

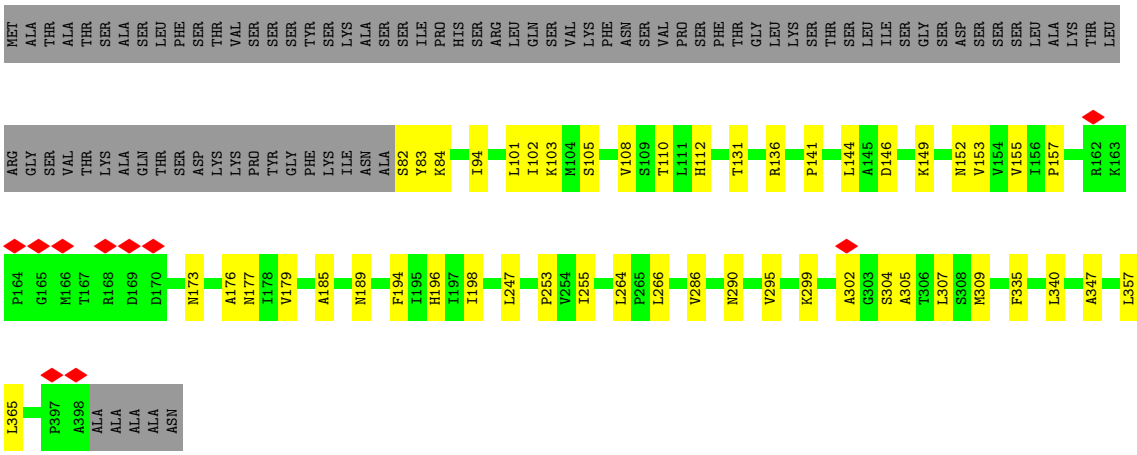


• Molecule 8: At4g28210



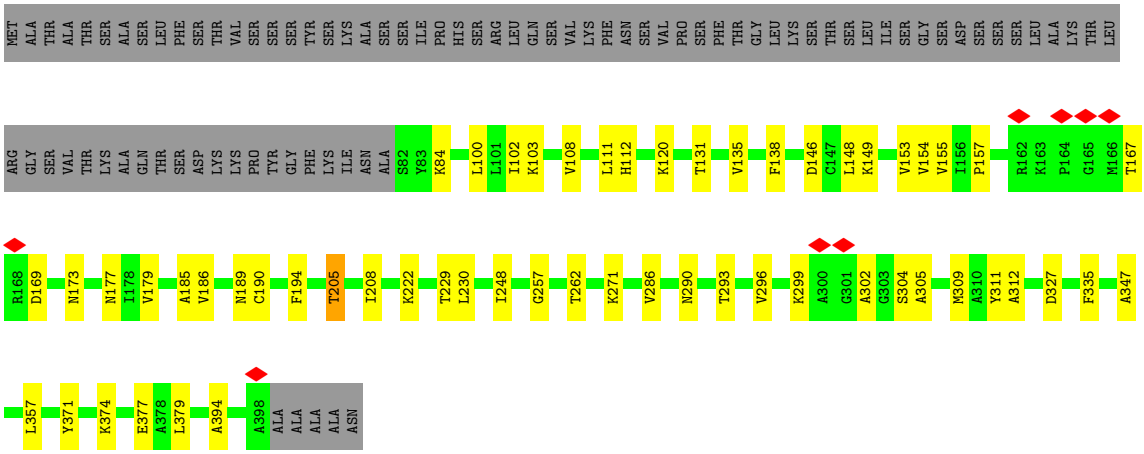
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain I:



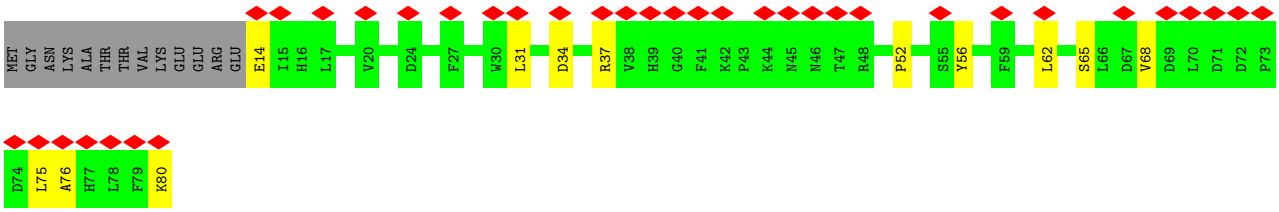
• Molecule 9: Malate dehydrogenase, chloroplastic

Chain J:



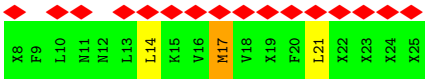
• Molecule 10: Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B

Chain K:



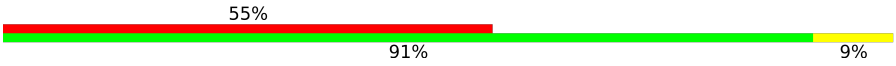
• Molecule 11: UNK

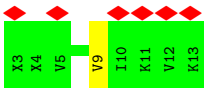
Chain L:



• Molecule 12: UNK

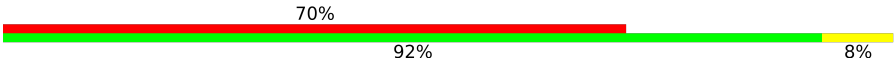
Chain M:

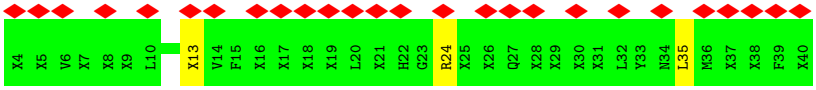




• Molecule 13: UNK

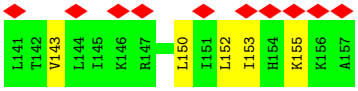
Chain N:





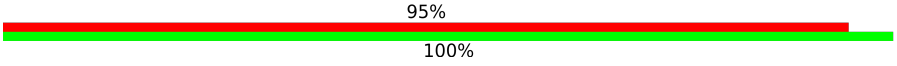
• Molecule 14: UNK

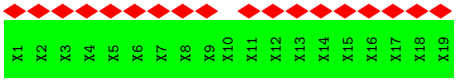
Chain O:



• Molecule 15: UNK

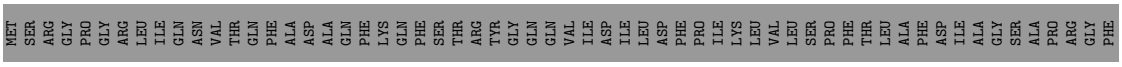
Chain P:

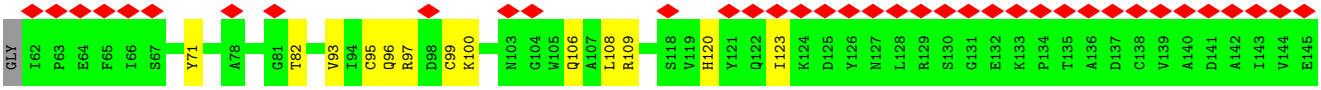


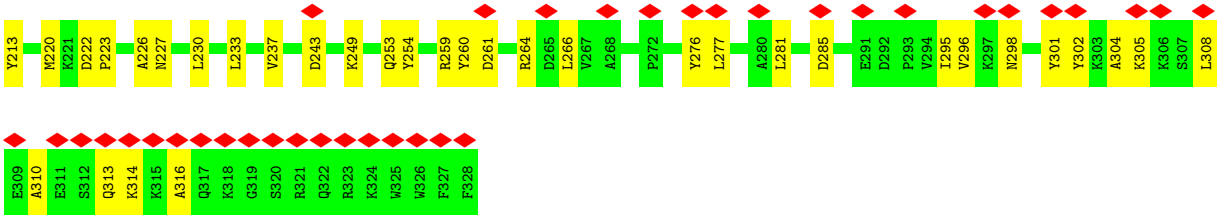


• Molecule 16: Embryo defective 2737

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

All (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
4	D	1659	LYS	CA-CB-CG	5.90	125.90	114.10
7	G	294	LEU	CA-CB-CG	5.47	135.44	116.30
2	B	623	GLU	CA-C-N	5.34	131.74	121.54
2	B	623	GLU	C-N-CA	5.34	131.74	121.54
9	J	205	THR	CA-C-N	5.20	123.52	120.24
9	J	205	THR	C-N-CA	5.20	123.52	120.24
6	F	625	ILE	N-CA-C	-5.04	107.42	111.91

There are no chirality outliers.

All (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	1982	VAL	Peptide
4	D	495	SER	Peptide
5	E	803	ASN	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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.

All (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
2:B:496:VAL:HG21	18:B:1103:ATP:N6	1.18	1.41
2:B:354:TRP:CZ2	20:B:1104:PX2:C16	2.15	1.29
2:B:496:VAL:CG2	18:B:1103:ATP:N6	2.02	1.21
2:B:354:TRP:CZ2	20:B:1104:PX2:C17	2.24	1.21
2:B:354:TRP:NE1	20:B:1104:PX2:H37	1.58	1.16
2:B:354:TRP:CZ2	20:B:1104:PX2:O8	1.99	1.15
2:B:496:VAL:CG2	18:B:1103:ATP:HN62	1.61	1.13
1:A:496:ILE:HD12	18:A:902:ATP:C6	1.85	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TRP:NE1	20:B:1104:PX2:H33	1.68	1.08
2:B:643:ASN:HD21	18:B:1103:ATP:PG	1.76	1.07
2:B:643:ASN:ND2	18:B:1103:ATP:O1G	1.88	1.06
2:B:354:TRP:CH2	20:B:1104:PX2:C17	2.37	1.05
1:A:496:ILE:CD1	18:A:902:ATP:C6	2.39	1.05
2:B:354:TRP:CD1	20:B:1104:PX2:H37	1.94	1.02
2:B:354:TRP:CH2	20:B:1104:PX2:O8	2.09	0.99
1:A:496:ILE:HD11	18:A:902:ATP:C5	2.00	0.97
1:A:532:GLN:HE22	18:A:902:ATP:C1'	1.79	0.95
2:B:496:VAL:HG21	18:B:1103:ATP:HN62	1.15	0.92
2:B:492:TYR:N	18:B:1103:ATP:N1	2.20	0.89
2:B:354:TRP:HH2	20:B:1104:PX2:C16	1.70	0.88
2:B:354:TRP:CD1	20:B:1104:PX2:C20	2.56	0.88
16:R:226:ALA:O	16:R:230:LEU:HB2	1.75	0.87
2:B:539:LYS:NZ	18:B:1103:ATP:O1B	2.06	0.87
1:A:532:GLN:NE2	18:A:902:ATP:H1'	1.88	0.87
1:A:361:GLY:CA	18:A:902:ATP:O1A	2.23	0.86
2:B:354:TRP:NE1	20:B:1104:PX2:C20	2.40	0.85
1:A:532:GLN:HE22	18:A:902:ATP:H1'	1.40	0.85
1:A:361:GLY:HA2	18:A:902:ATP:O1A	1.75	0.84
2:B:354:TRP:HZ2	20:B:1104:PX2:O8	1.61	0.84
2:B:354:TRP:CE2	20:B:1104:PX2:C19	2.63	0.82
1:A:532:GLN:CD	18:A:902:ATP:H1'	2.05	0.81
1:A:532:GLN:OE1	18:A:902:ATP:H1'	1.81	0.81
7:G:357:CYS:O	7:G:361:TYR:HB2	1.83	0.79
1:A:496:ILE:HD11	18:A:902:ATP:C6	2.15	0.79
4:D:1644:ILE:O	4:D:1789:ILE:HA	1.82	0.78
1:A:787:GLY:HA2	1:A:800:THR:O	1.84	0.78
2:B:643:ASN:ND2	18:B:1103:ATP:PG	2.55	0.77
2:B:354:TRP:CH2	20:B:1104:PX2:O7	2.36	0.77
2:B:468:GLN:HG3	2:B:472:MET:HE3	1.67	0.77
1:A:229:PHE:HB3	14:O:155:LYS:HG3	1.67	0.77
1:A:397:VAL:HG11	1:A:443:ILE:HG12	1.67	0.77
2:B:496:VAL:HG21	18:B:1103:ATP:HN61	0.96	0.76
2:B:354:TRP:CD1	20:B:1104:PX2:C21	2.68	0.76
2:B:426:GLN:HB2	4:D:92:ILE:HG23	1.70	0.74
1:A:496:ILE:CD1	18:A:902:ATP:C5	2.66	0.73
3:C:587:MET:SD	3:C:587:MET:N	2.62	0.73
1:A:790:THR:O	1:A:797:GLY:HA2	1.89	0.72
1:A:496:ILE:HD11	18:A:902:ATP:C4	2.23	0.72
4:D:1015:VAL:HG12	4:D:1017:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:TRP:CH2	20:B:1104:PX2:H30	2.26	0.71
1:A:496:ILE:HD12	18:A:902:ATP:N6	2.05	0.70
4:D:1734:ILE:HB	4:D:1769:LEU:HD22	1.73	0.70
2:B:935:ALA:HB1	2:B:968:LEU:HD12	1.74	0.69
1:A:169:ASN:ND2	14:O:153:ILE:O	2.26	0.69
2:B:139:TRP:HE1	16:R:304:ALA:HB3	1.57	0.69
1:A:542:THR:HG21	1:A:550:ILE:HA	1.75	0.68
2:B:496:VAL:HG23	18:B:1103:ATP:HN62	1.56	0.68
2:B:354:TRP:HE1	20:B:1104:PX2:H37	1.57	0.67
9:I:94:ILE:HD11	9:I:309:MET:HB3	1.77	0.67
14:O:150:LEU:HD22	16:R:95:CYS:HA	1.76	0.67
1:A:475:ARG:NH2	18:B:1103:ATP:O3A	2.28	0.67
3:C:1008:ALA:HB2	3:C:1063:LEU:HD13	1.77	0.67
3:C:500:VAL:HG23	11:L:21:LEU:HD12	1.77	0.67
1:A:301:ARG:NH2	1:A:387:GLU:OE1	2.27	0.67
7:G:388:ARG:O	7:G:388:ARG:NH1	2.25	0.66
1:A:497:LEU:HD21	1:A:520:ALA:HB2	1.77	0.66
2:B:330:LEU:HD11	16:R:233:LEU:HD13	1.76	0.66
2:B:410:GLU:HG2	4:D:1032:ARG:HD3	1.77	0.66
9:J:146:ASP:HA	9:J:149:LYS:HE3	1.78	0.66
3:C:822:ILE:HG22	3:C:950:PHE:HB2	1.78	0.66
9:J:155:VAL:HG12	9:J:157:PRO:HD3	1.78	0.65
4:D:134:ARG:NH1	16:R:213:TYR:OH	2.28	0.65
7:G:273:LEU:HD23	7:G:276:LEU:HD21	1.79	0.65
9:I:146:ASP:HA	9:I:149:LYS:HE3	1.77	0.65
9:J:262:THR:HA	9:J:379:LEU:HB2	1.78	0.65
1:A:712:MET:HE1	6:F:774:HIS:HB2	1.78	0.65
9:I:155:VAL:HG12	9:I:157:PRO:HD3	1.79	0.65
6:F:866:LYS:HA	6:F:869:MET:HE3	1.79	0.65
1:A:849:LEU:HG	7:G:182:GLN:HB3	1.77	0.64
1:A:383:THR:OG1	6:F:535:GLN:NE2	2.30	0.64
6:F:654:MET:HE3	6:F:655:LEU:H	1.62	0.64
4:D:1649:SER:HB2	4:D:1793:HIS:HB3	1.79	0.64
5:E:445:LEU:HD11	5:E:466:VAL:HG21	1.80	0.64
1:A:843:LYS:HE3	1:A:845:LYS:HE2	1.80	0.64
1:A:691:ARG:HG3	1:A:693:GLN:HE22	1.62	0.64
3:C:820:VAL:HG22	3:C:948:ARG:HB2	1.80	0.64
7:G:354:LEU:O	7:G:358:LEU:HB2	1.98	0.64
1:A:694:ARG:NH2	2:B:896:TRP:O	2.31	0.63
2:B:536:GLY:O	18:B:1103:ATP:H8	1.80	0.63
3:C:1240:ALA:HA	3:C:1291:LEU:HD11	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1372:VAL:HG11	16:R:82:THR:HG21	1.81	0.63
2:B:414:ASN:HB3	4:D:1029:LYS:HG3	1.81	0.63
1:A:827:LYS:HG2	4:D:1919:VAL:HA	1.81	0.63
3:C:312:ARG:NH2	4:D:1319:LEU:O	2.28	0.62
7:G:326:ARG:NH2	7:G:388:ARG:O	2.32	0.62
1:A:387:GLU:HA	6:F:485:GLY:HA3	1.81	0.62
2:B:581:ARG:NH2	2:B:617:GLN:OE1	2.33	0.62
4:D:1774:LEU:HD13	4:D:1807:LYS:HB3	1.80	0.62
1:A:680:THR:O	2:B:847:LYS:NZ	2.31	0.62
4:D:1644:ILE:HB	4:D:1789:ILE:HG22	1.81	0.62
6:F:692:THR:OG1	6:F:694:ASN:ND2	2.32	0.62
1:A:532:GLN:HE22	18:A:902:ATP:C2'	2.11	0.62
5:E:807:ILE:HD11	6:F:793:LEU:HD22	1.80	0.62
4:D:503:GLU:OE2	16:R:249:LYS:NZ	2.29	0.62
2:B:535:PRO:HB3	18:B:1103:ATP:O1G	2.00	0.62
2:B:493:LYS:HA	2:B:541:LEU:HD21	1.82	0.62
4:D:15:GLU:HG2	4:D:18:ARG:HH12	1.64	0.62
16:R:298:ASN:HB3	16:R:301:TYR:HB2	1.82	0.61
9:J:84:LYS:HB3	9:J:112:HIS:HE1	1.65	0.61
1:A:305:ILE:HG21	1:A:400:LEU:HD13	1.81	0.61
7:G:188:SER:O	7:G:192:TRP:HB3	2.01	0.61
2:B:203:ILE:HD11	2:B:300:MET:HE3	1.82	0.61
1:A:421:GLY:HA2	1:A:440:LEU:HD11	1.82	0.61
3:C:517:MET:HE1	4:D:505:HIS:HB3	1.83	0.61
2:B:875:VAL:HG12	2:B:903:PRO:HA	1.81	0.61
1:A:151:SER:HA	1:A:154:MET:HE3	1.83	0.61
20:B:1104:PX2:O6	7:G:155:TRP:CE3	2.54	0.61
3:C:237:ARG:NH1	3:C:277:GLU:OE2	2.34	0.60
3:C:578:CYS:SG	13:N:24:ARG:NH2	2.74	0.60
4:D:111:ILE:HG22	4:D:113:MET:H	1.66	0.60
4:D:1805:PRO:O	4:D:1809:ASN:ND2	2.34	0.60
1:A:504:LYS:NZ	6:F:439:GLY:O	2.34	0.60
16:R:264:ARG:HA	16:R:281:LEU:HD11	1.84	0.60
3:C:844:PRO:HG2	3:C:879:VAL:HG12	1.82	0.60
1:A:116:ARG:NE	2:B:364:TYR:OH	2.34	0.60
1:A:676:LEU:O	1:A:680:THR:OG1	2.17	0.60
5:E:442:LEU:HD13	5:E:483:ILE:HD11	1.82	0.60
2:B:820:MET:HE2	2:B:856:ILE:HG22	1.84	0.60
4:D:1658:VAL:HG13	4:D:1659:LYS:HD3	1.84	0.60
9:I:307:LEU:HB3	9:J:100:LEU:HD13	1.82	0.60
1:A:583:ARG:NH1	1:A:659:CYS:SG	2.75	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:13:UNK:O	16:R:259:ARG:NH1	2.34	0.59
1:A:179:PRO:HB2	1:A:197:ILE:HD11	1.84	0.59
2:B:139:TRP:HA	2:B:142:TRP:HB2	1.83	0.59
3:C:943:PRO:HG3	5:E:660:ARG:HH21	1.67	0.59
2:B:354:TRP:NE1	20:B:1104:PX2:C18	2.39	0.59
2:B:989:HIS:HD2	2:B:991:ASP:HA	1.67	0.59
3:C:539:VAL:HG23	3:C:554:ASP:HA	1.84	0.59
16:R:171:CYS:HB2	16:R:175:GLY:H	1.67	0.59
3:C:1178:ASN:ND2	3:C:1181:SER:OG	2.35	0.59
9:I:304:SER:OG	9:I:305:ALA:N	2.35	0.59
1:A:735:ASP:OD1	6:F:853:ARG:NH2	2.36	0.59
2:B:1005:LEU:HD13	9:J:248:ILE:HD13	1.85	0.59
9:J:112:HIS:HB3	9:J:138:PHE:HE2	1.67	0.59
2:B:791:LEU:HD13	2:B:947:LEU:HD23	1.85	0.59
5:E:435:ILE:HG22	5:E:438:ALA:HB3	1.85	0.59
1:A:364:LEU:HD22	18:A:902:ATP:H2'	1.84	0.58
2:B:425:ARG:NH1	4:D:94:ASN:O	2.35	0.58
3:C:536:ASP:HA	4:D:1323:LEU:HA	1.84	0.58
1:A:464:ASN:OD1	18:A:902:ATP:O3G	2.20	0.58
5:E:453:ASP:OD2	5:E:453:ASP:N	2.36	0.58
6:F:422:LEU:HD11	6:F:459:LEU:HD21	1.85	0.58
9:I:153:VAL:HG22	9:I:194:PHE:HB2	1.83	0.58
3:C:882:PHE:HD1	3:C:927:MET:HB3	1.68	0.58
3:C:506:ASN:O	3:C:510:SER:N	2.36	0.58
6:F:739:LEU:O	6:F:811:ARG:NH2	2.37	0.58
9:J:167:THR:HG23	9:J:169:ASP:H	1.68	0.58
9:J:103:LYS:NZ	9:J:131:THR:OG1	2.28	0.57
4:D:140:LEU:HD22	16:R:253:GLN:HE22	1.69	0.57
1:A:384:ASP:O	1:A:396:ARG:NH1	2.37	0.57
1:A:613:ILE:HG21	6:F:715:GLU:HB3	1.86	0.57
4:D:134:ARG:HH12	4:D:135:LEU:HD23	1.69	0.57
5:E:720:GLU:OE2	5:E:758:ARG:NH1	2.37	0.57
1:A:128:LEU:HD11	7:G:143:TRP:HD1	1.69	0.57
6:F:703:TYR:OH	6:F:705:ARG:NH2	2.38	0.57
16:R:96:GLN:O	16:R:189:ARG:NH1	2.37	0.57
8:H:114:ILE:HD12	8:H:117:TRP:HZ3	1.70	0.57
1:A:100:LEU:HA	1:A:103:MET:HG2	1.87	0.57
1:A:796:ILE:HD11	9:I:247:LEU:HG	1.86	0.57
1:A:810:GLN:NE2	1:A:814:ASP:OD1	2.38	0.57
2:B:354:TRP:CZ3	20:B:1104:PX2:H30	2.39	0.57
18:A:902:ATP:H4'	6:F:567:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:THR:O	4:D:1545:ARG:NH1	2.38	0.57
7:G:182:GLN:HA	7:G:185:ILE:HD12	1.87	0.57
9:J:305:ALA:HB3	9:J:309:MET:HE3	1.87	0.57
1:A:790:THR:OG1	1:A:805:ARG:NH1	2.34	0.57
1:A:169:ASN:HD22	14:O:152:LEU:HB3	1.69	0.56
2:B:448:ARG:HH11	4:D:1368:HIS:HA	1.70	0.56
3:C:575:MET:HB2	3:C:580:ILE:HB	1.87	0.56
9:I:286:VAL:O	9:I:290:ASN:ND2	2.38	0.56
4:D:1380:GLN:O	16:R:71:TYR:OH	2.23	0.56
2:B:365:PHE:HE2	2:B:408:LEU:HD11	1.70	0.56
7:G:262:GLY:HA3	7:G:353:LEU:HD21	1.87	0.56
3:C:821:LEU:HD11	3:C:930:THR:HG23	1.88	0.56
9:I:185:ALA:O	9:I:189:ASN:ND2	2.38	0.56
5:E:694:GLN:O	5:E:694:GLN:NE2	2.39	0.56
2:B:479:ILE:HB	2:B:554:PHE:HB3	1.86	0.56
2:B:672:ARG:NH2	2:B:807:GLU:OE2	2.39	0.56
3:C:1120:LEU:HG	3:C:1133:THR:HG23	1.88	0.56
3:C:211:LYS:HA	3:C:214:LYS:HD2	1.88	0.56
3:C:866:VAL:HA	3:C:869:LEU:HD12	1.86	0.56
4:D:104:TYR:O	16:R:203:TYR:OH	2.24	0.55
4:D:1748:ILE:HG23	4:D:1787:LEU:HB2	1.88	0.55
4:D:61:LEU:HD13	4:D:1546:ILE:HD11	1.88	0.55
3:C:533:ILE:HD11	3:C:584:VAL:HG22	1.86	0.55
4:D:138:SER:HA	4:D:142:LEU:HD12	1.89	0.55
1:A:496:ILE:CD1	18:A:902:ATP:N1	2.69	0.55
3:C:1201:TRP:NE1	5:E:777:THR:OG1	2.39	0.55
1:A:481:LYS:NZ	2:B:712:GLU:OE2	2.37	0.55
16:R:106:GLN:HE22	16:R:187:GLN:HG2	1.71	0.55
3:C:576:LEU:HD12	13:N:35:LEU:HD21	1.89	0.55
3:C:595:SER:OG	3:C:596:LEU:N	2.39	0.55
5:E:803:ASN:OD1	6:F:734:ARG:NH2	2.39	0.55
2:B:259:ILE:HD12	2:B:270:LYS:HE2	1.89	0.55
4:D:1844:THR:HG22	4:D:1845:ASN:H	1.71	0.55
2:B:624:LYS:HA	4:D:1535:VAL:HG11	1.88	0.55
7:G:330:TYR:HB3	7:G:361:TYR:HD1	1.71	0.55
7:G:192:TRP:CE2	7:G:260:MET:HE2	2.41	0.54
2:B:536:GLY:HA2	18:B:1103:ATP:O5'	2.08	0.54
4:D:1869:ILE:O	4:D:1872:THR:OG1	2.26	0.54
18:A:902:ATP:H4'	6:F:567:ARG:NH2	2.22	0.54
3:C:604:THR:HA	3:C:607:VAL:HG22	1.89	0.54
3:C:886:PHE:HB3	3:C:930:THR:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1297:ASN:H	5:E:775:SER:HB3	1.73	0.54
9:J:102:ILE:HG23	9:J:108:VAL:HG21	1.89	0.54
1:A:758:ILE:HD13	6:F:863:MET:HE1	1.89	0.54
2:B:390:MET:SD	2:B:391:LYS:N	2.81	0.54
2:B:798:THR:OG1	2:B:799:ALA:N	2.40	0.54
3:C:943:PRO:HG2	5:E:656:LEU:HD13	1.88	0.54
2:B:759:SER:OG	2:B:760:TYR:N	2.41	0.54
16:R:194:ASP:N	16:R:194:ASP:OD1	2.36	0.54
4:D:499:ASP:OD1	4:D:499:ASP:N	2.40	0.54
6:F:813:LEU:HD11	6:F:836:VAL:HA	1.90	0.54
1:A:428:ASP:OD1	1:A:428:ASP:N	2.39	0.54
3:C:467:LYS:NZ	10:K:65:SER:O	2.40	0.54
1:A:786:PRO:O	9:J:311:TYR:OH	2.21	0.54
18:A:902:ATP:O5'	6:F:567:ARG:NH2	2.41	0.54
2:B:354:TRP:HH2	20:B:1104:PX2:O7	1.81	0.54
6:F:417:LYS:O	6:F:420:LEU:HB2	2.08	0.54
4:D:1565:GLY:HA2	4:D:1824:LYS:HG2	1.89	0.53
6:F:422:LEU:HA	6:F:425:ILE:HD12	1.90	0.53
2:B:427:ILE:HG22	4:D:92:ILE:HG22	1.90	0.53
10:K:76:ALA:O	10:K:80:LYS:NZ	2.32	0.53
5:E:640:PRO:HG3	5:E:741:ARG:HD3	1.91	0.53
2:B:500:ASP:HB3	4:D:1894:LEU:HD22	1.89	0.53
1:A:216:TRP:HA	1:A:219:LEU:HB2	1.90	0.53
1:A:652:MET:SD	1:A:652:MET:N	2.82	0.53
2:B:588:VAL:HG23	2:B:638:PHE:HA	1.90	0.53
2:B:916:ARG:NH2	9:J:327:ASP:OD1	2.41	0.53
1:A:500:HIS:NE2	1:A:532:GLN:OE1	2.41	0.53
1:A:811:ILE:HD13	4:D:2255:GLU:HG3	1.91	0.53
2:B:396:LEU:HD11	4:D:539:GLU:HG3	1.91	0.53
4:D:1584:HIS:NE2	4:D:1785:ASN:O	2.40	0.53
7:G:195:LEU:HD22	7:G:205:LEU:HD13	1.91	0.53
1:A:608:THR:HB	1:A:743:ILE:HG22	1.90	0.53
4:D:50:ARG:HH22	7:G:229:ARG:HH12	1.57	0.53
4:D:540:ILE:HA	4:D:543:ILE:HD12	1.90	0.53
3:C:384:SER:HB3	16:R:276:TYR:HD2	1.73	0.53
5:E:914:GLN:CD	5:E:914:GLN:H	2.17	0.53
1:A:334:ILE:HG12	1:A:341:PHE:HD2	1.73	0.53
4:D:1568:MET:HG3	4:D:1569:ILE:HD12	1.91	0.53
4:D:2044:MET:SD	4:D:2045:MET:N	2.82	0.53
6:F:456:LYS:HD3	6:F:554:SER:HB2	1.91	0.53
1:A:569:GLY:HA3	6:F:576:PHE:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:ILE:HD11	4:D:1587:TYR:CG	2.44	0.52
1:A:489:SER:OG	1:A:490:LYS:N	2.42	0.52
1:A:851:ALA:O	1:A:855:PHE:N	2.43	0.52
9:J:299:LYS:HB3	9:J:302:ALA:HB3	1.89	0.52
2:B:164:LEU:HD12	16:R:316:ALA:HA	1.90	0.52
2:B:414:ASN:HD22	4:D:1032:ARG:HE	1.58	0.52
5:E:725:VAL:HG13	5:E:737:VAL:HG22	1.91	0.52
6:F:421:GLU:O	6:F:424:GLU:HB2	2.10	0.52
7:G:368:GLU:O	7:G:372:MET:HG2	2.09	0.52
16:R:168:CYS:HB3	16:R:171:CYS:SG	2.49	0.52
4:D:1857:ARG:NH1	4:D:1858:ASP:OD1	2.42	0.52
1:A:338:ASP:O	1:A:342:GLN:HB2	2.10	0.52
1:A:836:VAL:HG23	1:A:837:ILE:HG23	1.92	0.52
2:B:895:ARG:NH1	4:D:1996:GLU:OE2	2.40	0.52
5:E:800:ASN:O	6:F:734:ARG:NH1	2.43	0.52
9:J:153:VAL:HG22	9:J:194:PHE:HB2	1.92	0.52
16:R:108:LEU:N	16:R:177:MET:O	2.43	0.52
1:A:378:PHE:HB2	1:A:412:ILE:HG22	1.92	0.52
3:C:881:ILE:HG23	3:C:926:LEU:HA	1.91	0.52
1:A:128:LEU:HD11	7:G:143:TRP:CD1	2.45	0.52
1:A:148:ILE:O	1:A:205:ASP:N	2.34	0.52
2:B:129:THR:O	2:B:133:PHE:N	2.39	0.51
2:B:452:MET:HE3	4:D:1371:PHE:HD2	1.75	0.51
2:B:539:LYS:HD2	2:B:641:ALA:HB1	1.92	0.51
3:C:830:LYS:NZ	3:C:930:THR:O	2.43	0.51
5:E:759:LEU:HD23	5:E:861:MET:HG3	1.91	0.51
2:B:360:LEU:HB3	2:B:400:VAL:HG22	1.92	0.51
4:D:1029:LYS:HG2	4:D:1032:ARG:HH21	1.75	0.51
6:F:746:LEU:HB3	6:F:750:TRP:HZ2	1.76	0.51
3:C:1036:TRP:O	3:C:1040:THR:OG1	2.22	0.51
6:F:660:ARG:NH1	6:F:700:GLU:OE1	2.44	0.51
9:I:102:ILE:HG23	9:I:108:VAL:HG21	1.92	0.51
5:E:462:PRO:HD2	5:E:573:THR:HB	1.91	0.51
5:E:466:VAL:HG22	5:E:601:ARG:HB2	1.93	0.51
6:F:747:SER:OG	6:F:748:THR:N	2.41	0.51
9:I:103:LYS:NZ	9:I:131:THR:OG1	2.34	0.51
1:A:315:PHE:HE2	1:A:329:GLN:HG3	1.75	0.51
2:B:354:TRP:CD2	20:B:1104:PX2:H34	2.46	0.51
2:B:515:PRO:HA	2:B:525:PHE:HZ	1.76	0.51
3:C:979:LEU:HD23	3:C:1060:LYS:HE3	1.92	0.51
4:D:57:ILE:HG23	4:D:1553:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:869:LEU:HD22	5:E:876:LEU:HD22	1.92	0.51
7:G:189:VAL:HA	7:G:192:TRP:HE3	1.76	0.51
2:B:585:PRO:HD3	2:B:632:LEU:HD11	1.93	0.51
2:B:991:ASP:N	2:B:991:ASP:OD1	2.44	0.51
4:D:1642:ARG:NH1	4:D:1778:CYS:O	2.44	0.51
9:J:293:THR:HA	9:J:296:VAL:HG22	1.93	0.51
16:R:261:ASP:HA	16:R:264:ARG:HB3	1.93	0.51
9:I:299:LYS:HB3	9:I:302:ALA:HB3	1.93	0.50
9:J:371:TYR:HA	9:J:374:LYS:HE3	1.93	0.50
2:B:354:TRP:NE1	20:B:1104:PX2:C19	2.71	0.50
3:C:417:LEU:HD12	3:C:438:TRP:HE1	1.75	0.50
1:A:174:ILE:HB	1:A:207:MET:HE3	1.93	0.50
3:C:1119:ASN:HA	3:C:1268:LEU:O	2.11	0.50
4:D:1984:ASP:OD2	4:D:1986:LYS:NZ	2.44	0.50
8:H:112:PRO:HB2	8:H:117:TRP:HH2	1.76	0.50
1:A:789:VAL:HA	1:A:798:PHE:O	2.10	0.50
2:B:536:GLY:O	18:B:1103:ATP:C8	2.64	0.50
1:A:126:ARG:O	1:A:130:THR:OG1	2.29	0.50
1:A:388:MET:SD	1:A:388:MET:N	2.84	0.50
2:B:224:PHE:HB3	2:B:232:LEU:HD12	1.93	0.50
1:A:338:ASP:O	1:A:342:GLN:CB	2.59	0.50
2:B:973:PHE:HA	4:D:1986:LYS:HD3	1.92	0.50
2:B:341:THR:HG23	2:B:344:THR:HB	1.93	0.50
18:A:902:ATP:C5'	6:F:567:ARG:HH22	2.25	0.50
4:D:112:PRO:HB3	4:D:132:ILE:HD12	1.92	0.50
4:D:140:LEU:HD13	16:R:253:GLN:OE1	2.12	0.49
4:D:1677:PHE:HE1	4:D:1737:GLN:HE22	1.59	0.49
1:A:326:ARG:HG2	2:B:719:ARG:HH21	1.78	0.49
2:B:354:TRP:O	7:G:153:TRP:NE1	2.45	0.49
2:B:335:ILE:HD11	16:R:237:VAL:HA	1.95	0.49
2:B:372:SER:OG	4:D:1020:ARG:O	2.30	0.49
3:C:220:LEU:O	3:C:224:MET:HG3	2.11	0.49
7:G:190:PHE:CD1	7:G:216:TYR:HB3	2.47	0.49
7:G:299:SER:HB3	7:G:328:PRO:HG2	1.93	0.49
10:K:34:ASP:OD1	10:K:37:ARG:NH1	2.45	0.49
3:C:1017:ASP:N	3:C:1017:ASP:OD1	2.44	0.49
4:D:2006:LEU:HD13	4:D:2249:ARG:HB3	1.93	0.49
4:D:2277:THR:HA	4:D:2280:LYS:HE2	1.94	0.49
3:C:1215:ALA:HB2	5:E:814:TRP:HB3	1.95	0.49
6:F:585:ARG:NH2	6:F:608:ALA:O	2.45	0.49
9:J:185:ALA:O	9:J:189:ASN:ND2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LYS:HD3	2:B:239:VAL:HG11	1.94	0.49
10:K:62:LEU:HB3	16:R:249:LYS:HE2	1.95	0.49
1:A:352:VAL:HG23	1:A:458:LEU:HD11	1.93	0.49
2:B:526:VAL:HG13	2:B:659:ASP:HB2	1.95	0.49
20:B:1104:PX2:O5	7:G:199:ALA:HB1	2.13	0.49
3:C:532:ARG:NH1	3:C:550:GLU:OE1	2.45	0.49
4:D:1879:ASP:OD1	4:D:1879:ASP:N	2.37	0.49
6:F:628:ILE:O	6:F:630:MET:N	2.45	0.49
1:A:532:GLN:NE2	18:A:902:ATP:C1'	2.52	0.49
3:C:1113:ASN:ND2	3:C:1287:GLU:OE2	2.37	0.49
6:F:583:ILE:HA	6:F:586:MET:HG2	1.93	0.49
7:G:330:TYR:HB3	7:G:361:TYR:CD1	2.48	0.49
1:A:124:TRP:CD2	7:G:143:TRP:HB3	2.48	0.49
2:B:135:ASP:HA	2:B:138:LYS:HG3	1.95	0.49
3:C:772:ARG:NH2	3:C:847:ASN:O	2.40	0.49
3:C:1005:GLU:OE1	4:D:1601:ARG:NH2	2.36	0.49
5:E:756:LEU:HD22	5:E:861:MET:HE3	1.95	0.49
9:J:179:VAL:HG11	9:J:205:THR:HG23	1.95	0.49
4:D:1533:PHE:HB3	4:D:1733:TYR:HE1	1.77	0.48
1:A:701:VAL:HG13	6:F:780:TRP:HB3	1.94	0.48
2:B:354:TRP:CE2	20:B:1104:PX2:C17	2.75	0.48
4:D:1011:TRP:CD2	4:D:1012:LEU:HG	2.48	0.48
1:A:497:LEU:HD13	1:A:516:LEU:HB3	1.95	0.48
1:A:820:VAL:HA	1:A:823:ILE:HG22	1.95	0.48
2:B:822:MET:HA	2:B:822:MET:HE2	1.95	0.48
3:C:1109:LEU:HD11	3:C:1273:LEU:HB3	1.96	0.48
4:D:1903:ASP:OD1	4:D:1903:ASP:N	2.47	0.48
6:F:670:ILE:HG12	6:F:818:VAL:HG21	1.96	0.48
3:C:531:ALA:O	3:C:582:THR:HA	2.14	0.48
4:D:140:LEU:HD21	16:R:230:LEU:HD21	1.94	0.48
4:D:1985:GLU:HB3	4:D:1988:ARG:HD2	1.94	0.48
6:F:848:SER:OG	6:F:849:ILE:N	2.45	0.48
2:B:690:ASP:OD1	2:B:690:ASP:N	2.46	0.48
9:J:230:LEU:HD22	9:J:309:MET:HG2	1.96	0.48
16:R:100:LYS:HA	16:R:100:LYS:HD3	1.72	0.48
1:A:789:VAL:HG21	9:I:101:LEU:HD22	1.96	0.48
2:B:221:LEU:HD11	2:B:317:TYR:HB3	1.95	0.48
3:C:418:PHE:HE1	3:C:439:MET:HE1	1.78	0.48
4:D:1343:ARG:HD2	4:D:1347:VAL:HG11	1.94	0.48
9:J:286:VAL:O	9:J:290:ASN:ND2	2.39	0.48
2:B:643:ASN:CG	18:B:1103:ATP:O1G	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:828:THR:HG22	3:C:993:ARG:HG2	1.96	0.48
3:C:1240:ALA:HB2	3:C:1291:LEU:HD21	1.95	0.48
5:E:476:LYS:HG2	5:E:605:VAL:HG21	1.96	0.48
5:E:713:ARG:NH2	5:E:899:ASP:OD1	2.46	0.48
5:E:820:PHE:O	5:E:822:GLY:N	2.46	0.48
2:B:226:GLU:HB3	2:B:314:ALA:HB1	1.95	0.48
2:B:402:ILE:HD12	2:B:403:PRO:HD2	1.95	0.48
3:C:506:ASN:O	3:C:510:SER:CA	2.61	0.48
6:F:694:ASN:ND2	6:F:826:SER:OG	2.47	0.48
2:B:352:ARG:NE	7:G:204:TYR:HB3	2.28	0.48
3:C:1105:ALA:HB2	3:C:1120:LEU:HD21	1.95	0.48
4:D:2208:ASP:OD1	4:D:2208:ASP:N	2.43	0.48
9:J:257:GLY:N	9:J:262:THR:O	2.41	0.48
1:A:319:ALA:O	18:A:902:ATP:N6	2.35	0.48
4:D:1884:ARG:NH1	4:D:2287:ASP:OD2	2.46	0.47
16:R:120:HIS:HB3	16:R:163:LEU:HB2	1.95	0.47
1:A:170:TYR:OH	16:R:197:GLU:OE1	2.29	0.47
1:A:220:HIS:HA	1:A:223:ILE:HG22	1.96	0.47
1:A:361:GLY:C	18:A:902:ATP:O1A	2.57	0.47
2:B:355:ARG:HG2	2:B:356:TYR:H	1.80	0.47
3:C:599:GLN:HA	3:C:602:LEU:HD12	1.95	0.47
4:D:2031:THR:OG1	4:D:2032:LEU:N	2.47	0.47
6:F:444:GLY:HA2	6:F:550:ILE:HD12	1.95	0.47
10:K:52:PRO:HB3	10:K:56:TYR:HD2	1.80	0.47
3:C:498:ARG:NH2	16:R:243:ASP:OD2	2.43	0.47
1:A:777:ARG:HD3	2:B:912:GLU:HB2	1.96	0.47
3:C:254:LYS:O	3:C:258:LYS:NZ	2.44	0.47
6:F:652:ARG:HE	6:F:696:ARG:HD2	1.78	0.47
6:F:652:ARG:HH22	6:F:699:ARG:HH11	1.62	0.47
2:B:198:PRO:HD3	2:B:297:TRP:HE1	1.79	0.47
2:B:822:MET:HE3	2:B:973:PHE:CG	2.50	0.47
3:C:1101:ALA:HB1	3:C:1120:LEU:HD23	1.95	0.47
5:E:621:ALA:HB1	5:E:626:MET:HG3	1.96	0.47
6:F:744:ASP:OD1	6:F:745:GLN:NE2	2.48	0.47
3:C:1261:GLU:HA	3:C:1264:GLU:HG2	1.96	0.47
2:B:969:MET:HA	2:B:969:MET:HE2	1.96	0.47
4:D:1813:LYS:HD3	4:D:1815:ARG:HH12	1.79	0.47
9:I:141:PRO:O	9:I:144:LEU:HB2	2.14	0.47
16:R:220:MET:O	16:R:254:TYR:OH	2.30	0.47
1:A:822:GLU:O	1:A:826:LYS:HG2	2.15	0.47
3:C:506:ASN:O	3:C:510:SER:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1597:CYS:SG	4:D:1598:LEU:N	2.88	0.47
9:I:102:ILE:O	9:I:105:SER:OG	2.32	0.47
6:F:733:PRO:HB2	6:F:750:TRP:HB3	1.96	0.47
16:R:266:LEU:HG	16:R:277:LEU:HD13	1.96	0.47
2:B:770:GLU:OE1	2:B:801:SER:OG	2.32	0.47
3:C:505:TYR:HH	3:C:510:SER:HG	1.63	0.47
4:D:494:ARG:HH11	10:K:31:LEU:HA	1.79	0.47
4:D:2219:ILE:HD12	4:D:2219:ILE:H	1.80	0.47
6:F:472:PHE:O	6:F:507:PHE:N	2.44	0.47
7:G:320:GLY:O	7:G:323:ARG:HG2	2.15	0.47
1:A:215:VAL:O	1:A:219:LEU:N	2.48	0.46
1:A:640:ILE:HD13	1:A:718:LYS:HG2	1.96	0.46
3:C:175:LEU:HA	3:C:178:VAL:HG22	1.96	0.46
3:C:810:GLN:HE21	3:C:921:GLN:HB2	1.80	0.46
6:F:807:LEU:HD22	6:F:814:MET:HE2	1.96	0.46
7:G:349:SER:O	7:G:353:LEU:HG	2.15	0.46
1:A:214:ASP:O	1:A:217:LYS:HB3	2.15	0.46
1:A:504:LYS:HE3	1:A:535:LEU:HB3	1.97	0.46
1:A:746:ASP:OD1	1:A:746:ASP:N	2.47	0.46
9:J:111:LEU:HB3	9:J:135:VAL:HG22	1.97	0.46
2:B:421:LEU:HB2	4:D:105:LEU:HD21	1.96	0.46
3:C:512:TRP:CE2	3:C:549:LYS:HD3	2.50	0.46
3:C:766:ILE:HD11	3:C:865:ASN:HA	1.97	0.46
4:D:494:ARG:HG2	10:K:31:LEU:HD13	1.98	0.46
4:D:1325:SER:OG	4:D:1326:GLU:N	2.48	0.46
4:D:1852:MET:HG3	4:D:1925:PRO:HG2	1.97	0.46
6:F:818:VAL:O	6:F:822:VAL:HG23	2.15	0.46
8:H:110:ASP:OD1	8:H:110:ASP:N	2.47	0.46
16:R:310:ALA:O	16:R:313:GLN:HG3	2.14	0.46
1:A:845:LYS:NZ	7:G:178:ASN:OD1	2.41	0.46
6:F:693:ILE:HG23	6:F:821:LEU:HD22	1.96	0.46
6:F:725:ASP:O	6:F:728:THR:HB	2.14	0.46
2:B:782:ARG:HH22	2:B:809:MET:HB2	1.80	0.46
3:C:180:VAL:O	3:C:184:THR:HG23	2.15	0.46
3:C:312:ARG:HA	3:C:315:VAL:HG22	1.97	0.46
3:C:1040:THR:HG22	3:C:1042:VAL:H	1.80	0.46
4:D:1608:TYR:HA	4:D:1611:ILE:HD12	1.97	0.46
4:D:1823:ARG:NE	4:D:1848:GLU:OE2	2.45	0.46
5:E:555:GLN:HE22	6:F:481:GLU:HG3	1.81	0.46
5:E:795:ILE:HG23	5:E:801:LEU:HD12	1.98	0.46
7:G:197:PRO:HG3	7:G:264:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:334:MET:HE2	7:G:354:LEU:HA	1.97	0.46
1:A:93:ARG:HB3	2:B:258:ILE:HD11	1.97	0.46
1:A:532:GLN:NE2	18:A:902:ATP:O2'	2.49	0.46
2:B:348:TRP:CZ2	4:D:532:SER:HB2	2.51	0.46
3:C:245:ALA:HB2	3:C:274:MET:HE3	1.98	0.46
1:A:249:SER:HA	1:A:252:LEU:HG	1.98	0.46
2:B:738:LEU:HD23	2:B:788:PHE:HE1	1.80	0.46
2:B:989:HIS:CD2	2:B:991:ASP:HA	2.49	0.46
3:C:388:LYS:HB2	16:R:276:TYR:CG	2.51	0.46
4:D:45:HIS:ND1	4:D:47:GLU:OE2	2.49	0.46
18:A:902:ATP:C4'	6:F:567:ARG:HH22	2.28	0.46
2:B:528:GLY:HA3	2:B:658:ILE:HA	1.98	0.46
2:B:643:ASN:ND2	18:B:1103:ATP:O3G	2.49	0.46
4:D:2044:MET:SD	4:D:2045:MET:HG2	2.56	0.46
2:B:331:ARG:O	2:B:331:ARG:NE	2.49	0.45
4:D:1594:ASN:ND2	4:D:1600:GLU:HG2	2.31	0.45
4:D:1813:LYS:HB3	4:D:1813:LYS:HE3	1.77	0.45
6:F:755:ASP:HA	6:F:758:ARG:HG2	1.97	0.45
4:D:1911:ILE:HD12	4:D:2274:MET:HG2	1.98	0.45
7:G:302:TYR:HE2	7:G:320:GLY:HA3	1.81	0.45
2:B:151:LYS:HB2	2:B:151:LYS:HE2	1.79	0.45
4:D:1358:LEU:HD11	16:R:93:VAL:HG11	1.98	0.45
1:A:240:THR:O	1:A:244:THR:OG1	2.29	0.45
2:B:352:ARG:HE	7:G:204:TYR:HB3	1.80	0.45
4:D:495:SER:O	4:D:497:PHE:N	2.50	0.45
6:F:630:MET:HE1	6:F:642:ASP:HB3	1.99	0.45
6:F:869:MET:O	6:F:873:ARG:HG3	2.16	0.45
2:B:297:TRP:HA	2:B:300:MET:HE2	1.99	0.45
3:C:208:GLU:HA	3:C:211:LYS:HG2	1.97	0.45
3:C:1008:ALA:O	3:C:1011:SER:OG	2.32	0.45
4:D:134:ARG:NH1	4:D:135:LEU:HD23	2.31	0.45
4:D:494:ARG:NH1	10:K:34:ASP:HB3	2.31	0.45
7:G:228:LYS:HB3	7:G:228:LYS:HE3	1.68	0.45
8:H:114:ILE:HA	8:H:117:TRP:CZ3	2.52	0.45
16:R:296:VAL:HG11	16:R:302:TYR:HB2	1.97	0.45
1:A:817:TRP:HA	1:A:820:VAL:HG12	1.96	0.45
2:B:587:PHE:HD1	2:B:637:ILE:HB	1.81	0.45
9:I:84:LYS:HG2	9:I:110:THR:HB	1.99	0.45
16:R:281:LEU:HB3	16:R:295:ILE:HD11	1.97	0.45
1:A:411:ILE:HD12	1:A:458:LEU:HD23	1.99	0.45
1:A:653:PHE:O	1:A:657:ASN:ND2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:689:ILE:HD11	2:B:725:ILE:HG22	1.99	0.45
3:C:470:LEU:HD23	10:K:68:VAL:HB	1.99	0.45
5:E:522:LYS:HE2	5:E:575:LYS:HB3	1.99	0.45
3:C:238:ALA:HB2	3:C:281:ILE:HG21	1.97	0.45
4:D:494:ARG:NH1	10:K:31:LEU:HD12	2.31	0.45
9:I:155:VAL:HG22	9:I:196:HIS:HB2	1.99	0.45
1:A:520:ALA:HA	1:A:523:THR:HG22	1.99	0.45
2:B:632:LEU:H	4:D:15:GLU:HG3	1.82	0.45
3:C:308:ILE:HD13	4:D:1319:LEU:HA	1.98	0.45
3:C:972:MET:HA	4:D:1601:ARG:CZ	2.47	0.45
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.87	0.44
1:A:423:LYS:HG3	1:A:470:ASP:HB3	1.99	0.44
1:A:455:SER:O	1:A:455:SER:OG	2.33	0.44
2:B:139:TRP:NE1	16:R:304:ALA:HB3	2.28	0.44
16:R:147:ARG:O	16:R:147:ARG:NE	2.49	0.44
4:D:1609:GLN:HE21	4:D:1613:TYR:HD2	1.66	0.44
4:D:2281:LYS:HZ1	8:H:98:PRO:HA	1.82	0.44
5:E:476:LYS:NZ	5:E:584:ASN:OD1	2.42	0.44
5:E:601:ARG:HH21	6:F:628:ILE:HD11	1.82	0.44
11:L:17:MET:HE2	11:L:17:MET:O	2.17	0.44
3:C:194:GLU:HG3	3:C:196:ALA:H	1.82	0.44
3:C:968:ALA:HA	3:C:972:MET:HE2	1.98	0.44
3:C:1210:TYR:HD2	3:C:1219:LEU:HB2	1.83	0.44
4:D:34:ASN:HB3	4:D:1545:ARG:HH22	1.81	0.44
16:R:198:PRO:HG2	16:R:200:TRP:CZ2	2.52	0.44
9:I:335:PHE:HA	9:I:347:ALA:HA	1.99	0.44
2:B:370:ASP:OD2	4:D:1032:ARG:NH2	2.49	0.44
2:B:459:LYS:HE2	2:B:459:LYS:HB2	1.84	0.44
2:B:809:MET:HG2	2:B:891:LEU:HD21	1.99	0.44
3:C:1166:ILE:O	3:C:1170:MET:HG2	2.18	0.44
4:D:1643:SER:HB2	4:D:1788:VAL:HB	2.00	0.44
6:F:684:ASP:HB3	6:F:685:MET:HE3	2.00	0.44
6:F:779:PHE:HE2	6:F:788:ILE:HD11	1.83	0.44
1:A:777:ARG:HG2	2:B:908:VAL:HG22	2.00	0.44
18:A:902:ATP:C4'	6:F:567:ARG:NH2	2.81	0.44
3:C:602:LEU:HD23	4:D:1320:HIS:CE1	2.53	0.44
6:F:678:VAL:HG12	6:F:729:VAL:HG22	2.00	0.44
7:G:326:ARG:NH1	7:G:369:GLU:OE2	2.51	0.44
9:I:112:HIS:HE1	9:I:136:ARG:HD3	1.82	0.44
1:A:475:ARG:HH21	18:B:1103:ATP:PB	2.41	0.44
2:B:820:MET:HB2	2:B:856:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:379:ASP:N	3:C:379:ASP:OD1	2.51	0.44
3:C:1171:LEU:HD11	3:C:1255:LEU:HG	1.99	0.44
4:D:1584:HIS:CD2	4:D:1785:ASN:HB2	2.53	0.44
4:D:1647:ILE:HG12	4:D:1795:PRO:HB3	2.00	0.44
7:G:245:VAL:HG11	7:G:368:GLU:HA	1.99	0.44
3:C:828:THR:HA	3:C:993:ARG:HB3	1.99	0.44
7:G:193:LEU:HD21	7:G:259:ILE:HG22	2.00	0.44
1:A:594:LEU:HD23	1:A:594:LEU:HA	1.85	0.44
2:B:528:GLY:HA3	2:B:658:ILE:HD13	2.00	0.44
3:C:237:ARG:O	3:C:241:ILE:HG12	2.18	0.44
3:C:534:ARG:HE	3:C:539:VAL:HG12	1.83	0.44
3:C:1091:ARG:HH12	3:C:1095:PHE:HB2	1.82	0.44
4:D:1907:LEU:O	4:D:1911:ILE:HG12	2.17	0.44
7:G:259:ILE:O	7:G:263:HIS:ND1	2.49	0.44
9:I:157:PRO:HA	9:I:198:ILE:HB	2.00	0.44
4:D:1657:LEU:HD23	4:D:1657:LEU:HA	1.85	0.43
6:F:725:ASP:OD1	6:F:802:ARG:NH1	2.51	0.43
8:H:113:ILE:HG22	8:H:115:TRP:HZ3	1.82	0.43
9:I:253:PRO:HB2	9:I:266:LEU:HB2	2.00	0.43
16:R:206:LEU:HA	16:R:209:MET:HE2	1.99	0.43
1:A:464:ASN:ND2	18:A:902:ATP:O3G	2.50	0.43
2:B:811:ASP:HB3	4:D:1899:ARG:HD3	2.00	0.43
4:D:77:ILE:HA	4:D:80:VAL:HG12	2.00	0.43
9:I:83:TYR:HD1	9:I:152:ASN:HD22	1.65	0.43
9:J:208:ILE:HG12	9:J:394:ALA:HB2	2.00	0.43
2:B:354:TRP:CD2	20:B:1104:PX2:C19	3.01	0.43
3:C:509:LYS:NZ	3:C:511:ARG:HH21	2.15	0.43
3:C:1209:VAL:O	5:E:789:SER:OG	2.30	0.43
4:D:1850:ILE:HD13	4:D:1884:ARG:HE	1.83	0.43
6:F:734:ARG:HG2	6:F:800:TYR:HE2	1.83	0.43
1:A:355:HIS:CE1	1:A:484:ARG:HB3	2.53	0.43
2:B:516:MET:HG3	4:D:14:ARG:HB2	2.00	0.43
2:B:978:GLN:N	2:B:978:GLN:OE1	2.52	0.43
3:C:212:LEU:O	3:C:216:ILE:HG13	2.19	0.43
3:C:461:LYS:O	3:C:465:GLU:HG2	2.18	0.43
6:F:516:ARG:HD3	6:F:520:LEU:HD11	2.01	0.43
3:C:1006:SER:O	4:D:1609:GLN:HG3	2.18	0.43
4:D:35:SER:OG	4:D:1547:ASP:OD2	2.29	0.43
6:F:859:GLU:O	6:F:862:GLU:HG3	2.19	0.43
1:A:216:TRP:HZ2	2:B:403:PRO:HB2	1.83	0.43
1:A:263:ASP:OD2	1:A:264:SER:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:817:PHE:HE1	4:D:1990:THR:HB	1.83	0.43
2:B:863:SER:HB3	2:B:895:ARG:HH22	1.84	0.43
2:B:902:MET:HE2	2:B:902:MET:HA	2.00	0.43
2:B:1005:LEU:HD23	2:B:1005:LEU:HA	1.87	0.43
3:C:1046:MET:HA	3:C:1046:MET:HE2	2.00	0.43
5:E:820:PHE:HB3	5:E:821:VAL:H	1.64	0.43
6:F:590:GLN:O	6:F:594:ARG:HG2	2.18	0.43
10:K:75:LEU:HD12	10:K:75:LEU:HA	1.89	0.43
16:R:97:ARG:HA	16:R:189:ARG:HH11	1.84	0.43
2:B:460:ARG:HG3	4:D:16:ILE:HD11	2.00	0.43
2:B:869:LEU:HD22	2:B:874:LEU:HD21	2.01	0.43
4:D:1780:ARG:HD2	4:D:1780:ARG:HA	1.72	0.43
9:J:222:LYS:HA	9:J:357:LEU:HD12	2.00	0.43
2:B:353:TRP:CZ2	2:B:354:TRP:HD1	2.37	0.43
2:B:990:LYS:HE2	4:D:1981:PRO:HB3	2.00	0.43
4:D:1911:ILE:HG23	4:D:2274:MET:HG2	2.01	0.43
4:D:1957:LYS:HA	4:D:1957:LYS:HD3	1.67	0.43
4:D:2281:LYS:NZ	8:H:99:ASP:H	2.17	0.43
5:E:660:ARG:HH22	5:E:677:ARG:HH12	1.67	0.43
6:F:565:LEU:HD23	6:F:565:LEU:HA	1.88	0.43
6:F:728:THR:HG23	6:F:803:ALA:HB2	2.00	0.43
1:A:464:ASN:OD1	18:A:902:ATP:PG	2.77	0.43
3:C:517:MET:O	3:C:520:PRO:HD2	2.18	0.43
3:C:1275:ARG:O	3:C:1279:GLU:HG2	2.19	0.43
7:G:198:PRO:HB2	7:G:205:LEU:HD21	2.01	0.43
9:J:374:LYS:HA	9:J:377:GLU:HG3	2.00	0.43
1:A:148:ILE:HG22	1:A:204:VAL:HG13	2.01	0.43
1:A:361:GLY:N	18:A:902:ATP:O1A	2.50	0.43
1:A:685:PHE:HZ	1:A:700:LEU:HB3	1.83	0.43
2:B:405:ASP:N	2:B:405:ASP:OD1	2.51	0.43
3:C:190:LYS:HA	3:C:190:LYS:HD3	1.77	0.43
3:C:474:LEU:HD23	3:C:474:LEU:HA	1.86	0.43
4:D:7:LYS:HD2	4:D:7:LYS:HA	1.78	0.43
4:D:1652:THR:HG21	4:D:1857:ARG:HE	1.84	0.43
5:E:537:ARG:HH21	5:E:591:PRO:HG3	1.84	0.43
6:F:585:ARG:HE	6:F:608:ALA:HB1	1.84	0.43
1:A:130:THR:HA	1:A:135:LEU:HB2	2.00	0.42
1:A:378:PHE:HZ	1:A:407:TYR:HD1	1.66	0.42
1:A:780:ILE:HD11	9:J:271:LYS:HB3	2.00	0.42
3:C:1115:ASP:HB3	3:C:1137:LYS:HA	2.00	0.42
3:C:1204:ASP:OD1	3:C:1204:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLY:N	1:A:322:GLU:OE2	2.51	0.42
3:C:188:VAL:HA	3:C:193:GLY:H	1.85	0.42
16:R:123:ILE:HG23	16:R:148:ALA:HB1	2.00	0.42
1:A:124:TRP:CE2	7:G:143:TRP:HB3	2.54	0.42
1:A:208:PRO:HG2	16:R:109:ARG:HH21	1.84	0.42
3:C:169:ASP:HA	3:C:172:ARG:HD2	2.01	0.42
7:G:289:ILE:O	7:G:292:THR:OG1	2.36	0.42
16:R:93:VAL:HG12	16:R:192:ALA:HB2	2.01	0.42
1:A:536:ASN:ND2	6:F:441:LYS:HB2	2.34	0.42
3:C:221:TYR:HB3	3:C:225:ARG:HH21	1.84	0.42
3:C:470:LEU:HA	3:C:473:LYS:HG2	2.01	0.42
3:C:1052:ASN:OD1	3:C:1057:ASN:ND2	2.49	0.42
9:J:148:LEU:HB3	9:J:190:CYS:SG	2.59	0.42
9:J:335:PHE:HA	9:J:347:ALA:HA	2.00	0.42
16:R:260:TYR:CD2	16:R:285:ASP:HB3	2.55	0.42
1:A:843:LYS:HD2	1:A:843:LYS:HA	1.77	0.42
3:C:1222:GLY:HA3	5:E:848:ASP:HB3	2.01	0.42
7:G:305:ARG:O	7:G:305:ARG:NH1	2.51	0.42
9:J:154:VAL:HG11	9:J:186:VAL:HG21	2.01	0.42
1:A:165:MET:SD	1:A:223:ILE:HD13	2.59	0.42
18:A:902:ATP:O2G	6:F:570:ARG:NH2	2.41	0.42
2:B:142:TRP:O	2:B:148:TRP:NE1	2.49	0.42
3:C:516:PRO:O	3:C:519:VAL:HB	2.19	0.42
4:D:1924:CYS:HA	4:D:1925:PRO:HD3	1.93	0.42
5:E:915:ASN:O	5:E:918:SER:OG	2.35	0.42
16:R:223:PRO:O	16:R:227:ASN:HB2	2.20	0.42
1:A:314:THR:OG1	1:A:315:PHE:N	2.52	0.42
2:B:650:LEU:HD12	2:B:650:LEU:HA	1.89	0.42
5:E:695:CYS:O	5:E:699:THR:OG1	2.33	0.42
6:F:607:VAL:O	6:F:611:THR:HG22	2.20	0.42
7:G:186:VAL:HG11	7:G:220:PHE:CZ	2.55	0.42
7:G:262:GLY:HA3	7:G:353:LEU:CD2	2.50	0.42
7:G:389:HIS:CE1	7:G:394:PHE:HA	2.55	0.42
9:J:229:THR:HB	9:J:312:ALA:HB1	2.02	0.42
1:A:418:ASP:OD1	1:A:418:ASP:N	2.51	0.42
1:A:713:ARG:NH1	1:A:717:GLU:OE2	2.51	0.42
1:A:845:LYS:HA	1:A:845:LYS:HD3	1.85	0.42
2:B:134:ILE:O	2:B:138:LYS:N	2.53	0.42
2:B:406:PRO:HB3	16:R:211:TYR:HA	2.02	0.42
20:B:1104:PX2:O6	7:G:155:TRP:CZ3	2.72	0.42
3:C:801:ALA:O	3:C:804:GLN:NE2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:HG22	2:B:439:PRO:HG2	2.02	0.42
1:A:497:LEU:HB2	1:A:516:LEU:HD12	2.02	0.42
2:B:257:LYS:HD2	2:B:257:LYS:HA	1.77	0.42
2:B:685:LEU:HB3	2:B:689:ILE:HG13	2.01	0.42
3:C:401:LEU:HD12	3:C:401:LEU:HA	1.85	0.42
3:C:936:ILE:HB	3:C:941:ARG:HD3	2.01	0.42
4:D:1379:LEU:HD12	4:D:1379:LEU:HA	1.88	0.42
5:E:457:LYS:HZ3	5:E:458:MET:HG2	1.85	0.42
8:H:121:LEU:O	8:H:125:VAL:HG22	2.20	0.42
4:D:50:ARG:HG3	4:D:51:LYS:HG3	2.01	0.42
4:D:558:PRO:HA	4:D:1052:PHE:CD2	2.55	0.42
4:D:1588:LEU:HD23	4:D:1588:LEU:HA	1.89	0.42
4:D:1852:MET:HB3	4:D:1853:GLY:H	1.68	0.42
7:G:259:ILE:HD13	7:G:259:ILE:HA	1.91	0.42
9:I:357:LEU:HD23	9:I:357:LEU:HA	1.90	0.42
1:A:110:ALA:HA	4:D:546:ILE:HG23	2.02	0.41
1:A:634:ASP:OD1	1:A:634:ASP:N	2.53	0.41
1:A:707:LEU:HG	1:A:772:LEU:HD21	2.01	0.41
2:B:824:MET:SD	2:B:853:ILE:HG23	2.60	0.41
3:C:539:VAL:HG21	3:C:552:TYR:CZ	2.55	0.41
3:C:1187:LYS:HB2	3:C:1187:LYS:HE3	1.67	0.41
3:C:1253:ARG:HH21	3:C:1280:ASN:HA	1.85	0.41
4:D:1864:ASN:O	4:D:1868:SER:OG	2.33	0.41
4:D:2247:PHE:O	4:D:2251:ASN:ND2	2.40	0.41
5:E:765:GLY:O	5:E:769:GLU:HG2	2.20	0.41
6:F:685:MET:HB2	6:F:706:VAL:HG21	2.02	0.41
9:J:173:ASN:O	9:J:177:ASN:ND2	2.40	0.41
1:A:444:LEU:HD22	1:A:478:ARG:HD3	2.01	0.41
3:C:1019:LEU:HD12	4:D:1610:THR:HG21	2.02	0.41
8:H:95:SER:OG	8:H:96:THR:N	2.52	0.41
9:I:255:ILE:HD11	9:I:264:LEU:HD23	2.02	0.41
9:J:296:VAL:HG12	9:J:304:SER:HA	2.03	0.41
12:M:9:VAL:HG11	16:R:222:ASP:HB2	2.02	0.41
4:D:1776:ARG:HA	4:D:1776:ARG:HD2	1.90	0.41
10:K:14:GLU:OE1	10:K:14:GLU:N	2.52	0.41
11:L:14:LEU:HD12	11:L:14:LEU:HA	1.85	0.41
16:R:95:CYS:O	16:R:189:ARG:N	2.40	0.41
1:A:849:LEU:HD12	7:G:172:HIS:CE1	2.56	0.41
2:B:534:PRO:O	2:B:537:THR:OG1	2.35	0.41
3:C:938:GLU:HA	3:C:941:ARG:HG2	2.01	0.41
4:D:21:LYS:O	4:D:22:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:892:GLU:H	5:E:892:GLU:HG3	1.62	0.41
7:G:209:PRO:HG2	7:G:273:LEU:HD11	2.02	0.41
9:J:84:LYS:HB3	9:J:112:HIS:CE1	2.51	0.41
13:N:24:ARG:HD2	13:N:24:ARG:HA	1.70	0.41
1:A:92:LEU:HD12	2:B:277:LEU:HD22	2.02	0.41
1:A:512:LYS:HB3	1:A:512:LYS:HE2	1.86	0.41
2:B:221:LEU:HD13	2:B:319:VAL:HG12	2.02	0.41
2:B:506:ASP:O	2:B:510:ILE:HG23	2.20	0.41
2:B:534:PRO:HG2	2:B:666:LEU:HG	2.01	0.41
2:B:568:SER:O	2:B:568:SER:OG	2.35	0.41
3:C:227:LEU:HA	3:C:227:LEU:HD23	1.79	0.41
3:C:1120:LEU:HB2	3:C:1268:LEU:HB2	2.02	0.41
9:I:176:ALA:HA	9:I:179:VAL:HG12	2.02	0.41
16:R:99:CYS:SG	16:R:100:LYS:N	2.90	0.41
2:B:572:LYS:O	2:B:576:MET:HG3	2.20	0.41
3:C:892:VAL:HG12	3:C:937:ASP:HA	2.01	0.41
1:A:212:TRP:HA	1:A:215:VAL:HB	2.02	0.41
2:B:355:ARG:HH22	2:B:395:PRO:HB2	1.85	0.41
4:D:50:ARG:HH12	7:G:229:ARG:NH1	2.17	0.41
4:D:1343:ARG:HB3	4:D:1344:SER:H	1.65	0.41
11:L:21:LEU:HD23	11:L:21:LEU:HA	1.95	0.41
2:B:821:LYS:HB3	2:B:821:LYS:HE2	1.82	0.41
3:C:246:LEU:O	3:C:250:LYS:HG2	2.20	0.41
3:C:463:GLN:HG2	3:C:467:LYS:NZ	2.36	0.41
3:C:601:LEU:HA	3:C:604:THR:HG22	2.02	0.41
3:C:849:GLU:HG2	3:C:852:GLU:HG2	2.01	0.41
3:C:996:GLU:O	3:C:1000:VAL:HG23	2.21	0.41
5:E:775:SER:O	5:E:775:SER:OG	2.37	0.41
7:G:291:ILE:HG13	7:G:292:THR:N	2.36	0.41
1:A:100:LEU:HD22	2:B:265:ILE:HG21	2.02	0.41
1:A:231:VAL:HG12	14:O:155:LYS:HG2	2.03	0.41
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.94	0.41
1:A:497:LEU:HD13	1:A:516:LEU:HD12	2.02	0.41
2:B:156:LEU:HG	16:R:308:LEU:HD11	2.01	0.41
2:B:852:LYS:HE2	2:B:856:ILE:HD11	2.02	0.41
2:B:939:ILE:HG12	2:B:965:LEU:HD13	2.03	0.41
3:C:562:PHE:HD2	3:C:565:PHE:HB2	1.85	0.41
3:C:941:ARG:NH1	3:C:946:MET:HG2	2.36	0.41
4:D:1597:CYS:SG	4:D:1598:LEU:HD23	2.61	0.41
6:F:446:ILE:HD11	6:F:552:ILE:HG12	2.03	0.41
6:F:621:ASN:O	6:F:625:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:854:LYS:HA	6:F:854:LYS:HD2	1.85	0.41
9:I:295:VAL:HG11	9:I:305:ALA:HB2	2.02	0.41
9:I:340:LEU:HB3	9:I:365:LEU:HD12	2.03	0.41
2:B:572:LYS:HB3	2:B:572:LYS:HE2	1.82	0.41
2:B:820:MET:HE3	2:B:860:MET:HB2	2.02	0.41
3:C:411:LYS:HE3	3:C:411:LYS:HB2	1.81	0.41
5:E:790:TRP:O	5:E:793:ARG:HB2	2.21	0.41
7:G:367:MET:O	7:G:370:GLU:HG3	2.20	0.41
1:A:326:ARG:O	1:A:330:GLU:HG2	2.22	0.40
3:C:229:LYS:HA	3:C:229:LYS:HD2	1.94	0.40
3:C:1016:THR:HG23	4:D:1610:THR:HG23	2.02	0.40
4:D:496:PHE:CZ	13:N:24:ARG:HG2	2.56	0.40
6:F:419:ARG:HA	6:F:422:LEU:HB2	2.03	0.40
6:F:816:GLU:HG3	6:F:839:TYR:CZ	2.56	0.40
16:R:301:TYR:O	16:R:305:LYS:HB3	2.21	0.40
1:A:157:LEU:O	1:A:222:GLN:NE2	2.42	0.40
1:A:496:ILE:HG13	18:A:902:ATP:C2	2.57	0.40
1:A:517:GLN:O	1:A:521:GLU:HG2	2.21	0.40
2:B:587:PHE:CD1	2:B:637:ILE:HB	2.56	0.40
2:B:990:LYS:H	2:B:990:LYS:HG2	1.57	0.40
3:C:509:LYS:HZ2	3:C:511:ARG:HH21	1.68	0.40
6:F:611:THR:HA	6:F:614:MET:HE3	2.04	0.40
1:A:691:ARG:HG3	1:A:693:GLN:NE2	2.33	0.40
2:B:865:GLN:O	4:D:1988:ARG:NE	2.54	0.40
3:C:229:LYS:HE3	3:C:233:LEU:HG	2.02	0.40
3:C:410:LYS:HA	3:C:410:LYS:HD2	1.89	0.40
4:D:1645:LEU:HB2	4:D:1808:LEU:HG	2.04	0.40
5:E:742:LEU:HB2	5:E:747:TYR:HE1	1.87	0.40
9:J:335:PHE:HD2	9:J:347:ALA:HB2	1.86	0.40
1:A:254:LEU:HD22	8:H:138:TRP:CH2	2.56	0.40
1:A:476:LYS:HD2	1:A:476:LYS:HA	1.79	0.40
2:B:211:TRP:HB3	2:B:243:ALA:HB1	2.03	0.40
2:B:429:TYR:CD1	16:R:196:MET:HE1	2.57	0.40
9:I:82:SER:O	9:I:82:SER:OG	2.33	0.40
2:B:739:LEU:HD22	2:B:742:MET:HE1	2.04	0.40
3:C:255:LEU:HD11	3:C:260:ALA:HB3	2.02	0.40
7:G:290:VAL:O	7:G:294:LEU:HG	2.22	0.40
9:I:173:ASN:O	9:I:177:ASN:ND2	2.43	0.40
16:R:310:ALA:O	16:R:314:LYS:HG3	2.21	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	724/855 (85%)	691 (95%)	31 (4%)	2 (0%)	37	69
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

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	MET
1	A	494	LEU
2	B	273	LEU
2	B	348	TRP
2	B	537	THR
2	B	974	VAL
3	C	1114	PHE
4	D	1666	TYR

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Mol	Chain	Res	Type
6	F	577	ILE
6	F	831	GLU
7	G	219	PHE
9	J	120	LYS
14	O	143	VAL
16	R	196	MET
16	R	203	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	169	ASN
1	A	337	ASN
1	A	601	GLN
1	A	692	ASN
2	B	137	ASN
2	B	202	ASN
2	B	643	ASN
2	B	711	ASN
2	B	773	HIS
2	B	790	GLN
2	B	812	GLN
2	B	823	GLN
2	B	828	HIS
2	B	938	HIS
2	B	989	HIS
3	C	213	GLN
3	C	901	GLN
3	C	935	GLN
3	C	1065	ASN
3	C	1165	HIS
3	C	1178	ASN
3	C	1270	HIS
3	C	1295	ASN
3	C	1297	ASN
4	D	537	ASN
4	D	1019	GLN
4	D	1321	ASN
4	D	1555	HIS
4	D	1558	HIS
4	D	1590	ASN

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Mol	Chain	Res	Type
4	D	1917	GLN
4	D	1975	GLN
4	D	2206	GLN
4	D	2232	GLN
5	E	555	GLN
6	F	470	ASN
6	F	590	GLN
6	F	645	GLN
6	F	687	ASN
6	F	721	GLN
6	F	745	GLN
7	G	202	ASN
7	G	378	GLN
9	I	96	GLN
9	I	112	HIS
9	I	128	HIS
9	I	134	GLN
9	J	203	ASN
16	R	96	GLN
16	R	106	GLN
16	R	187	GLN
16	R	215	HIS
16	R	271	ASN
16	R	278	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 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	-

All (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
20	B	1104	PX2	P1-O1	-2.23	1.46	1.54
20	B	1104	PX2	C17-C16	-2.22	1.44	1.50

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	A	902	ATP	PA-O3A-PB	-4.28	118.13	132.83
18	B	1103	ATP	PA-O3A-PB	-4.28	118.15	132.83
20	B	1104	PX2	C3-O5-C4	4.01	131.99	117.12
18	B	1103	ATP	C3'-C2'-C1'	3.99	106.98	100.98
18	A	902	ATP	C3'-C2'-C1'	3.99	106.98	100.98
20	B	1104	PX2	O1-P1-O4	-3.73	96.81	106.73
20	B	1104	PX2	O7-C16-O8	-3.64	114.91	123.70
20	B	1104	PX2	O5-C4-O6	-3.64	114.41	123.59
20	B	1104	PX2	O7-C2-C3	-3.61	95.33	108.40
18	B	1103	ATP	N3-C2-N1	-3.53	123.16	128.68
18	A	902	ATP	N3-C2-N1	-3.52	123.18	128.68
20	B	1104	PX2	O4-P1-O2	3.37	115.94	106.47
20	B	1104	PX2	C8-C7-C6	-2.88	99.82	114.42
18	B	1103	ATP	N6-C6-N1	2.72	124.21	118.57
18	A	902	ATP	N6-C6-N1	2.71	124.21	118.57
20	B	1104	PX2	C7-C6-C5	-2.66	103.64	113.19
20	B	1104	PX2	C2-O7-C16	2.64	124.30	117.79
20	B	1104	PX2	P1-O4-C1	2.51	125.21	118.30
20	B	1104	PX2	O1-P1-O2	2.36	119.93	110.68
18	B	1103	ATP	C5-C6-N6	-2.02	117.28	120.35

There are no chirality outliers.

All (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
20	B	1104	PX2	C4-C5-C6-C7
20	B	1104	PX2	O8-C16-O7-C2
20	B	1104	PX2	C17-C16-O7-C2
20	B	1104	PX2	C7-C8-C9-C10
20	B	1104	PX2	O6-C4-O5-C3
20	B	1104	PX2	C5-C4-O5-C3
18	A	902	ATP	C5'-O5'-PA-O3A
18	B	1103	ATP	C5'-O5'-PA-O3A
18	A	902	ATP	PG-O3B-PB-O1B
18	B	1103	ATP	PG-O3B-PB-O1B

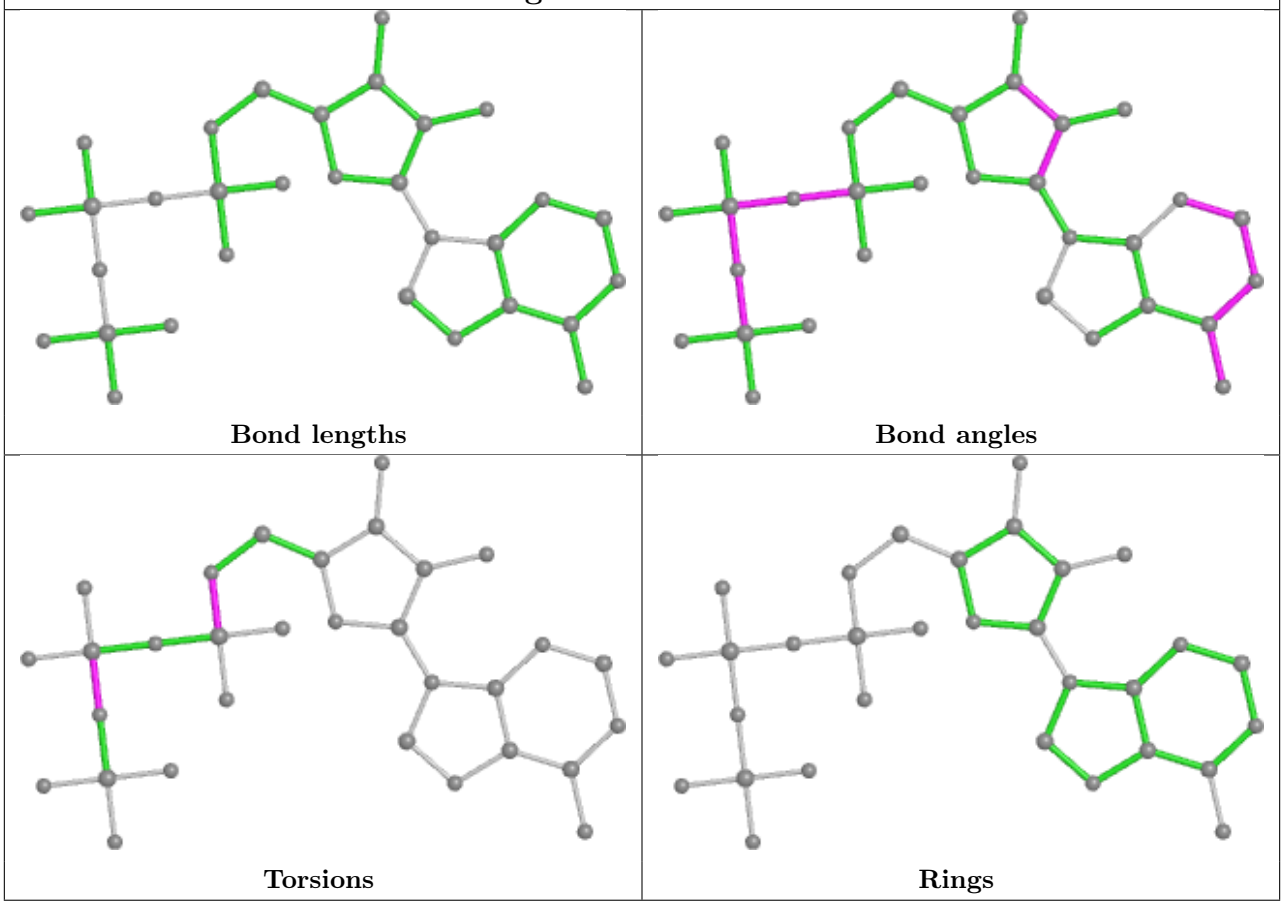
There are no ring outliers.

3 monomers are involved in 84 short contacts:

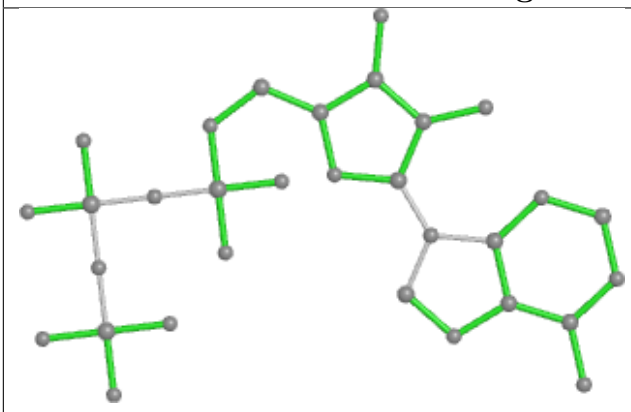
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	902	ATP	33	0
18	B	1103	ATP	19	0
20	B	1104	PX2	32	0

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.

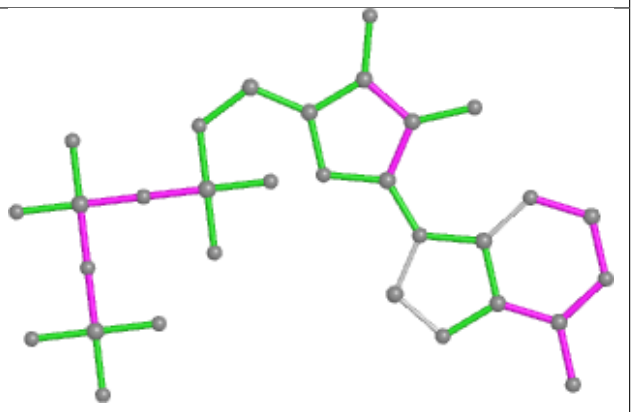
Ligand ATP A 902



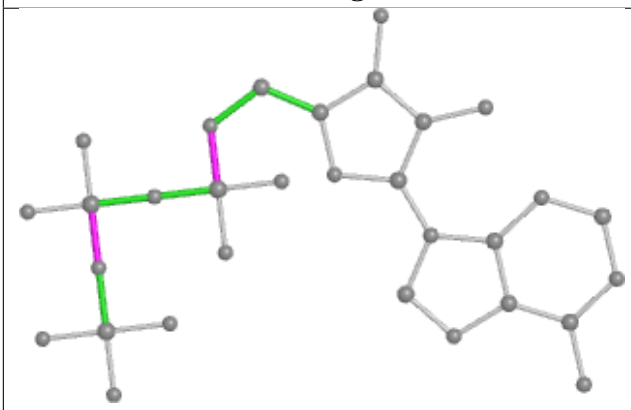
Ligand ATP B 1103



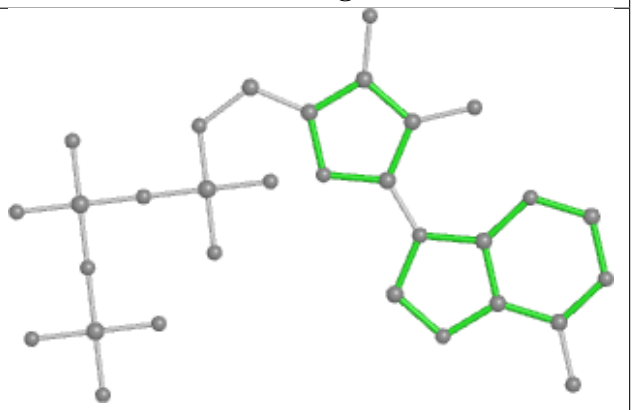
Bond lengths



Bond angles

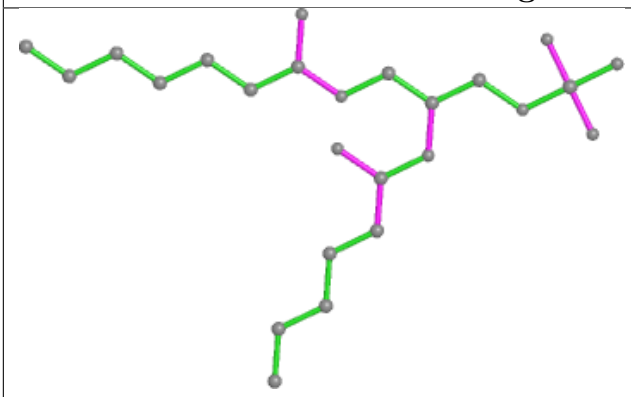


Torsions

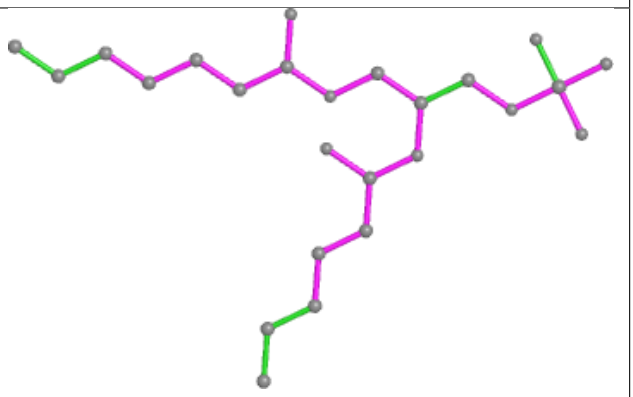


Rings

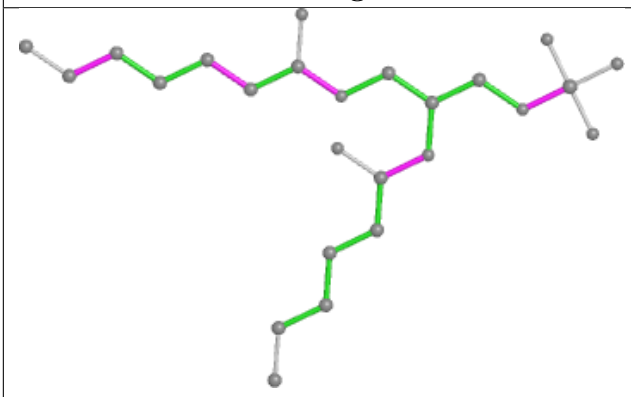
Ligand PX2 B 1104



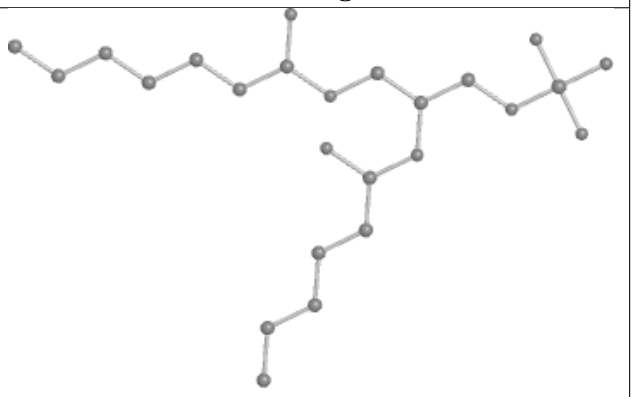
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

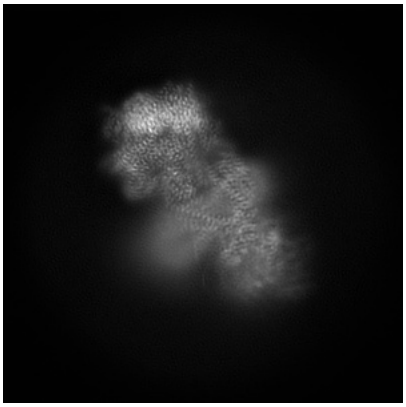
6 Map visualisation

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

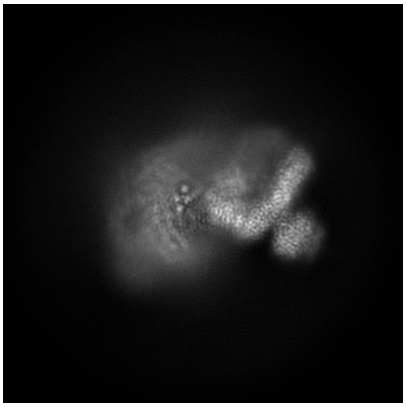
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

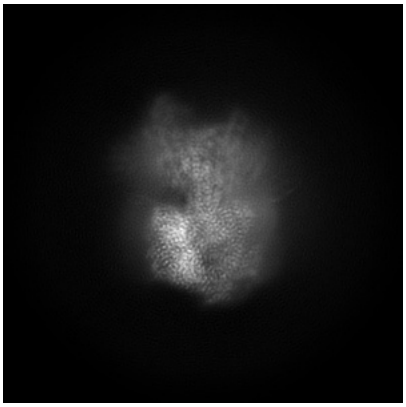
6.1.1 Primary map



X



Y

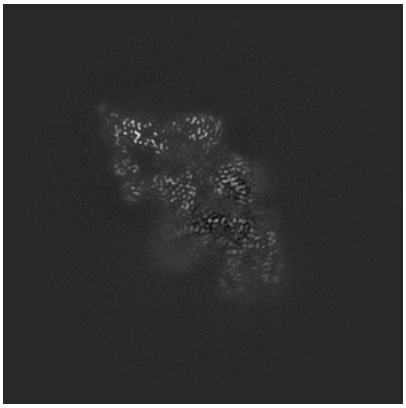


Z

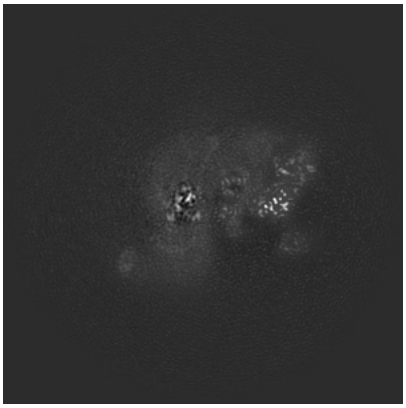
The images above show the map projected in three orthogonal directions.

6.2 Central slices

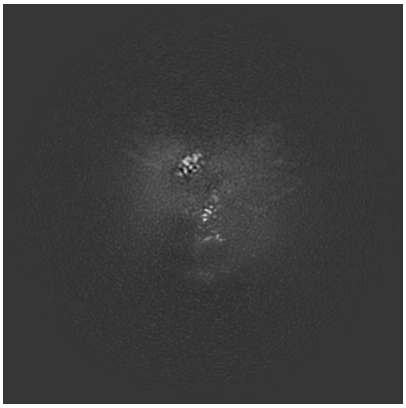
6.2.1 Primary map



X Index: 180



Y Index: 180

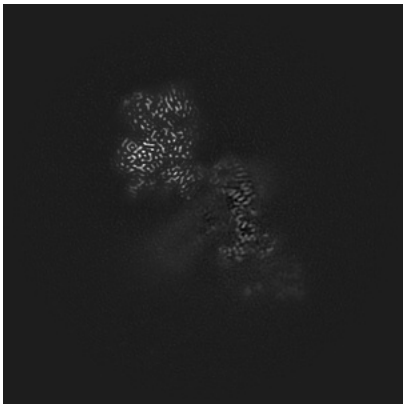


Z Index: 180

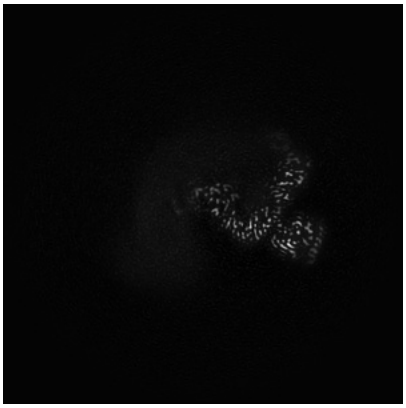
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

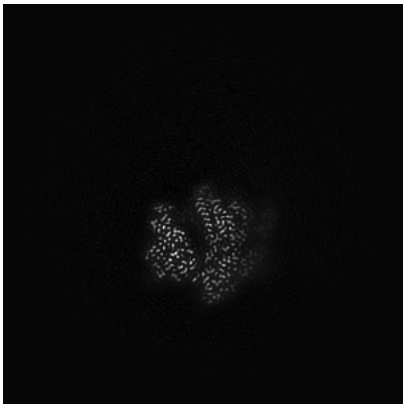
6.3.1 Primary map



X Index: 163



Y Index: 156

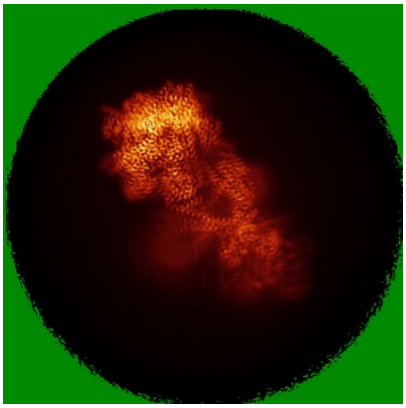


Z Index: 254

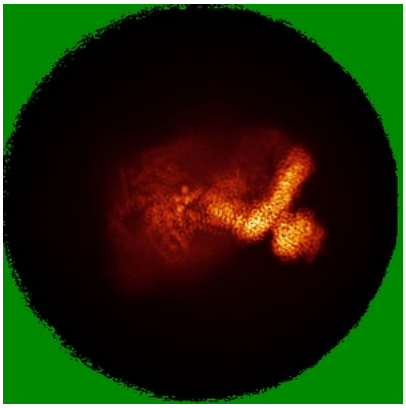
The images above show the largest variance slices of the map in three orthogonal directions.

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

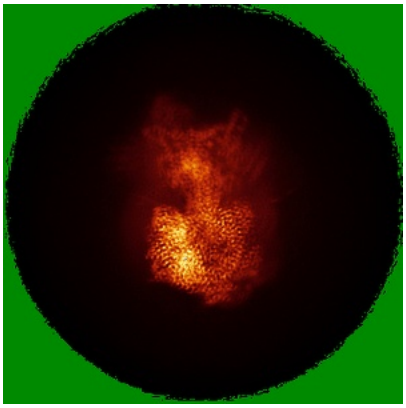
6.4.1 Primary map



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.

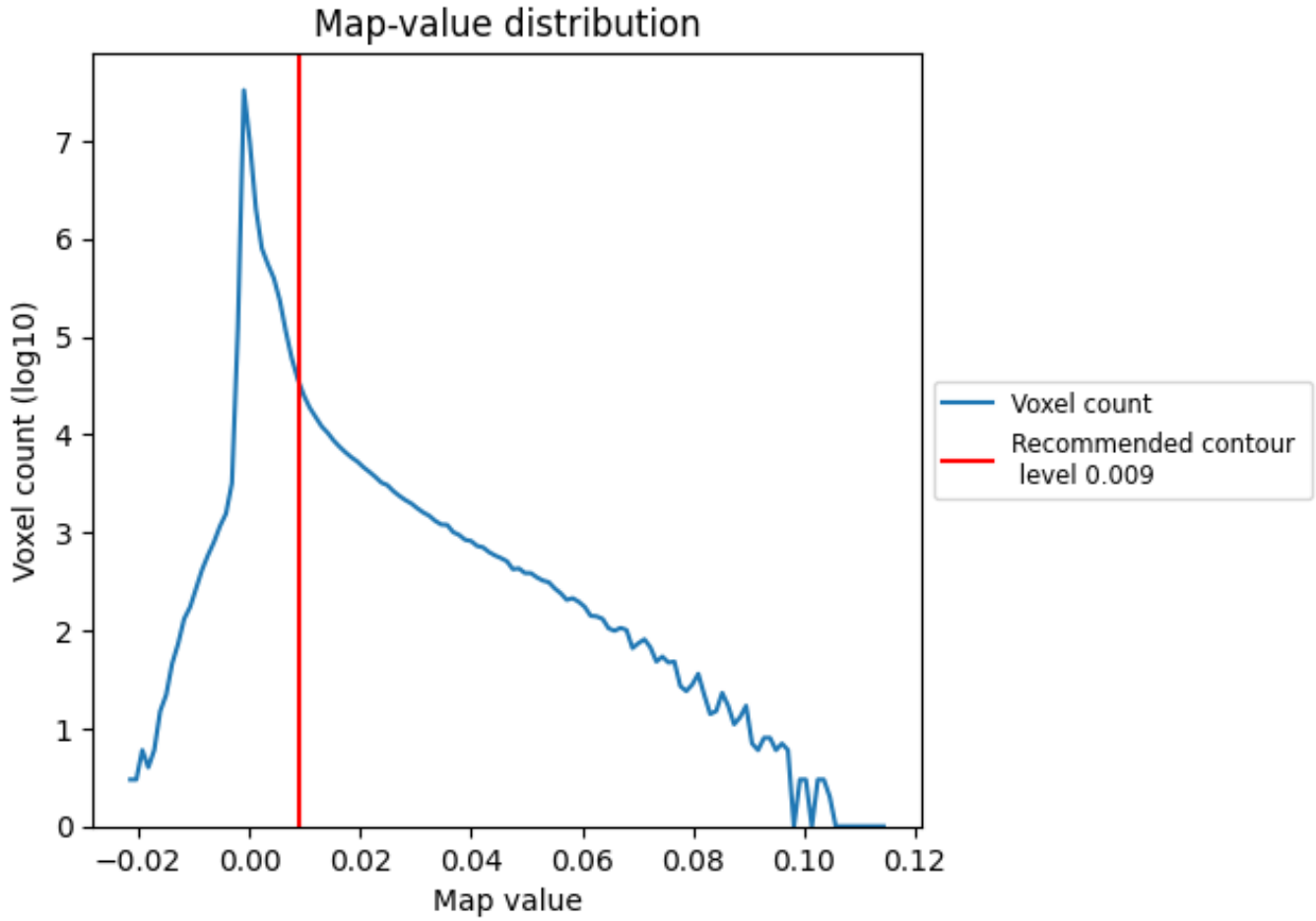
6.6 Mask visualisation (i)

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

7 Map analysis

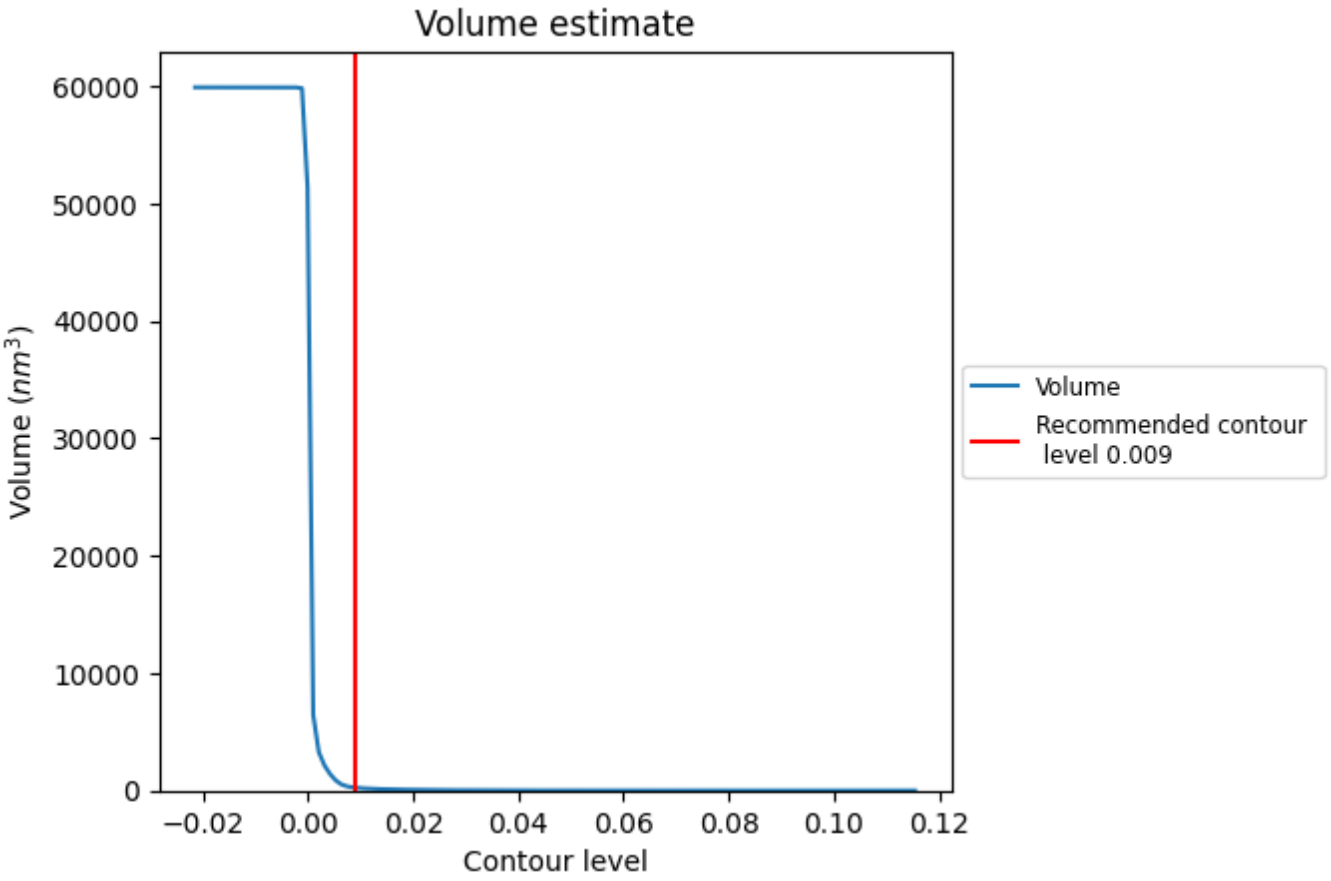
This section contains the results of statistical analysis of the map.

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.

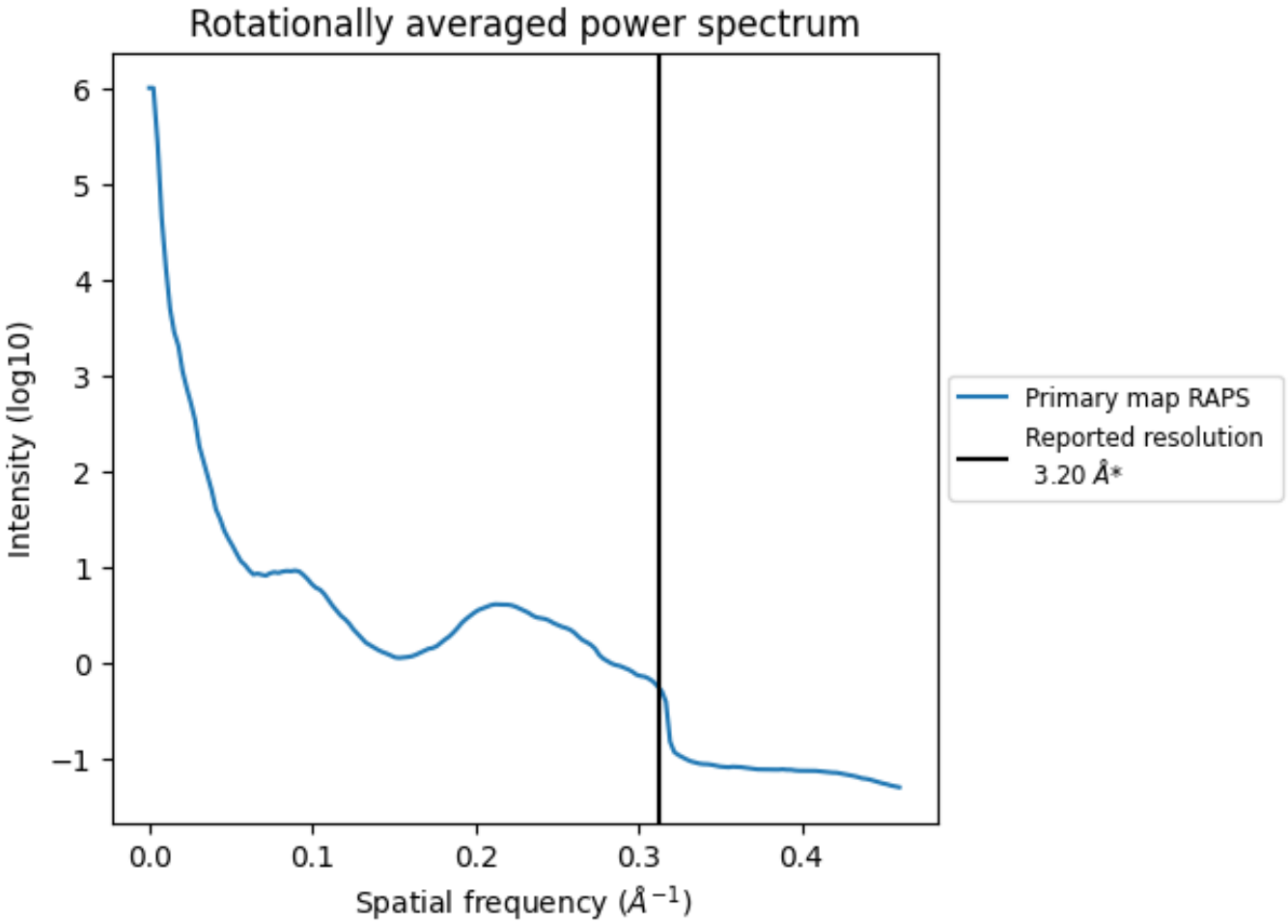
7.2 Volume estimate



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 $Å^{-1}$

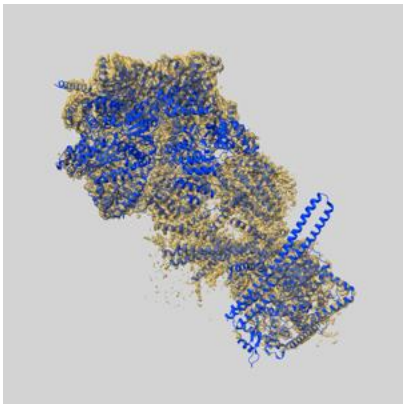
8 Fourier-Shell correlation

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

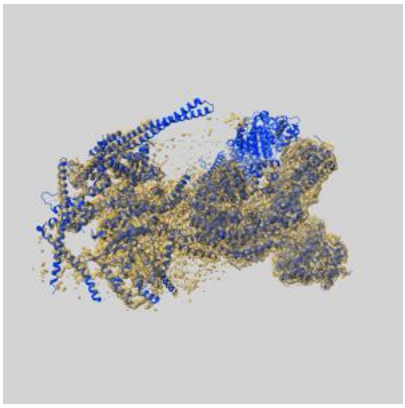
9 Map-model fit

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.

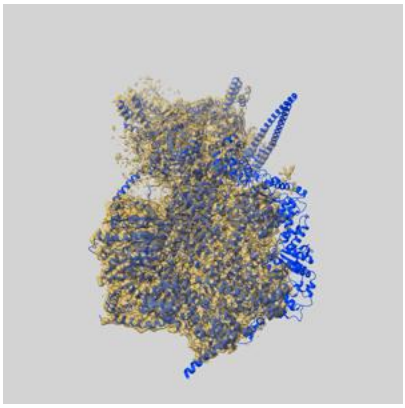
9.1 Map-model overlay



X



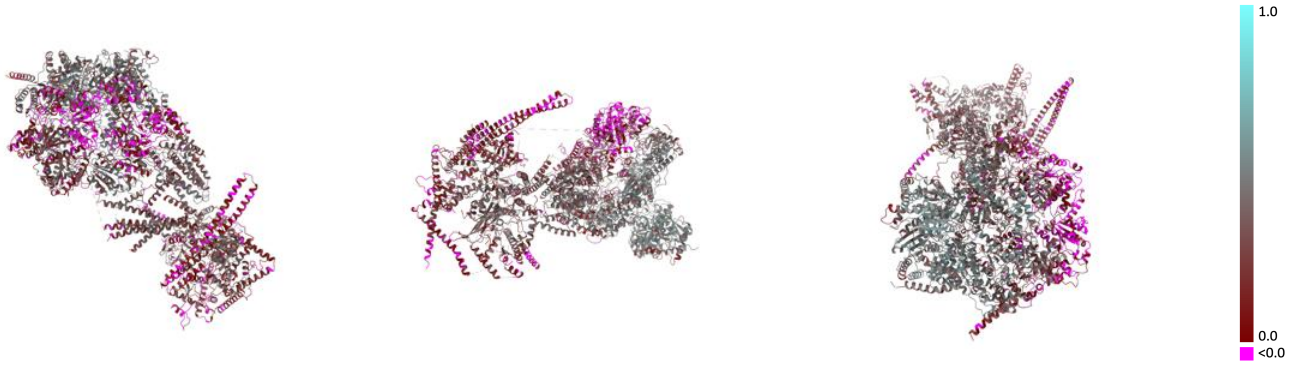
Y



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.

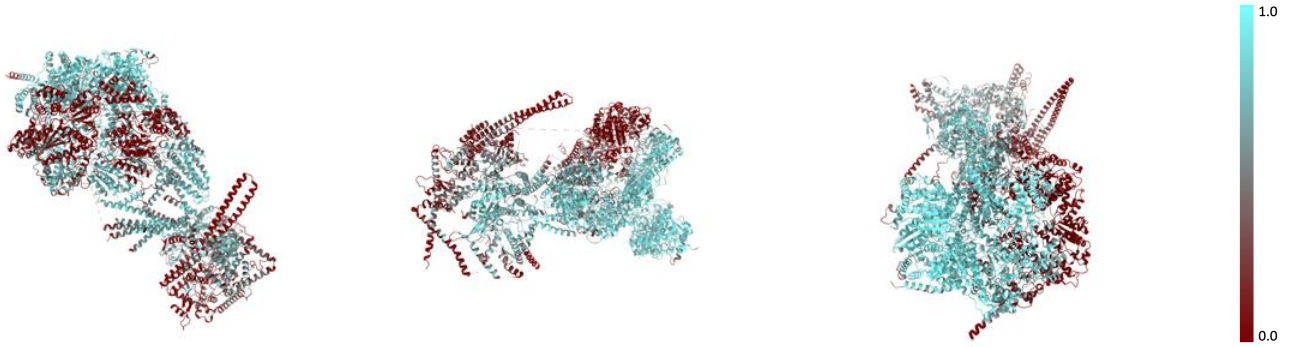
9.2 Q-score mapped to coordinate model (i)



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.

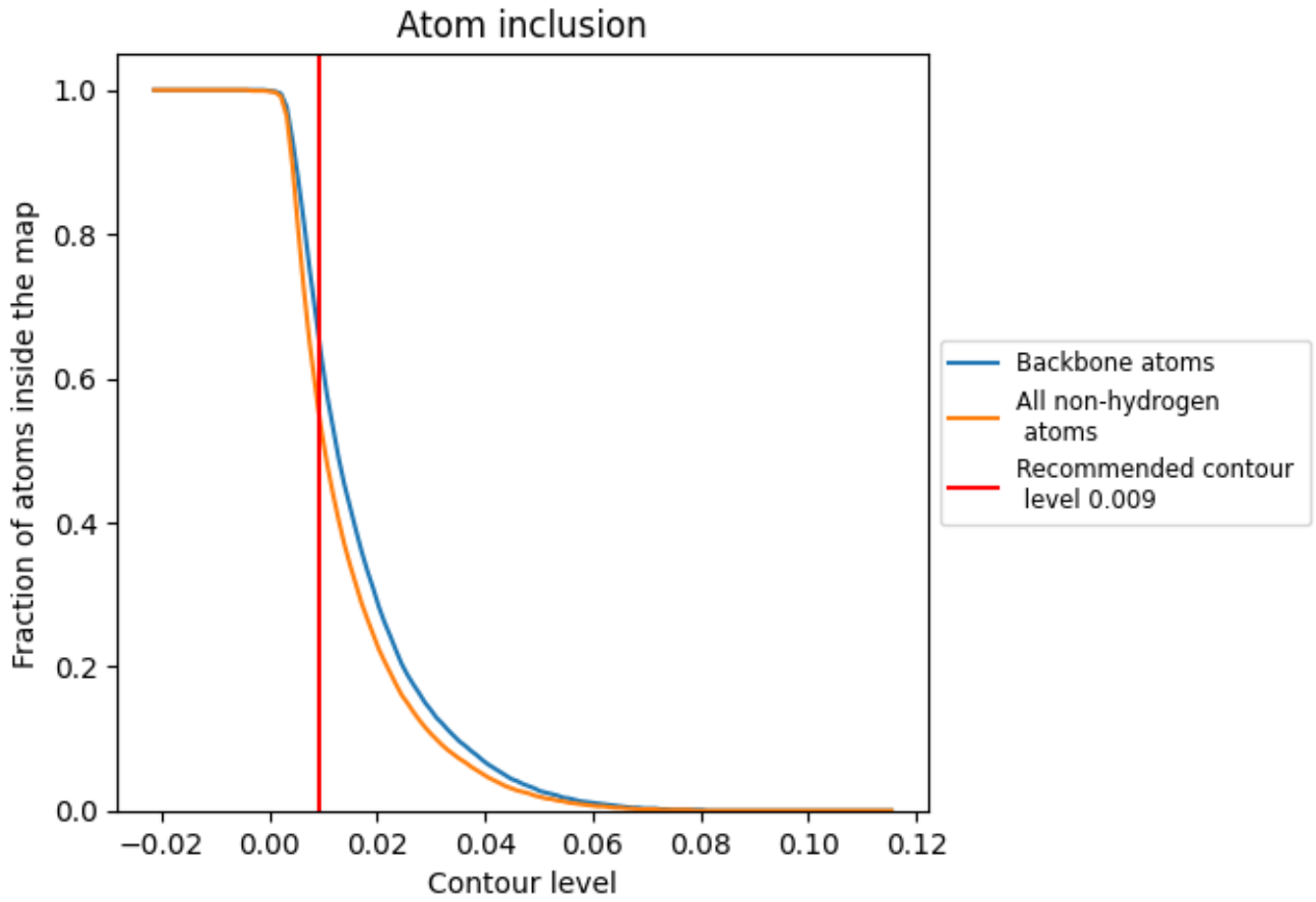
9.3 Atom inclusion mapped to coordinate model (i)



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