Full wwPDB EM Validation Report

Nov 10, 2024 – 10:19 PM EST

PDB ID	:	8TEU
EMDB ID	:	EMD-41202
Title	:	Human cytomegalovirus portal vertex, non-infectious enveloped particle (NIEP) configuration 2 - inverted (NC2-inv)
Authors	:	Jih, J.; Liu, Y.T.; Liu, W.; Zhou, H.
Deposited on	:	2023-07-07
Resolution	:	4.01 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:

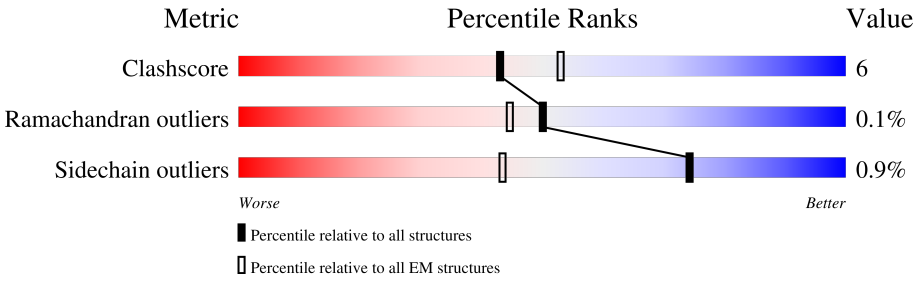
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.01 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	2241	32% 23% 9% 68%
1	C	2241	98%
2	E	642	76% 52% 24% 23%
2	F	642	13% 11% 87%
3	G	594	59% 67% 12% 21%
4	H	1370	45% 79% 16%
4	I	1370	50% 81% 17%
4	J	1370	64% 83% 12%

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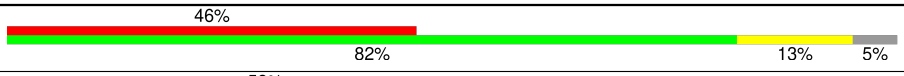
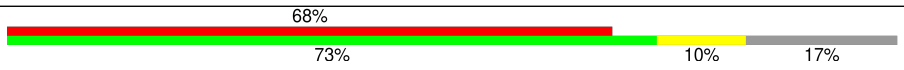
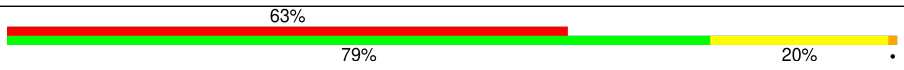
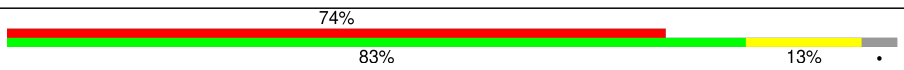
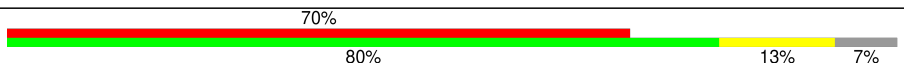
Mol	Chain	Length	Quality of chain
4	K	1370	
4	L	1370	
4	M	1370	
5	N	75	
5	O	75	
5	P	75	
5	Q	75	
5	R	75	
5	S	75	
6	T	290	
6	W	290	
7	U	306	
7	V	306	
7	X	306	
7	Y	306	
8	Z	1048	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 96759 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 Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	722	Total	C	N	O	S	0	0
			5830	3723	1027	1058	22		
1	C	40	Total	C	N	O	S	0	0
			332	213	60	58	1		

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	495	Total	C	N	O	S	0	0
			3992	2559	706	715	12		
2	F	85	Total	C	N	O	S	0	0
			710	442	138	126	4		

- Molecule 3 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	471	Total	C	N	O	S	0	0
			3862	2416	740	692	14		

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	1309	Total	C	N	O	S	0	0
			10391	6619	1800	1911	61		
4	I	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		
4	J	1317	Total	C	N	O	S	0	0
			10433	6641	1814	1919	59		
4	K	1296	Total	C	N	O	S	0	0
			10259	6529	1787	1884	59		
4	L	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	1350	Total	C	N	O	S	0	0
			10693	6809	1853	1970	61		

- Molecule 5 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	O	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	P	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	Q	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
5	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

- Molecule 6 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	242	Total	C	N	O	S	0	0
			1939	1248	338	342	11		
6	W	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 7 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	292	Total	C	N	O	S	0	0
			2317	1489	399	411	18		
7	V	288	Total	C	N	O	S	0	0
			2292	1471	397	407	17		
7	X	295	Total	C	N	O	S	0	0
			2334	1501	402	412	19		
7	Y	285	Total	C	N	O	S	0	0
			2266	1456	387	405	18		

- Molecule 8 is a protein called Large structural phosphoprotein.

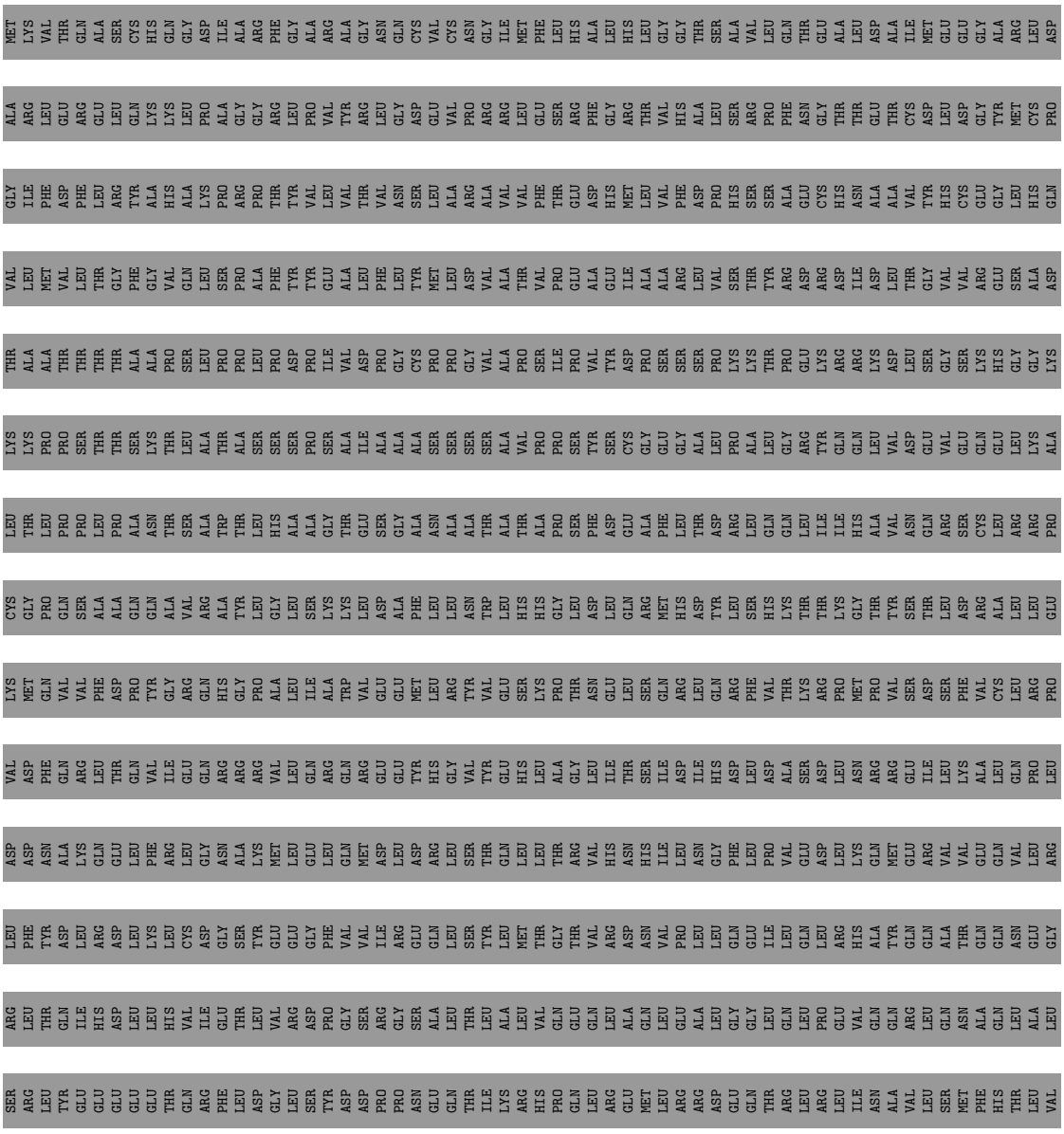
Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

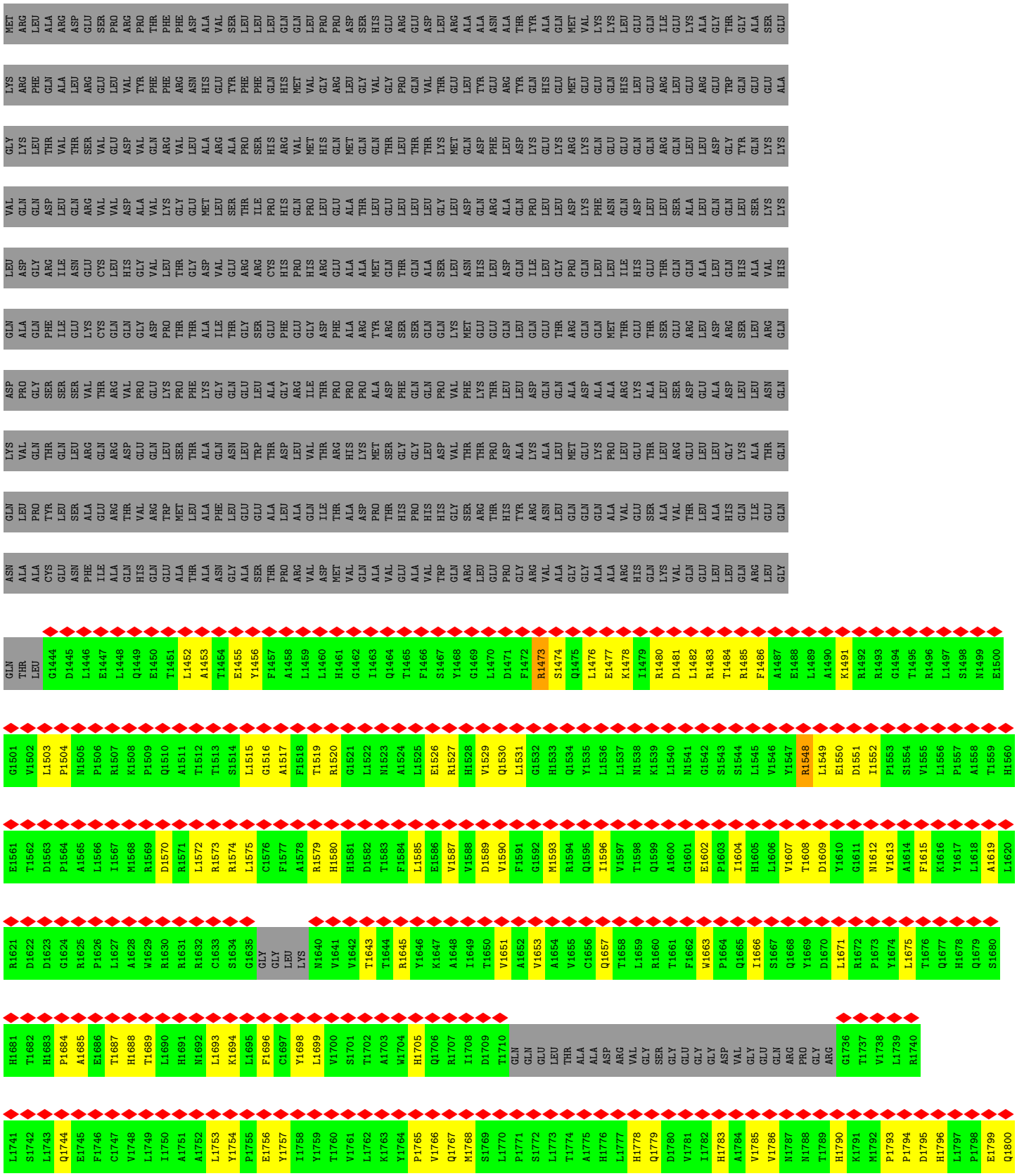
3 Residue-property plots (i)

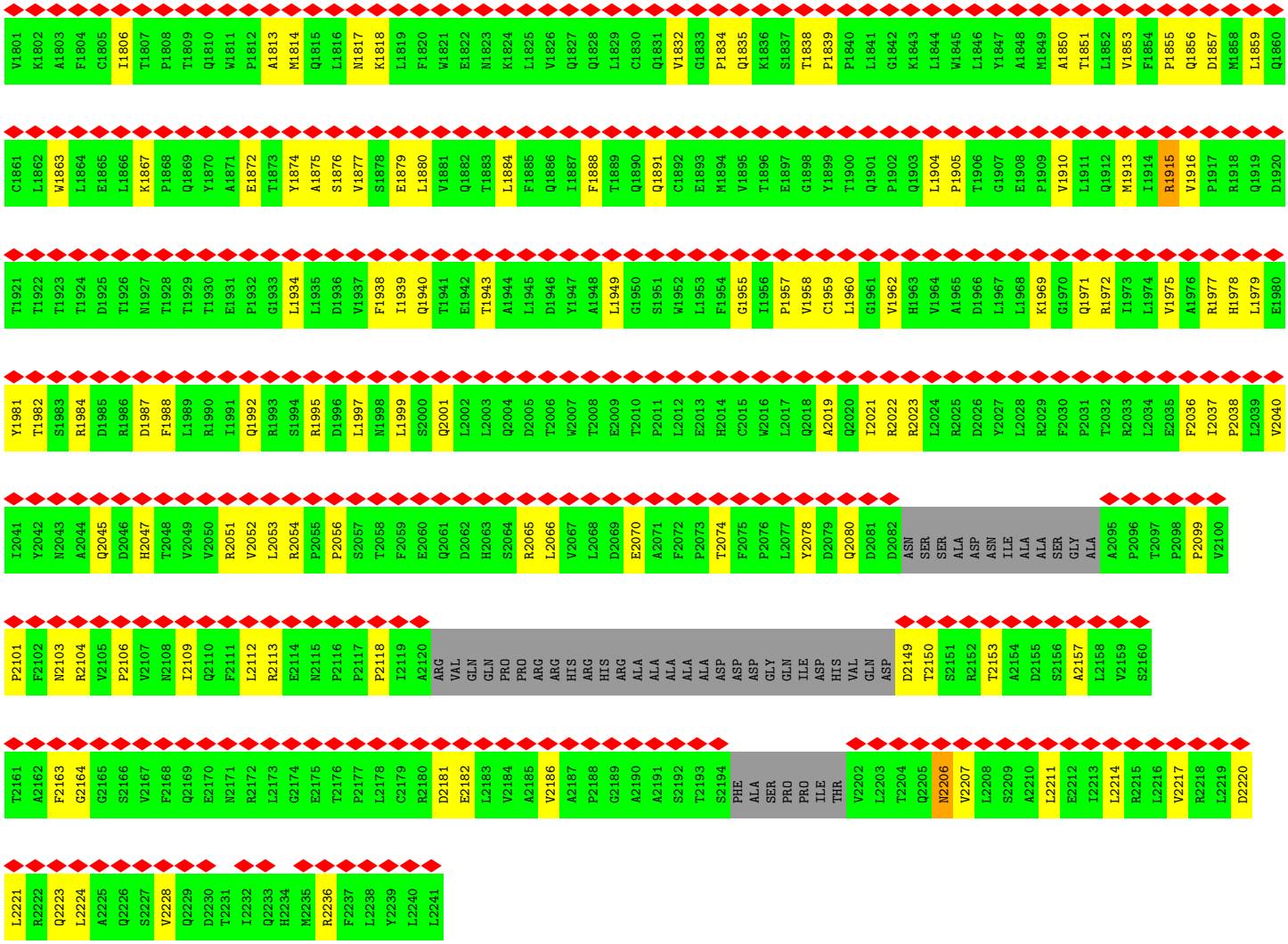
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:

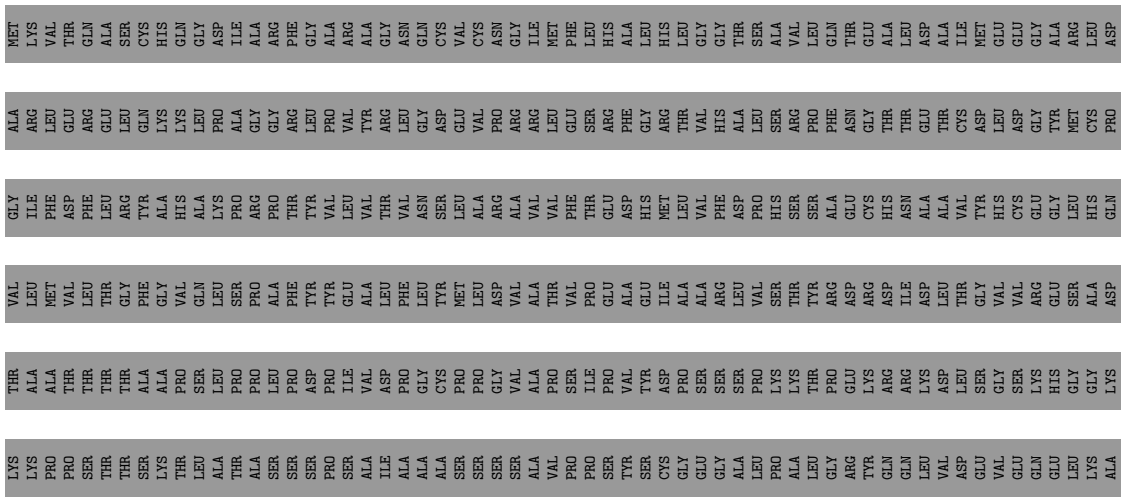


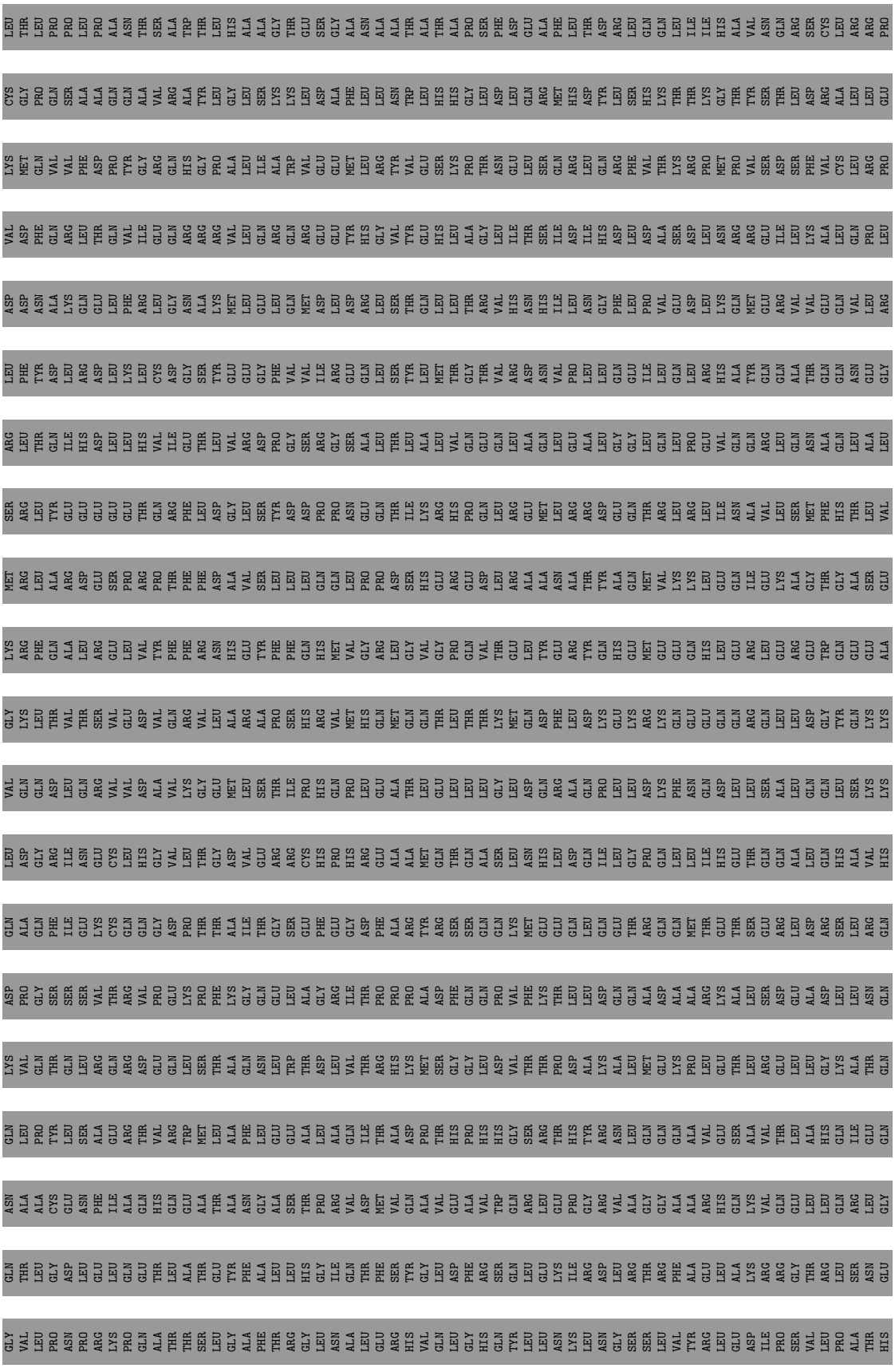

MET ARG LEU ALA ARG ASP GLU SER PRO ARG PRO THR PHE PHE ASP ALA VAL SER LEU LEU LEU GLN GLN LEU PRO PRO ASP SER HIS GLU ARG GLU ASP LEU ARG ARG ALA ALA ASN ALA THR TYR ALA GLN MET VAL LYS LYS LEU GLU GLN ILE GLU LYS ALA GLY THR GLY ALA SER GLU
LYS ARG PHE GLN ALA LEU ARG GLU LEU VAL TYR PHE PHE ARG ASN HIS GLU TYR PHE PHE HIS GLN HIS MET VAL GLY ARG LEU GLY VAL GLY PRO GLN VAL THR GLU LEU TYR GLU ARG TYR GLN HIS GLU MET GLU GLU GLN HIS LEU GLU GLN ARG LEU GLU ARG GLU TRP GLN GLU GLU ALA
GLY LYS LEU THR VAL THR SER VAL GLU ASP VAL GLN ARG VAL LEU ALA ARG ALA PRO SER HIS ARG VAL MET HIS GLN MET GLN GLN THR LEU THR THR THR LYS MET GLN ASP PHE LEU ASP LYS GLU LYS ARG GLN GLU GLN GLN ARG GLN LEU LEU ASP GLY TYR GLN GLU LYS LYS
VAL GLN GLN ASP LEU GLN ARG VAL VAL ASP ALA VAL LYS GLY GLU MET LEU SER THR ILE PRO HIS GLN PRO LEU GLU LEU LEU LEU GLY LEU ASP GLN ARG ALA GLN PRO LEU LEU ASP LYS PHE ASN GLN ASP LEU GLN LEU LEU SER ALA LEU GLN GLN LEU SER LYS LYS
LEU ASP GLY ARG ILE ASN GLU CYS LEU HIS GLY VAL LEU THR GLY ASP VAL GLU ARG ARG CYS HIS PRO HIS ARG GLU GLU ALA ALA MET GLN THR GLN LEU GLU LEU LEU GLY PRO GLN LEU ASP ILE LEU GLY PRO GLN ILE HIS GLU THR GLN ALA LEU SER LEU ASN HIS LEU ASP GLN ARG ALA GLN LEU ASP ARG SER VAL HIS
GLN ALA GLN PHE ILE GLU LYS CYS GLN GLN GLY GLY ASP PRO THR THR ALA ILE THR GLY SER GLU PHE GLU GLY ASP PHE ALA ARG TYR ARG SER SER GLN GLN LYS GLN GLU LEU GLN GLN GLU THR ARG GLN GLN MET MET THR GLU THR SER GLU ARG LEU ARG GLN
ASP PRO GLY SER SER SER VAL THR ARG VAL PRO GLU LYS PRO PHE LYS GLY GLN GLU LEU ALA GLY ARG ILE THR PRO PRO ALA ASP PHE GLN GLN PRO VAL PHE LYS THR LEU LEU ASP GLN GLN GLU THR ARG ALA ALA LEU SER ASP GLU ALA ALA ASP LEU ASN ASN
LYS VAL GLN THR GLN LEU ARG GLN ARG ASP GLU GLN LEU SER THR ALA GLN ASN LEU TRP THR ASP LEU VAL THR ARG HIS LYS MET SER GLY GLY LEU ASP VAL THR THR PRO ASP ALA LYS ALA LEU MET GLU LYS PRO LEU GLU THR LEU GLU LEU GLY LYS ALA THR GLN
GLN LEU PRO TYR LEU SER ALA GLU ARG THR VAL ARG TRP MET LEU ALA PHE LEU GLU GLU ALA LEU ALA GLN ILE THR ALA ASP PRO HIS HIS GLY SER ARG THR HIS TYR ARG ASN LEU GLN GLN GLN ALA VAL GLU SER ALA VAL THR LEU ALA HIS GLN ILE GLU GLN
ASN ALA ALA CYS GLU ASN PHE ILE ALA GLN HIS GLN GLU ALA THR ALA ALA ASN GLY ALA SER THR PRO ARG VAL ASP MET VAL GLN ALA ALA VAL GLU ALA VAL ALA PRO THR HIS TYR ARG VAL ALA GLY GLY ALA ALA ARG HIS GLN LYS VAL GLN GLU LEU LEU LEU GLN ARG LEU GLY
GLN THR LEU G1444 D1445 L1446 E1447 L1448 Q1449 E1450 T1451 L1452 A1453 T1454 E1455 Y1456 F1457 A1458 L1459 L1460 H1461 G1462 I1463 Q1464 T1465 F1466 S1467 Y1468 G1469 L1470 D1471 F1472 R1473 S1474 Q1475 L1476 E1477 K1478 I1479 R1480 D1481 L1482 R1483 T1484 R1485 F1486 A1487 E1488 L1489 A1490 K1491 R1492 R1493 G1494 T1495 R1496 L1497 S1498 N1499 E1500
G1501 V1502 L1503 P1504 N1505 P1506 R1507 K1508 P1509 Q1510 A1511 T1512 T1513 S1514 L1515 G1516 A1517 F1518 T1519 R1520 G1521 L1522 N1523 A1524 L1525 E1526 R1527 H1528 V1529 Q1530 L1531 G1532 H1533 Q1534 Y1535 L1536 L1537 N1538 K1539 L1540 N1541 G1542 S1543 S1544 L1545 V1546 Y1547 R1548 L1549 E1550 D1551 I1552 P1553 S1554 V1555 L1556 P1557 A1558 T1559 H1560
E1561 T1562 D1563 P1564 A1565 L1566 I1567 M1568 R1569 D1570 R1571 L1572 R1573 R1574 L1575 C1576 F1577 A1578 R1579 H1580 H1581 D1582 T1583 F1584 L1585 E1586 V1587 V1588 D1589 V1590 F1591 G1592 M1593 R1594 Q1595 I1596 V1597 T1598 Q1599 A1600 G1601 E1602 P1603 I1604 H1605 L1606 V1607 T1608 D1609 Y1610 G1611 N1612 V1613 A1614 F1615 K1616 Y1617 L1618 A1619 L1620
R1621 D1622 D1623 G1624 R1625 P1626 L1627 A1628 W1629 R1630 R1631 R1632 C1633 S1634 G1635 GLY GLY LEU LYS N1640 V1641 V1642 T1643 T1644 R1645 Y1646 K1647 A1648 I1649 T1650 V1651 A1652 V1653 A1654 V1655 C1656 Q1657 T1658 L1659 R1660 T1661 F1662 W1663 P1664 Q1665 I1666 S1667 Q1668 Y1669 D1670 L1671 R1672 P1673 Y1674 L1675 T1676 Q1677 H1678 Q1679 S1680
H1681 T1682 H1683 P1684 A1685 E1686 T1687 H1688 T1689 L1690 H1691 N1692 L1693 K1694 L1695 F1696 C1697 Y1698 L1699 V1700 S1701 T1702 A1703 W1704 H1705 Q1706 R1707 I1708 D1709 T1710 GLN GLU LEU THR ALA ALA ASP ARG VAL GLY SER GLY GLU GLY GLY GLY ASP VAL GLY GLU GLN ARG PRO GLY ARG G1736 T1737 V1738 L1739 R1740
L1741 S1742 L1743 Q1744 E1745 F1746 C1747 V1748 L1749 I1750 A1751 A1752 L1753 Y1754 P1755 E1756 Y1757 I1758 Y1759 T1760 V1761 L1762 K1763 Y1764 P1765 V1766 Q1767 M1768 S1769 L1770 P1771 S1772 L1773 T1774 A1775 H1776 L1777 H1778 Q1779 D1780 V1781 I1782 H1783 A1784 V1785 V1786 N1787 N1788 T1789 H1790 K1791 M1792 P1793 P1794 D1795 H1796 L1797 P1798 E1799 Q1800

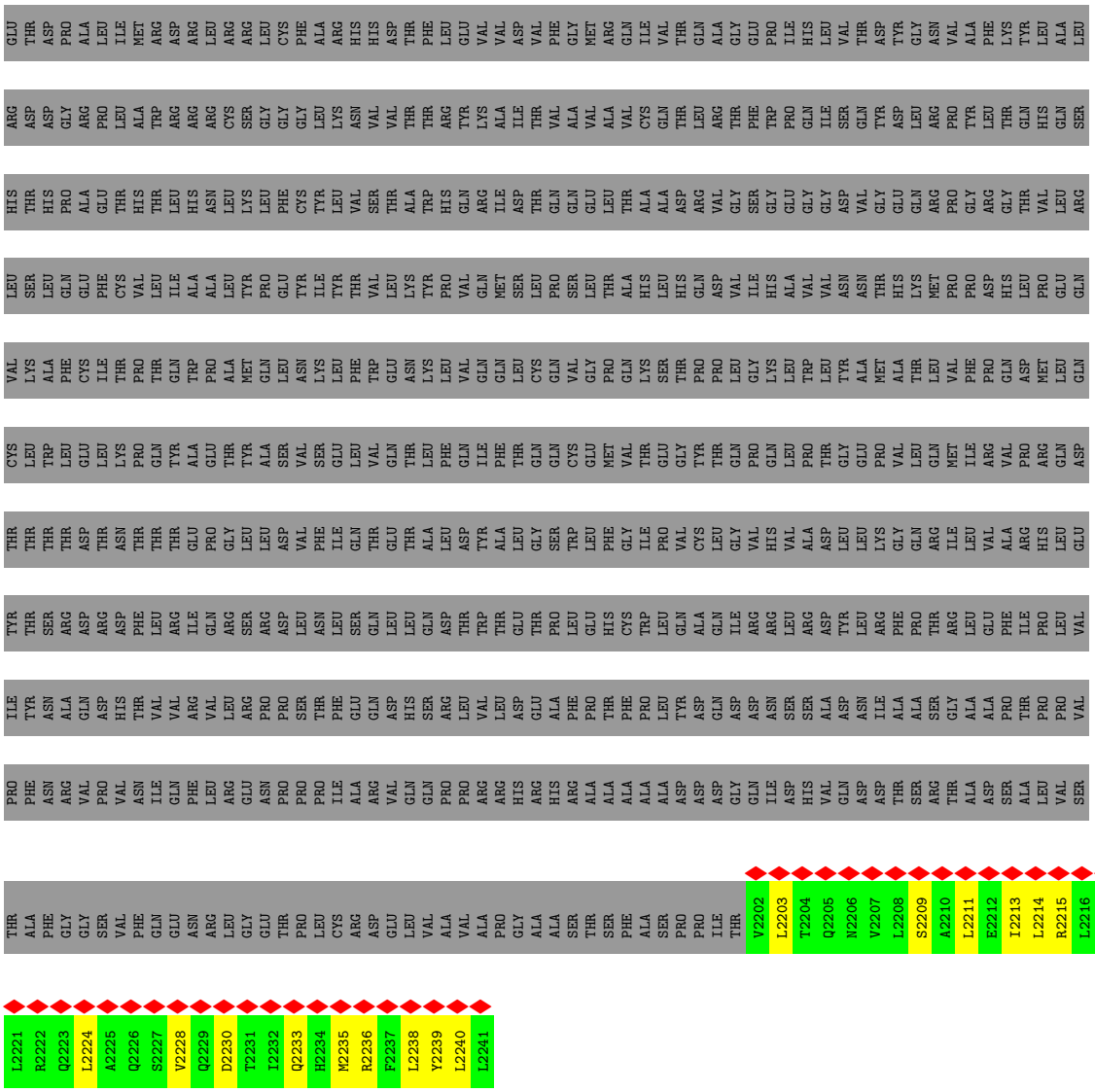


• Molecule 1: Large tegument protein deneddylase

Chain C: 98%




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



• Molecule 2: Capsid vertex component 2

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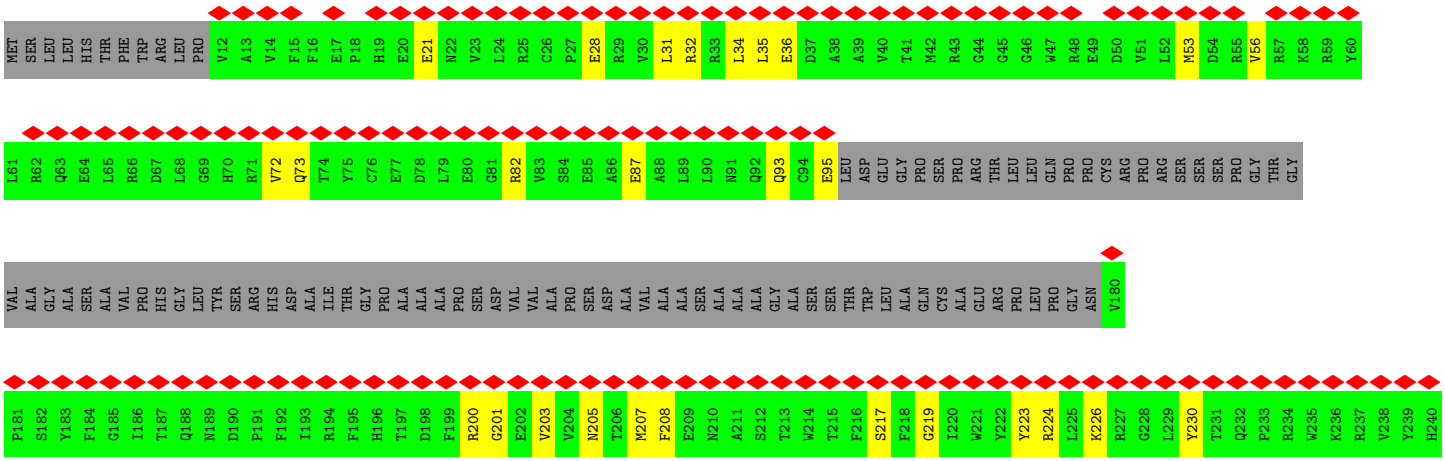

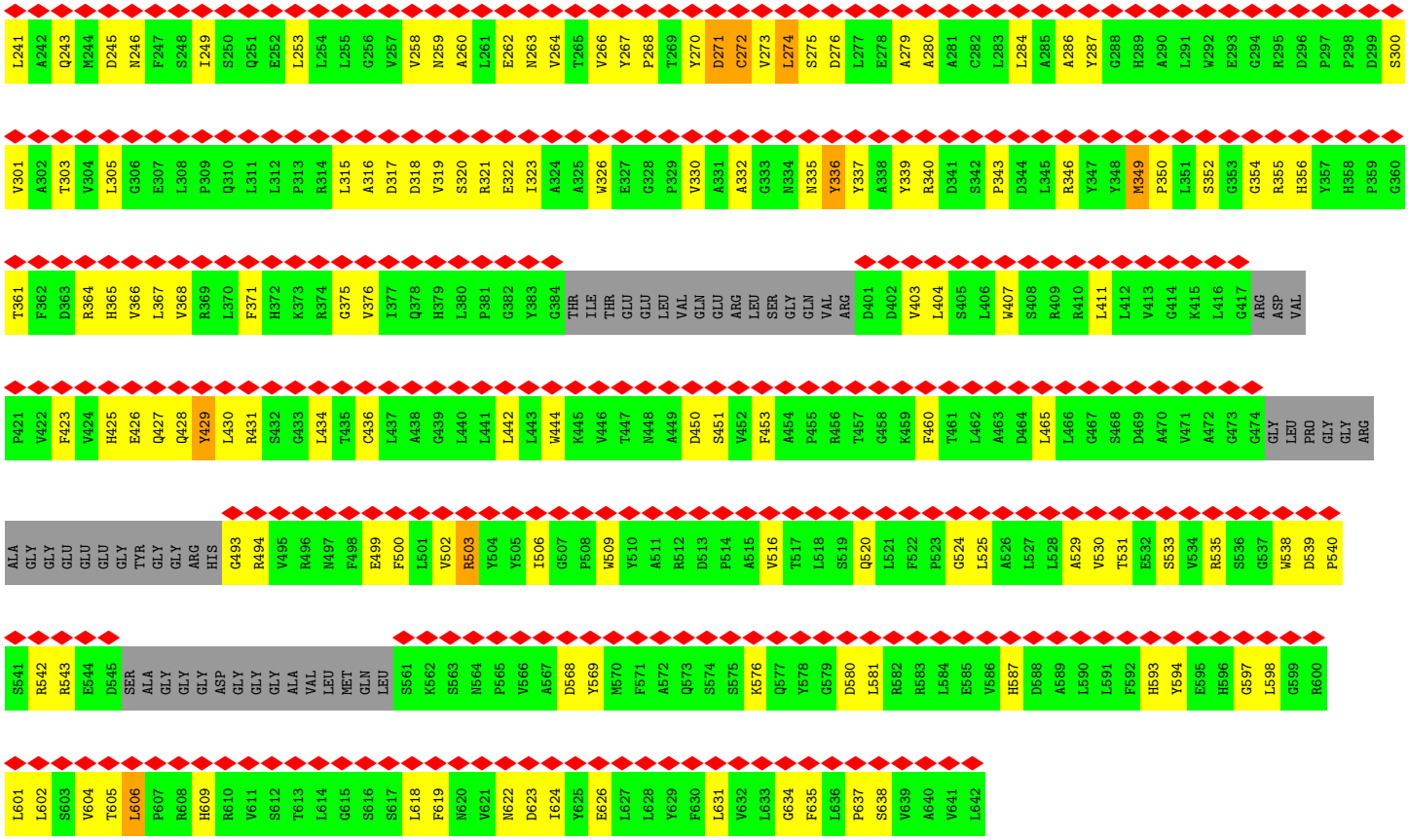

• Molecule 2: Capsid vertex component 2

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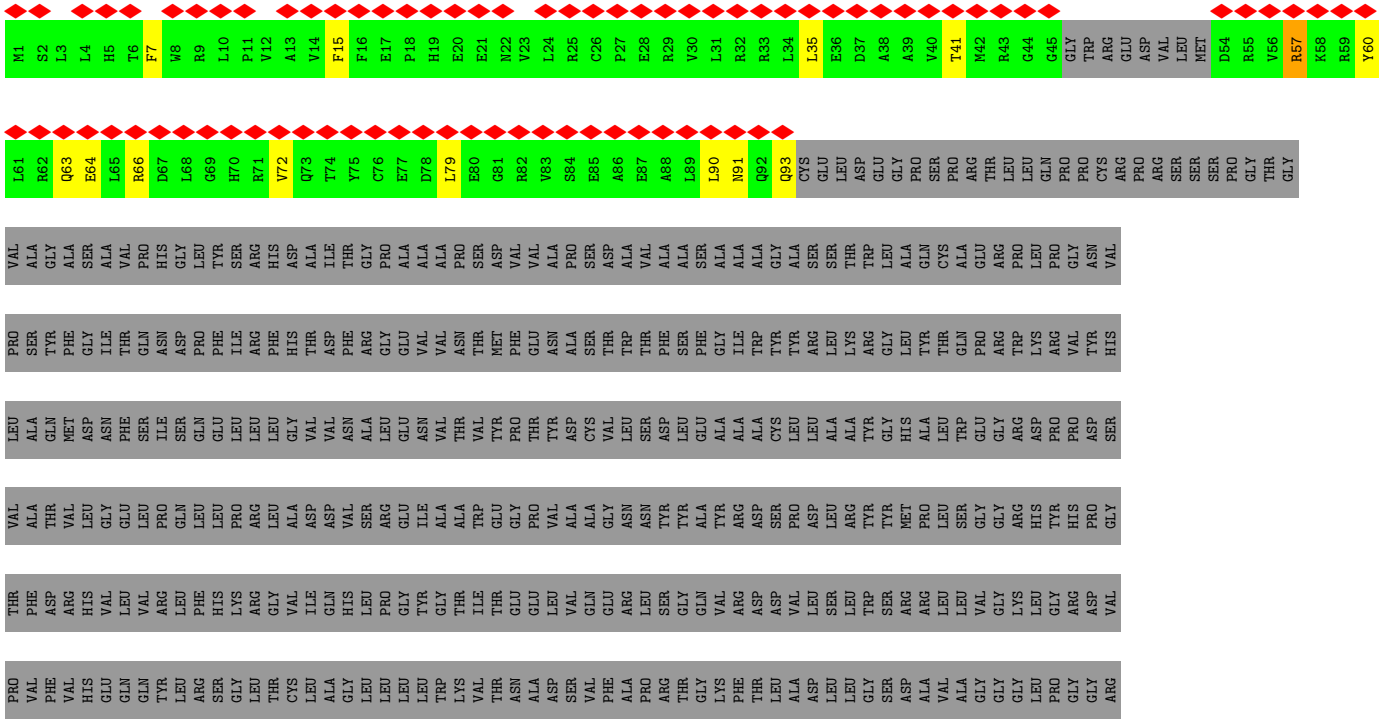

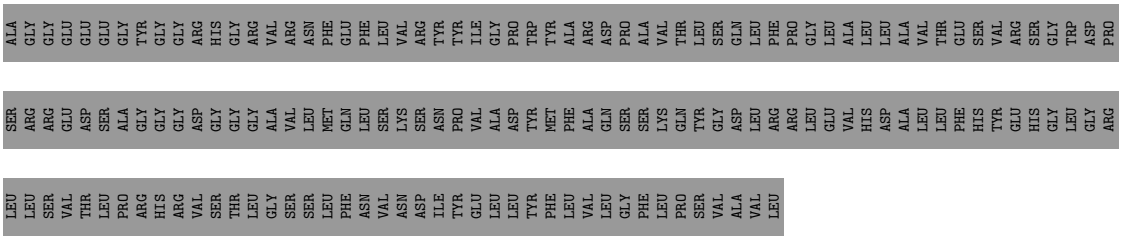

• Molecule 3: Capsid vertex component 1

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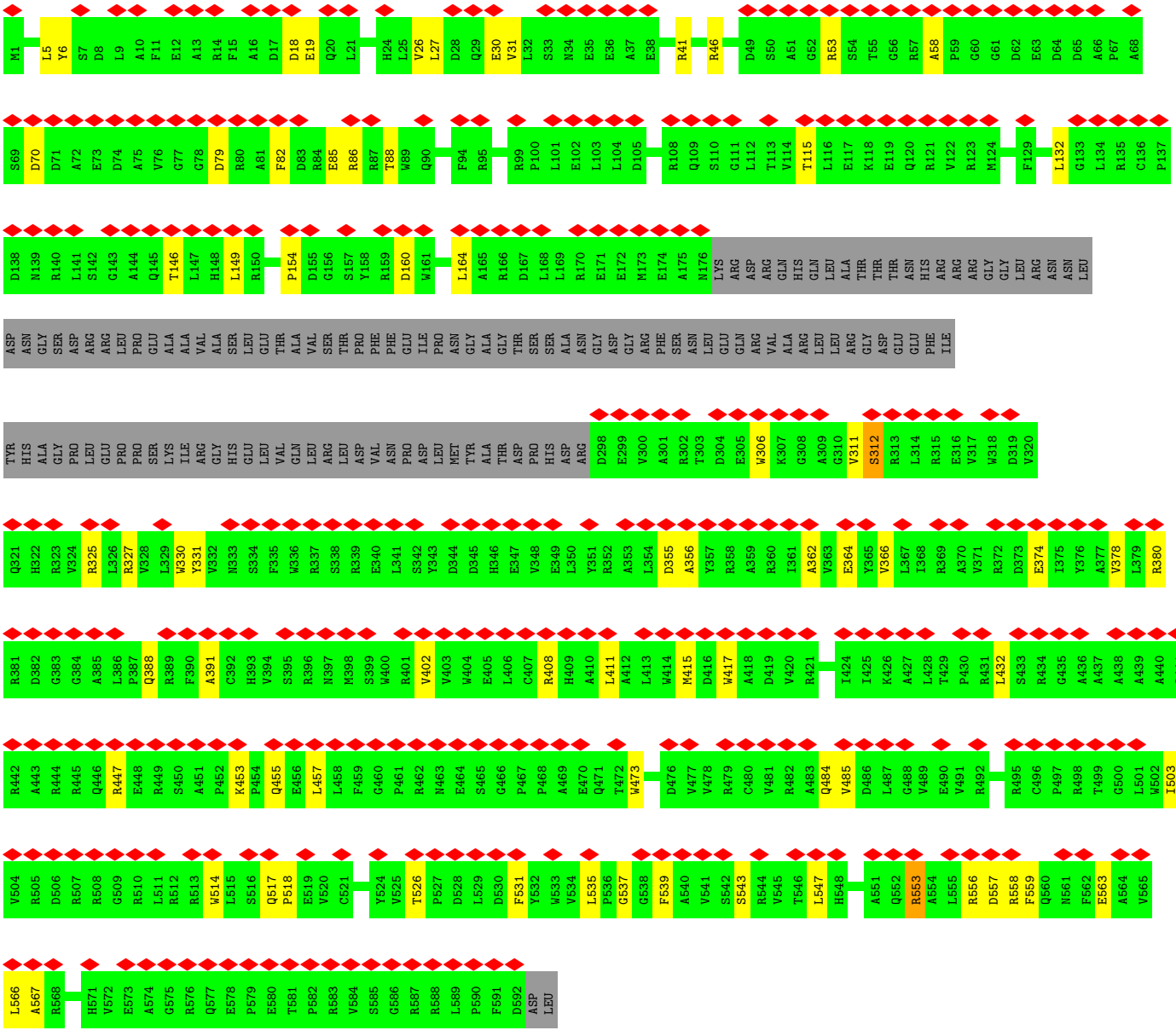

• Molecule 4: Major capsid protein

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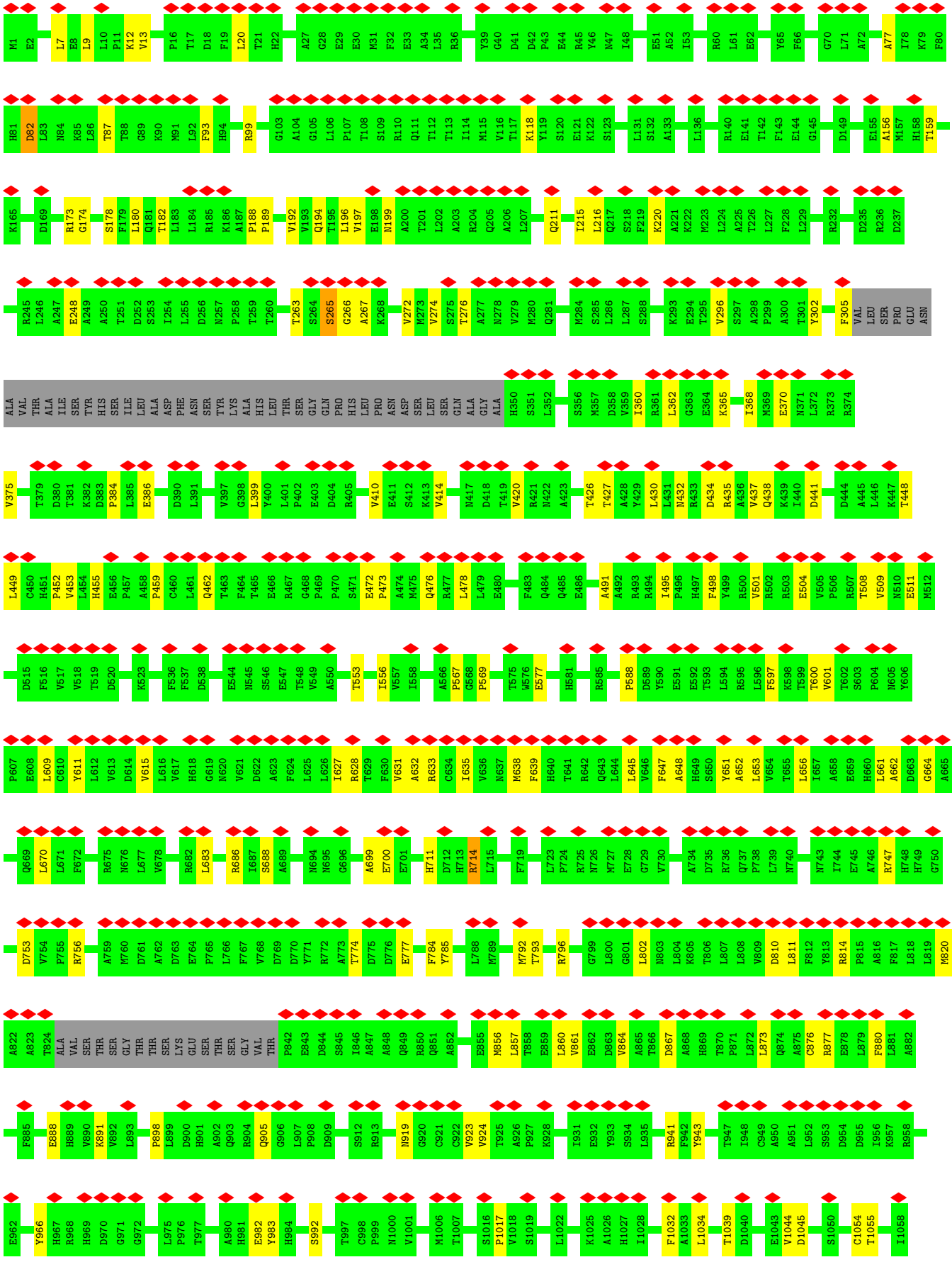
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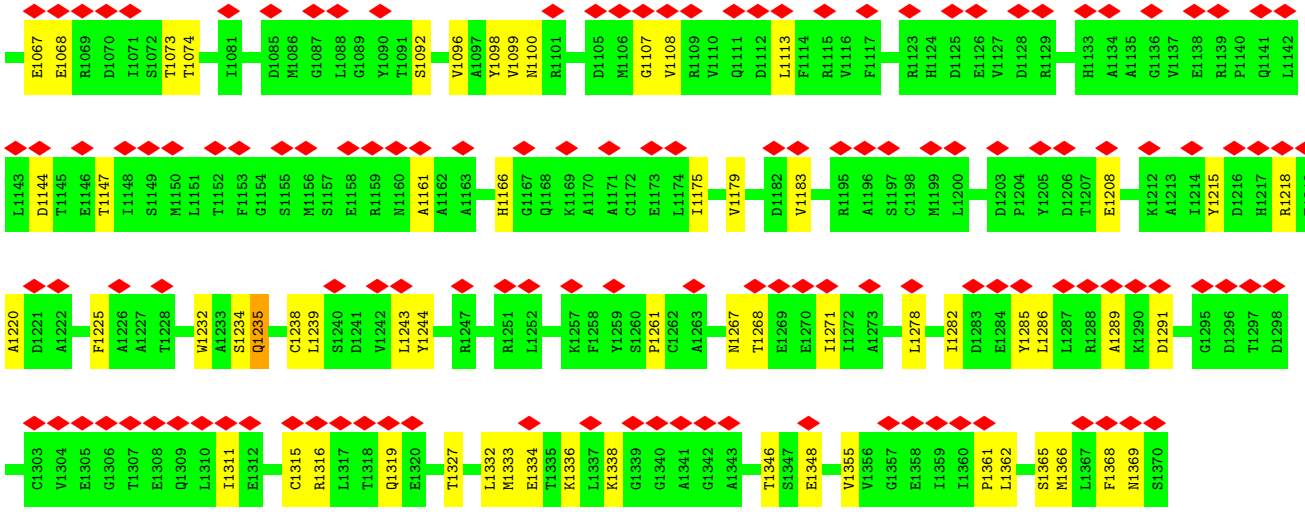

• Molecule 4: Major capsid protein

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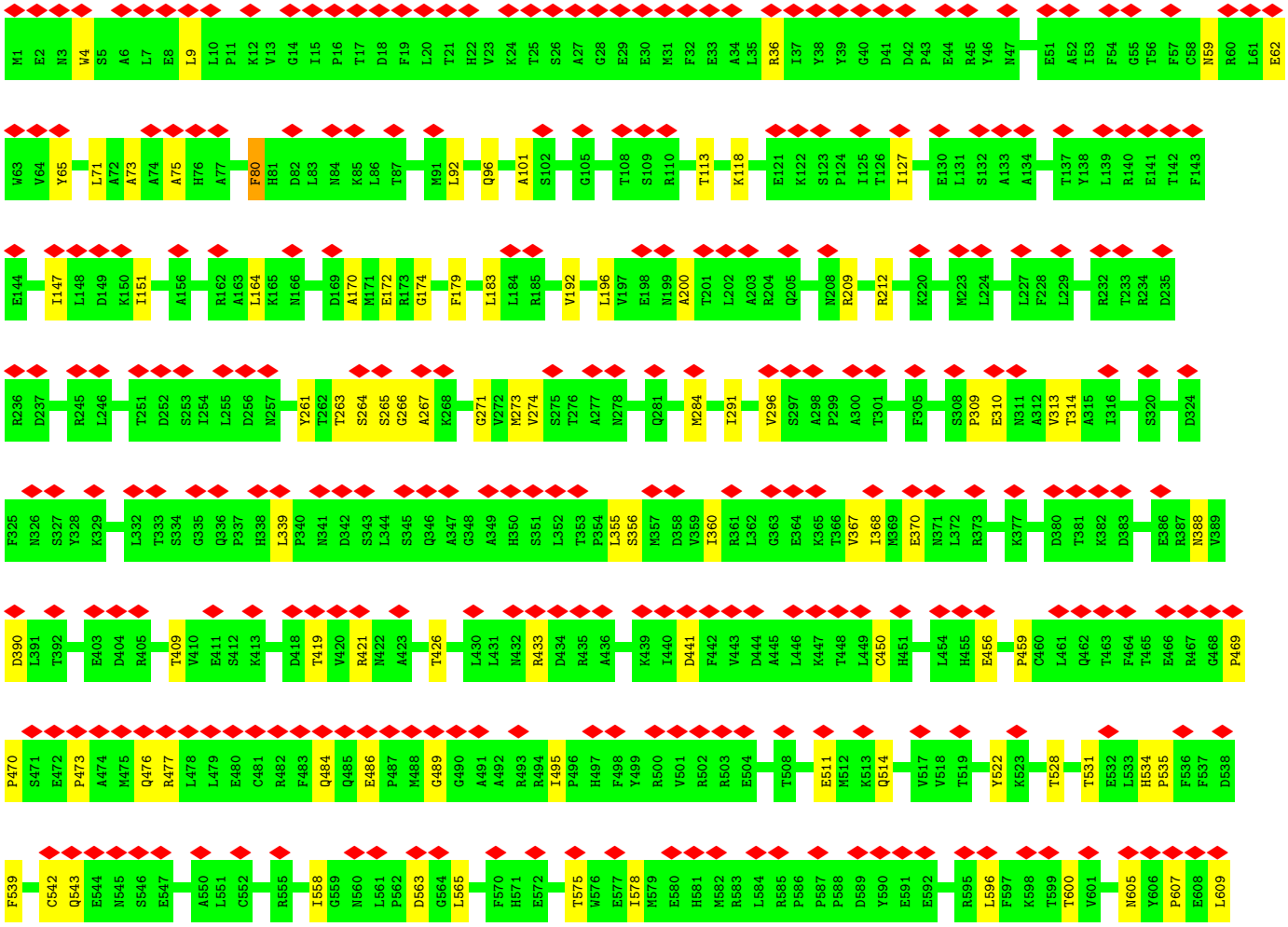

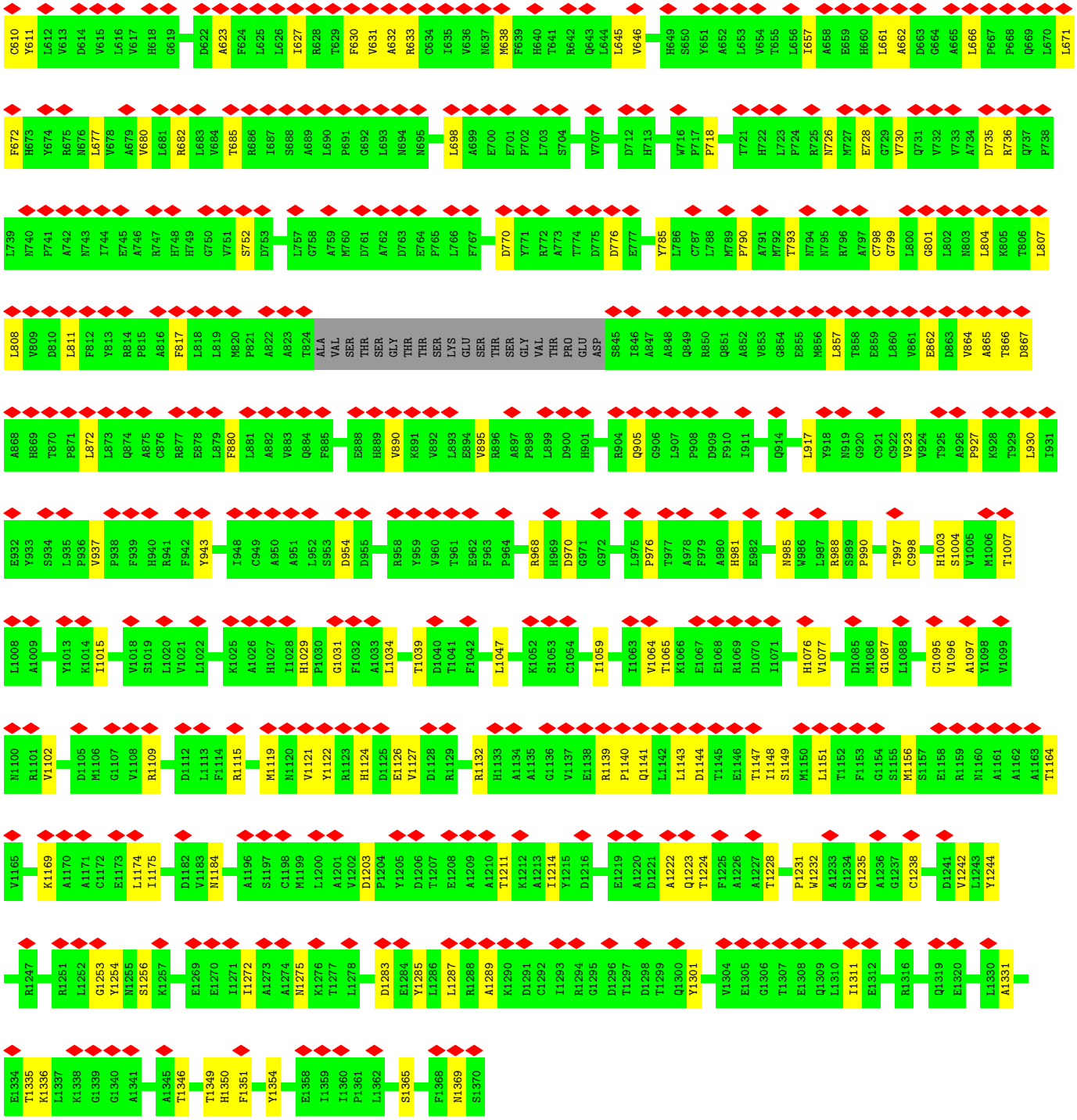

- Molecule 4: Major capsid protein

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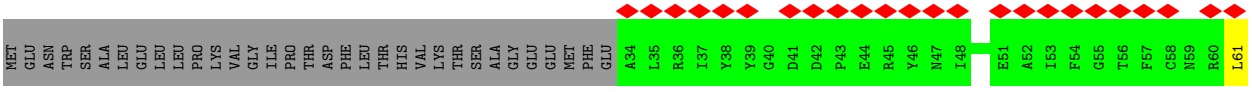

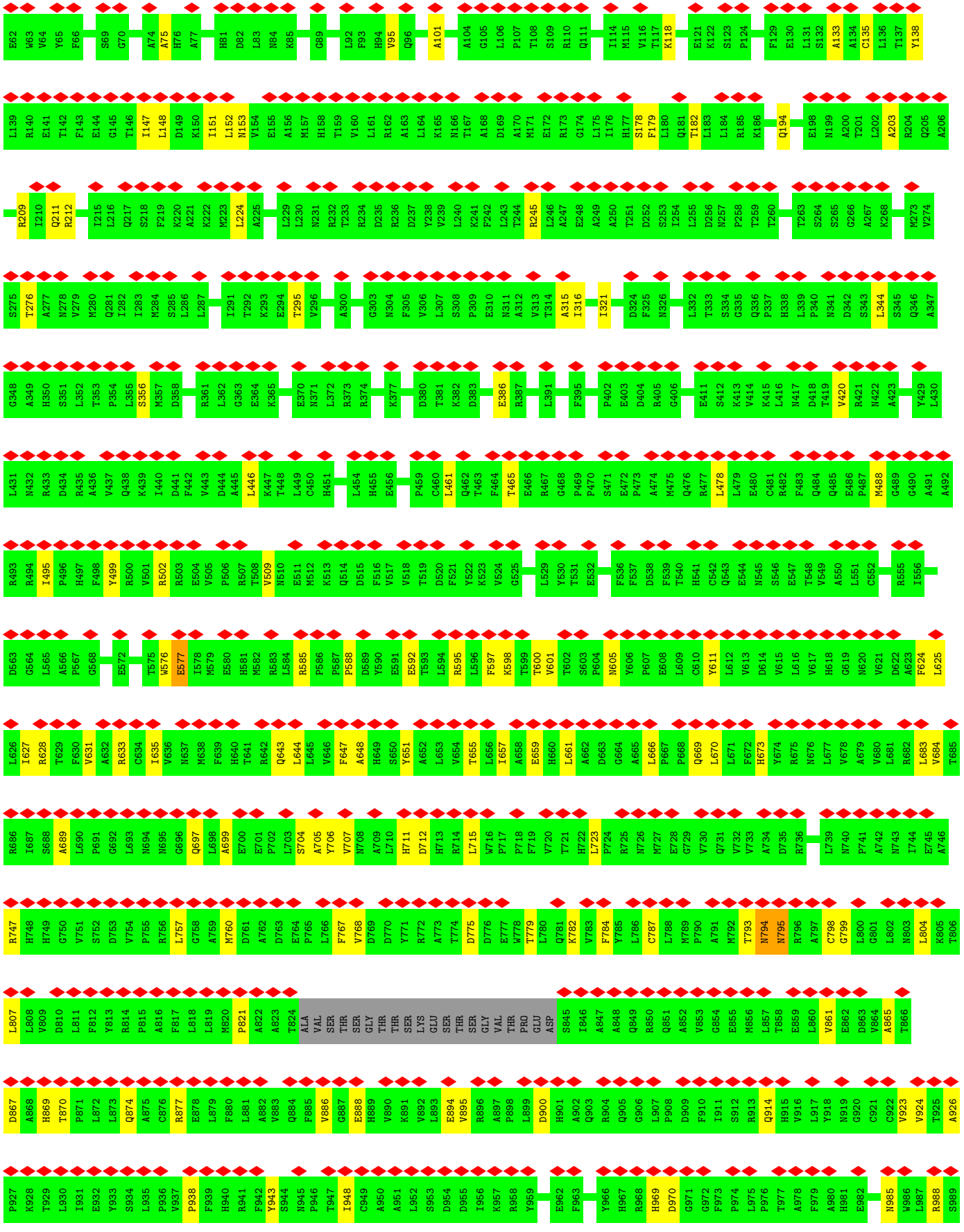
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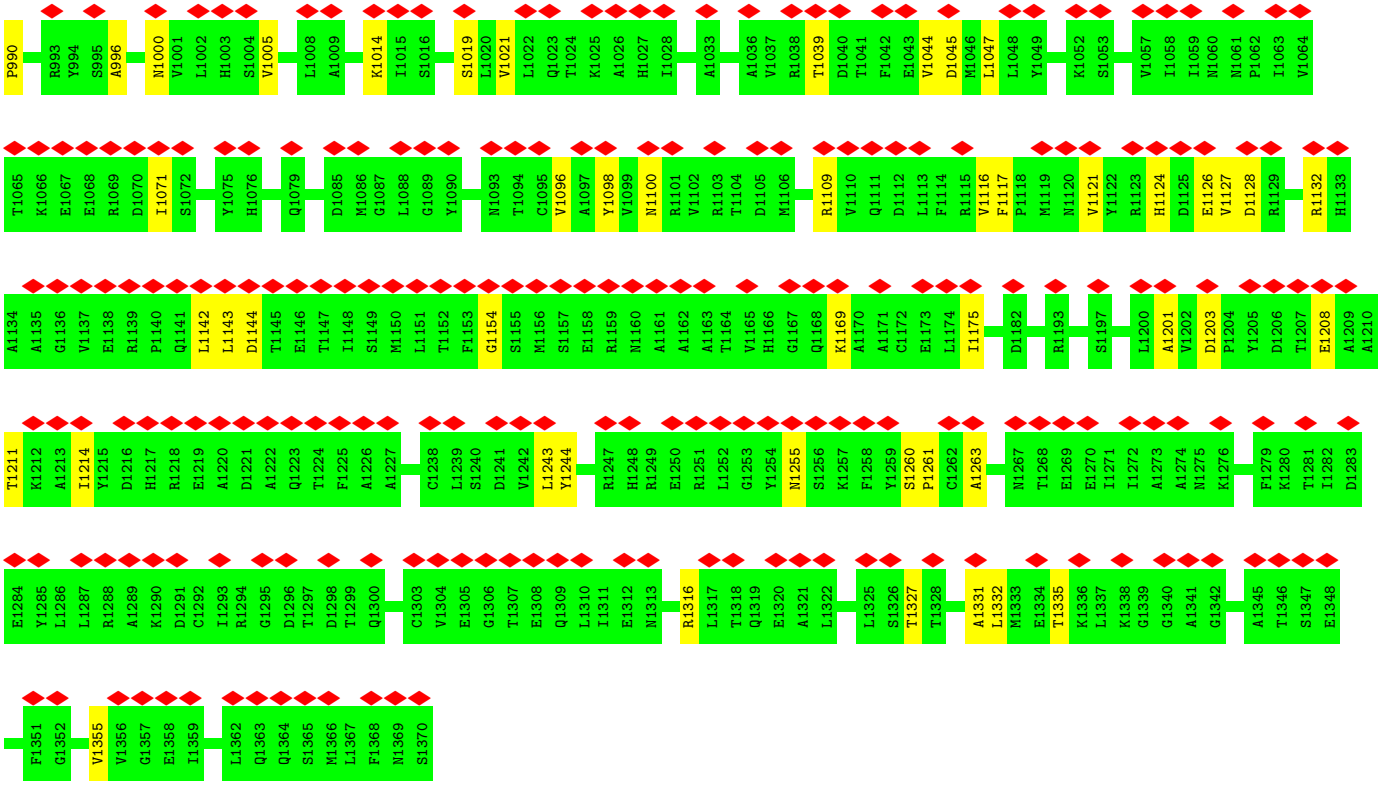

• Molecule 4: Major capsid protein

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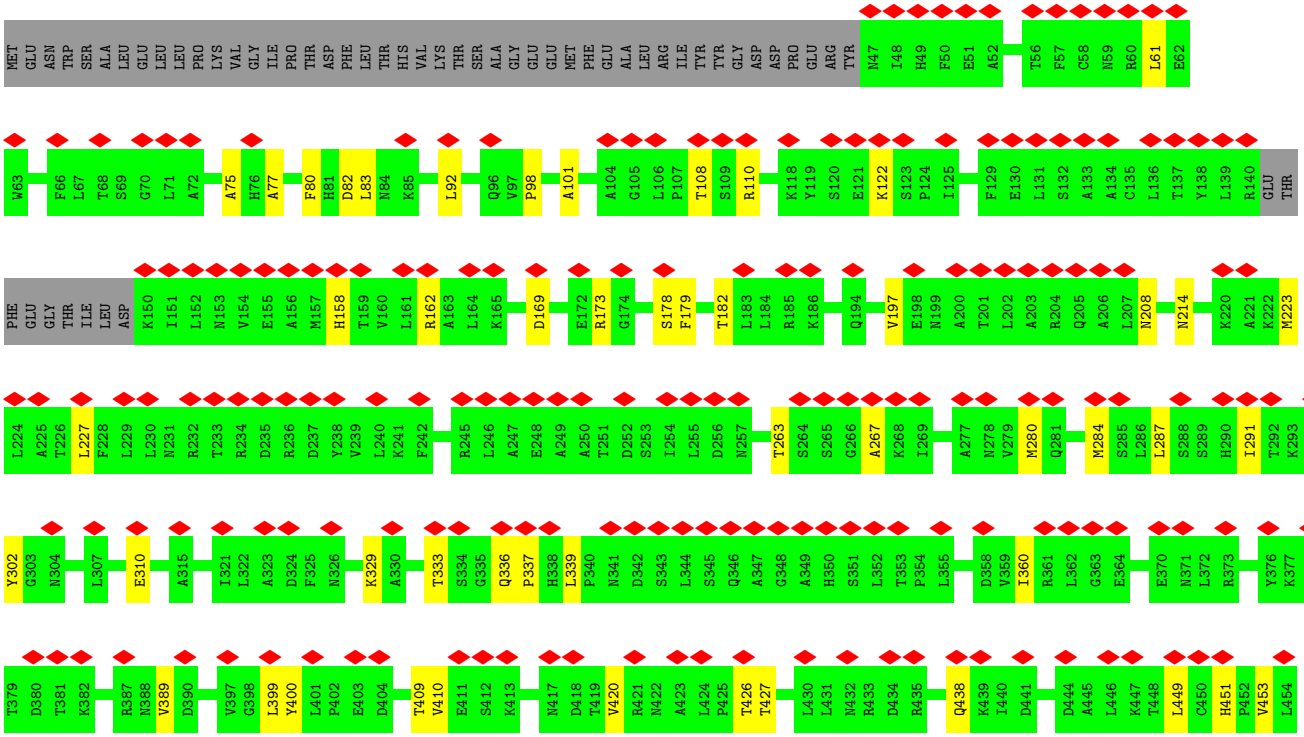

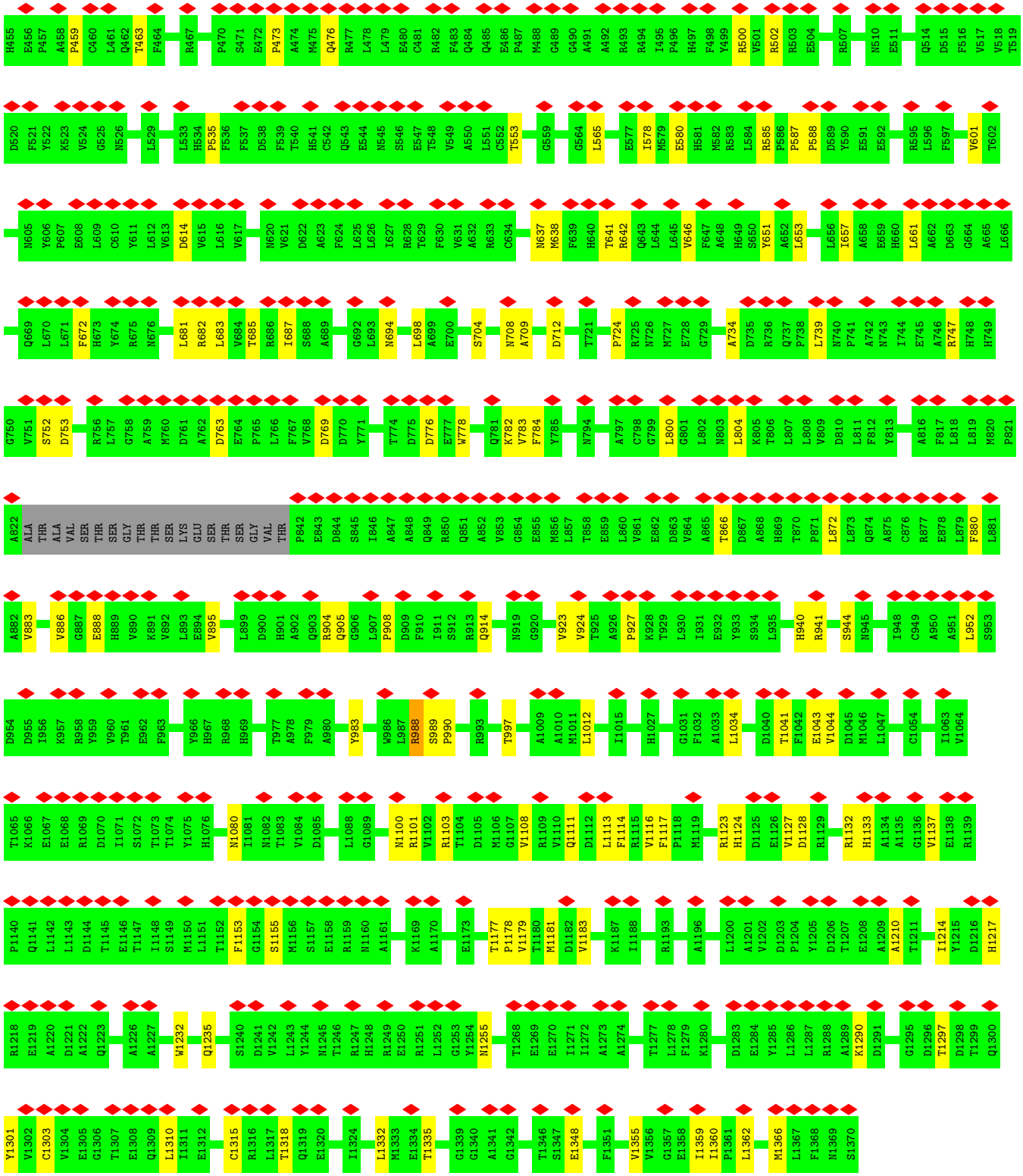

• Molecule 4: Major capsid protein

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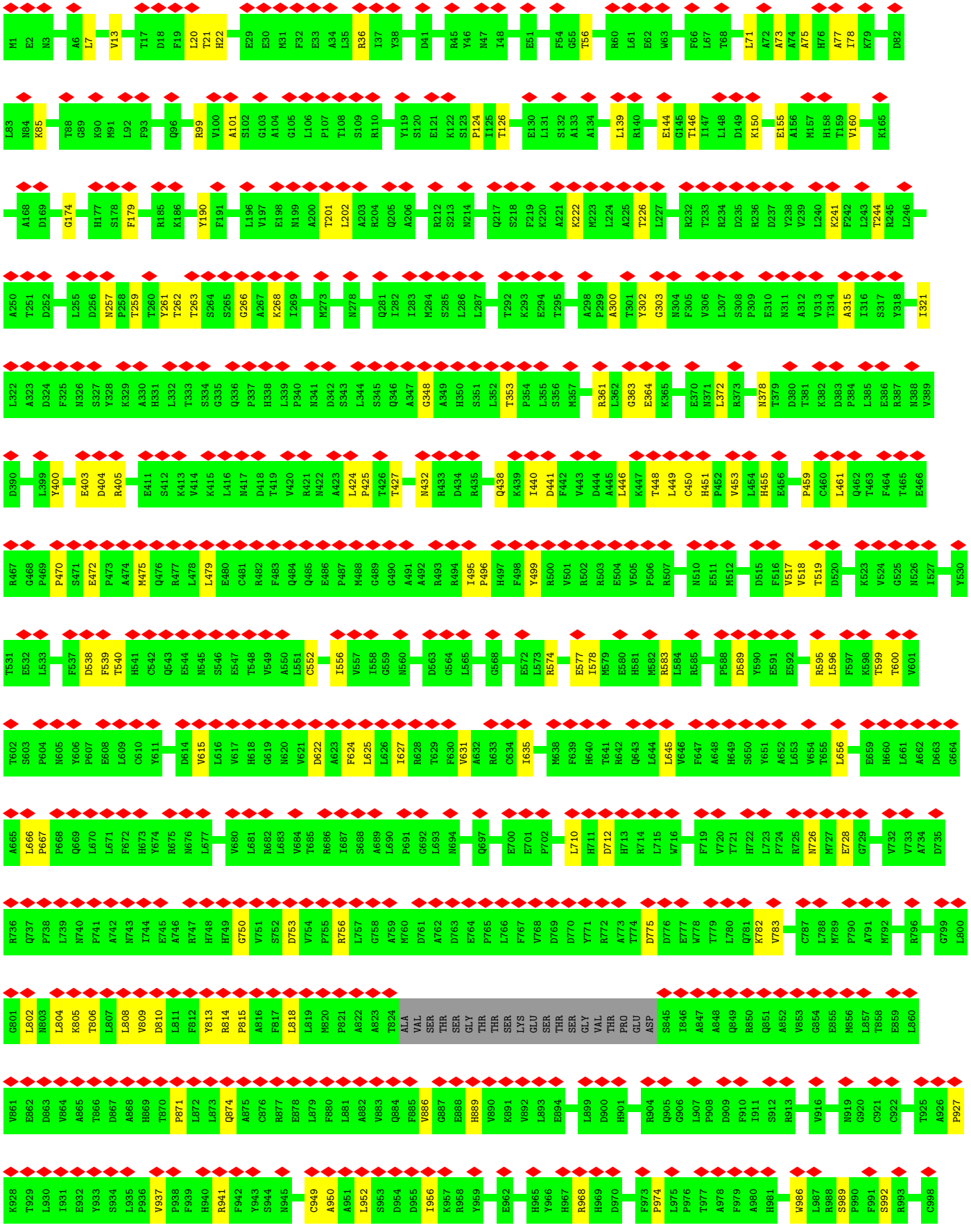
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T602 S603 P604 N605 Y606 P607 E608 L609 C610 Y611 D614 V615 L616 V617 H618 G619 N620 V621 D622 A623 F624 L625 L626 I627 R628 T629 F630 V631 A632 R633 C634 I635 M638 F639 H640 T641 R642 Q643 L644 L645 V646 F647 A648 H649 S650 Y651 A652 L653 V654 T655 L656 E659 H660 L661 A662 D663 G664
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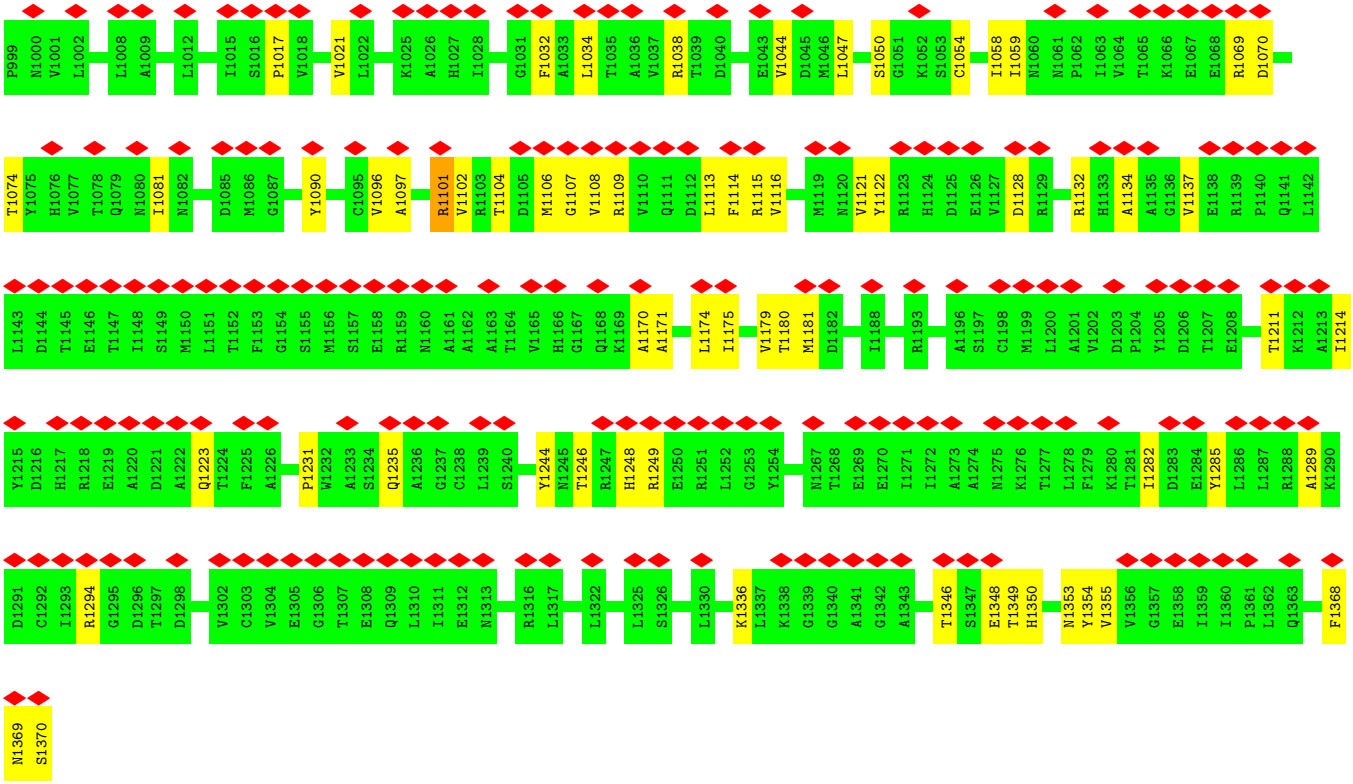
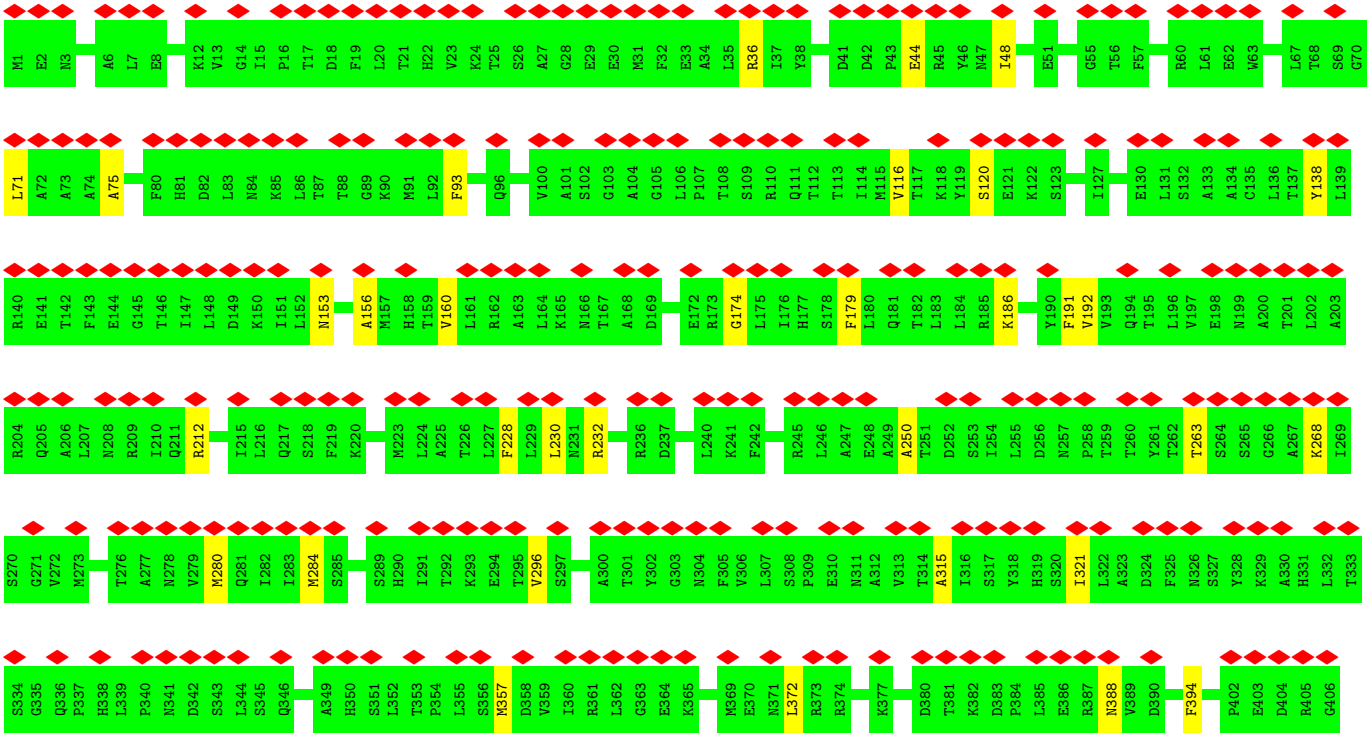
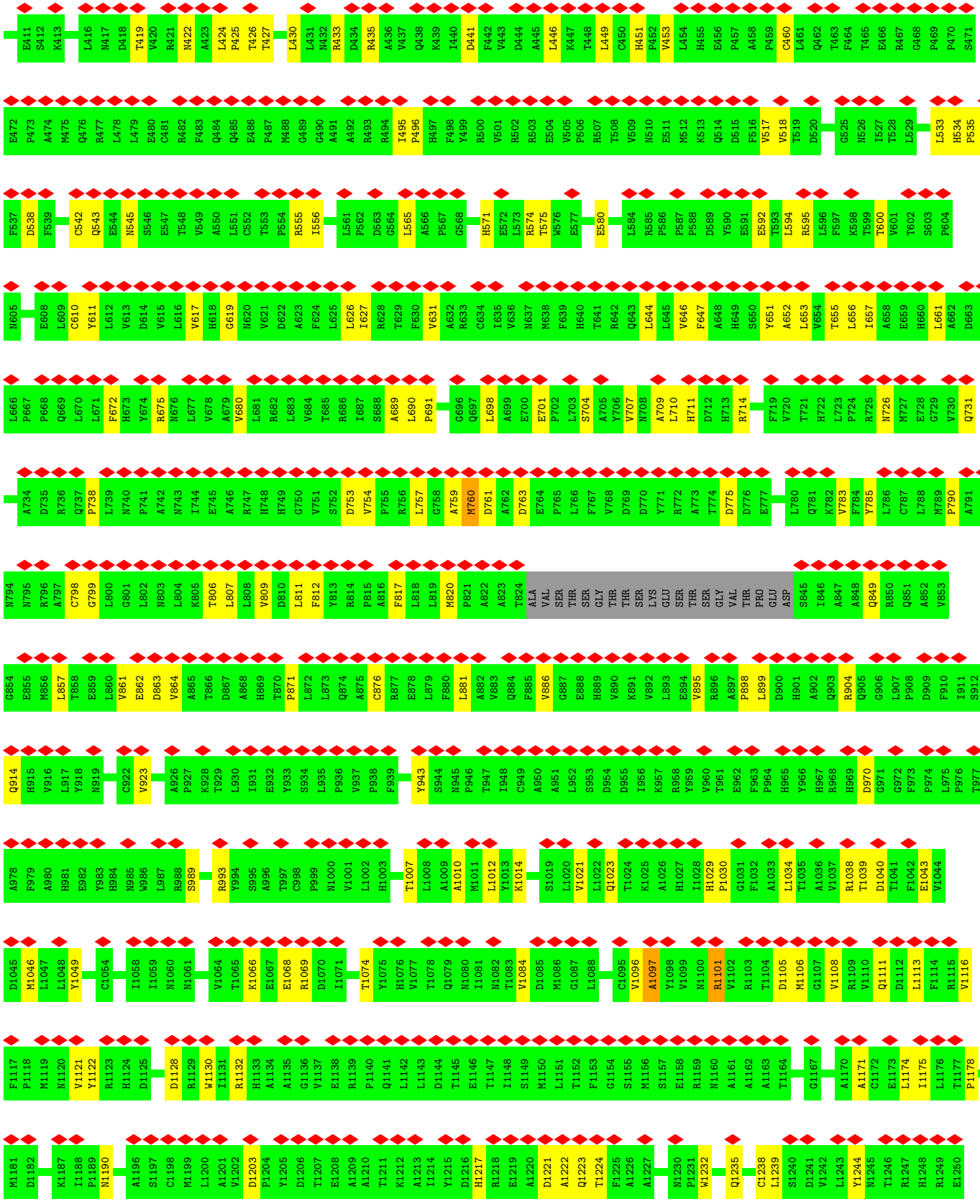


• Molecule 4: Major capsid protein

Chain M:

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E472 P473 A474 M475 Q476 R477 L478 L479 E480 C481 R482 F483 Q484 Q485 E486 P487 M488 G489 G490 A491 A492 R493 R494 I495 P496 H497 F498 Y499 R500 V501 R502 R503 E504 V505 P506 R507 T508 V509 N510 E511 M512 K513 Q514 D515 F516 V517 V518 T519 D520 G525 N526 I527 T528 L529 L533 H534 P535 F536
F537 D538 F539 C542 Q543 E544 N545 S546 E547 T548 V549 A550 L551 C552 T553 P554 R555 I556 L561 P562 D563 G564 L565 A566 P567 G568 H571 E572 L573 R574 T575 W576 E577 E580 L584 R585 P586 P587 P588 D589 Y590 E591 E592 T593 L594 R595 L596 F597 K598 T599 T600 V601 T602 S603 P604
N605 E608 L609 C610 Y611 L612 V613 D614 V615 L616 V617 H618 G619 N620 V621 D622 A623 F624 L625 L626 I627 R628 T629 F630 V631 A632 R633 C634 I635 V636 N637 M638 F639 H640 T641 R642 Q643 L644 L645 V646 F647 A648 H649 S650 Y651 A652 L653 V654 T655 L656 I657 A658 E659 H660 L661 A662 D663 G664 A665
L666 P667 P668 Q669 L670 L671 F672 H673 Y674 R675 N676 L677 V678 A679 V680 L681 R682 L683 V684 T685 R686 I687 S688 A689 L690 P691 G696 Q697 L698 A699 E700 E701 P702 L703 S704 A705 Y706 V707 N708 A709 L710 H711 D712 H713 R714 F719 V720 T721 H722 L723 P724 R725 N726 M727 E728 G729 V730 Q731
A734 D735 R736 Q737 P738 L739 N740 P741 A742 N743 I744 E745 A746 R747 H748 H749 G750 V751 S752 D753 V754 P755 R756 L757 G758 A759 M760 D761 A762 D763 E764 P765 L766 F767 V768 D769 D770 Y771 R772 A773 T774 D775 D776 E777 L780 Q781 K782 V783 F784 Y785 L786 C787 L788 M789 P790 A791 M792 T793
N794 N795 R796 A797 C798 G799 L800 G801 L802 N803 L804 K805 T806 L807 L808 V809 D810 L811 F812 Y813 R814 P815 A816 F817 L818 L819 M820 P821 A822 A823 T824 ALA VAL SER THR SER GLY THR THR SER LYS GLU SER THR SER GLY VAL THR PRO GLU ASP S845 I846 A847 A848 Q849 R850 Q851 A852 V853
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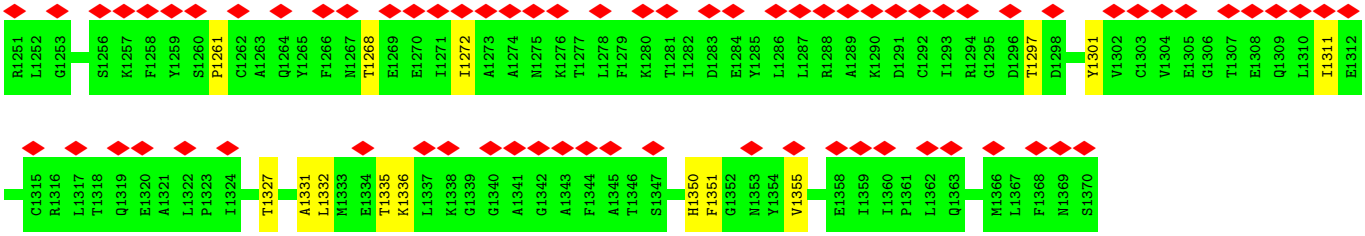
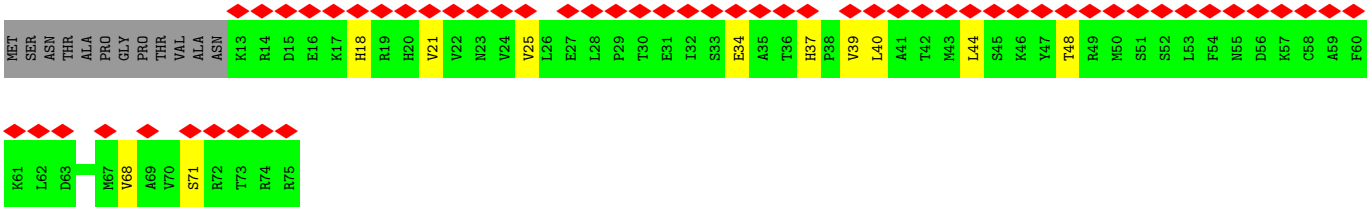
Q914 H915 V916 L917 Y918 N919 C922 V923 A926 P927 K928 T929 L930 I931 E932 Y933 S934 L935 P936 V937 P938 F939 Y943 S944 N945 P946 T947 I948 C949 A950 A951 L952 S953 D954 D955 I956 K957 R958 Y959 V960 T961 E962 F963 P964 H965 Y966 H967 R968 H969 D970 G971 G972 F973 P974 L975 P976 T977
A978 P979 A980 H981 E982 Y983 H984 N985 W986 L987 R988 S989 R993 Y994 S995 A996 T997 C998 P999 N1000 V1001 L1002 H1003 T1007 L1008 A1009 A1010 M1011 L1012 Y1013 K1014 S1019 L1020 V1021 L1022 Q1023 T1024 K1025 A1026 H1027 I1028 H1029 P1030 G1031 F1032 A1033 L1034 T1035 A1036 V1037 R1038 T1039 D1040 T1041 F1042 E1043 V1044
D1045 M1046 L1047 L1048 Y1049 C1054 I1058 I1059 N1060 N1061 V1064 T1065 K1066 E1067 E1068 R1069 D1070 I1071 T1074 Y1075 H1076 V1077 T1078 Q1079 N1080 I1081 N1082 T1083 V1084 D1085 M1086 G1087 L1088 C1095 V1096 A1097 Y1098 V1099 N1100 R1101 V1102 R1103 T1104 D1105 M1106 G1107 V1108 R1109 V1110 Q1111 D1112 L1113 F1114 R1115 V1116
F1117 P1118 M1119 N1120 V1121 Y1122 R1123 H1124 D1125 D1128 R1129 W1130 I1131 R1132 H1133 A1134 A1135 G1136 V1137 E1138 R1139 P1140 Q1141 L1142 L1143 D1144 T1145 E1146 T1147 I1148 S1149 M1150 L1151 T1152 F1153 G1154 S1155 M1156 S1157 E1158 R1159 N1160 A1161 A1162 A1163 T1164 G1167 A1170 A1171 C1172 E1173 L1174 I1175 L1176 T1177 P1178
M1181 D1182 K1187 I1188 P1189 N1190 A1196 S1197 C1198 M1199 L1200 A1201 V1202 D1203 P1204 Y1205 D1206 T1207 E1208 A1209 A1210 T1211 K1212 A1213 I1214 Y1215 D1216 H1217 R1218 E1219 A1220 D1221 A1222 Q1223 T1224 F1225 A1226 A1227 N1230 P1231 W1232 Q1235 C1238 L1239 S1240 D1241 V1242 L1243 Y1244 N1245 T1246 R1247 H1248 R1249 E1250



• Molecule 5: Small capsomere-interacting protein

Chain N:



• Molecule 5: Small capsomere-interacting protein

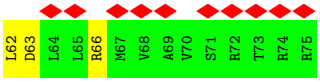
Chain O:

• Molecule 5: Small capsomere-interacting protein

Chain P:

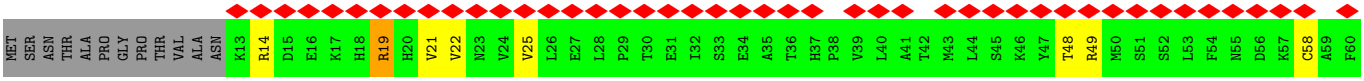
• Molecule 5: Small capsomere-interacting protein

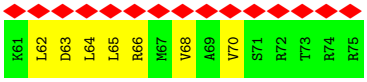
Chain Q:



• Molecule 5: Small capsomere-interacting protein

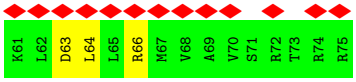
Chain R:





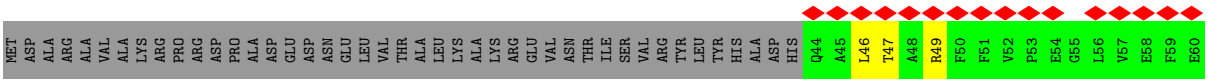
• Molecule 5: Small capsomere-interacting protein

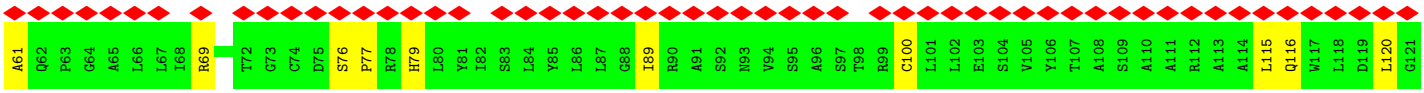
Chain S:

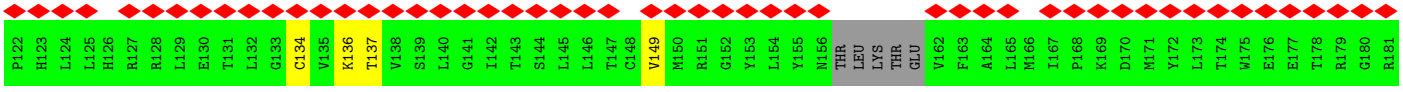


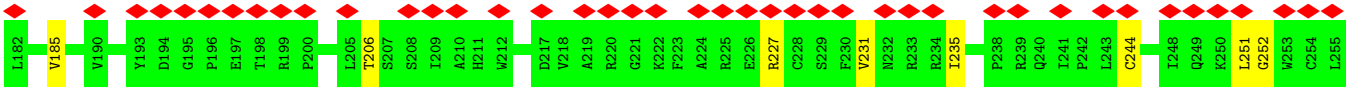
• Molecule 6: Triplex capsid protein 1

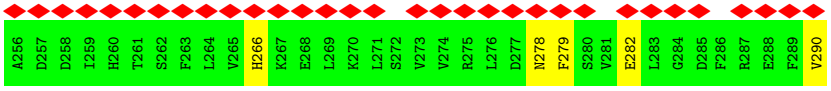
Chain T:





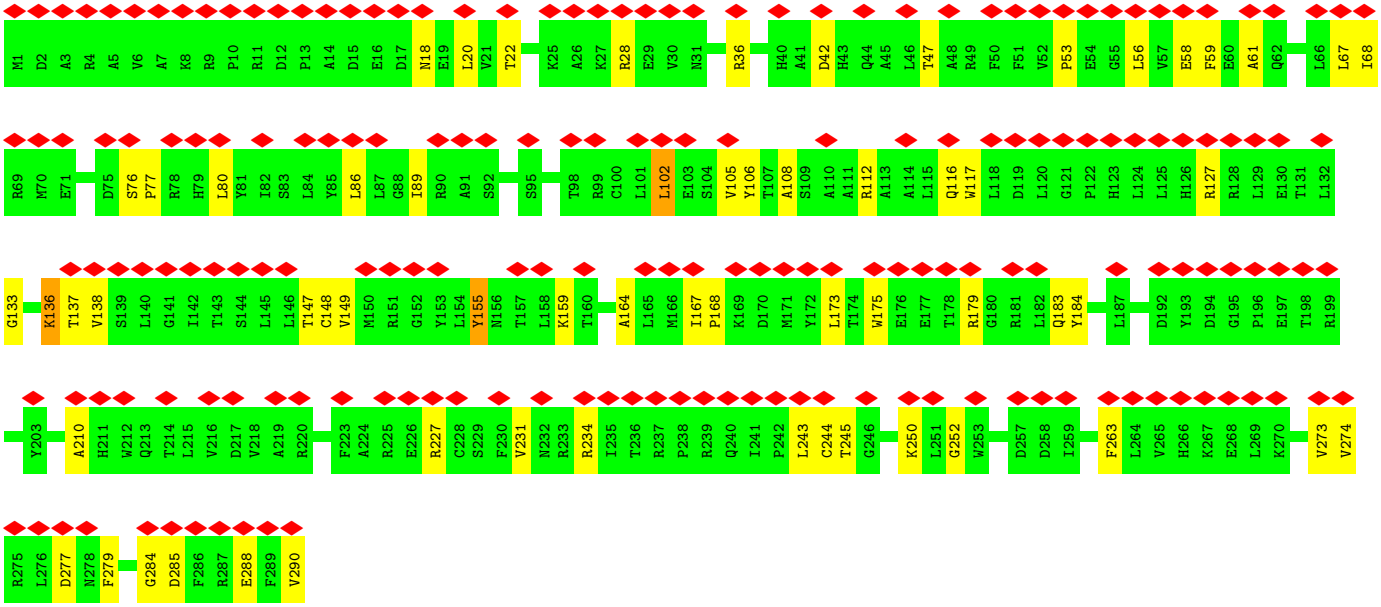






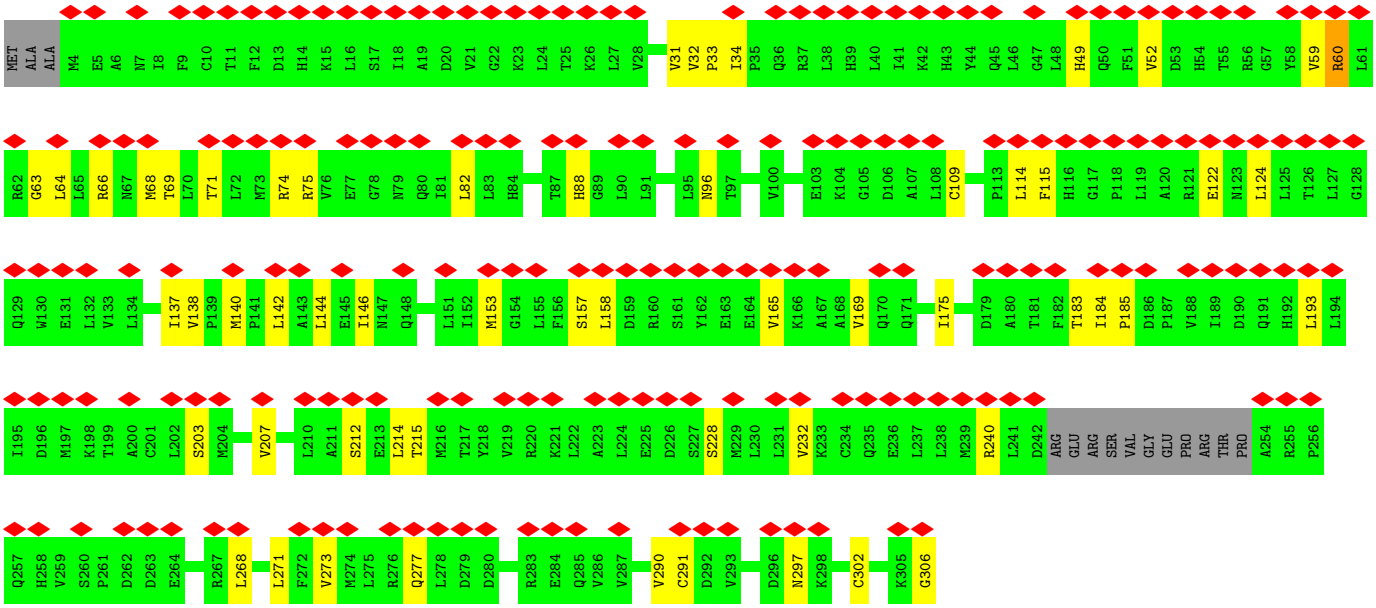
• Molecule 6: Triplex capsid protein 1

Chain W:



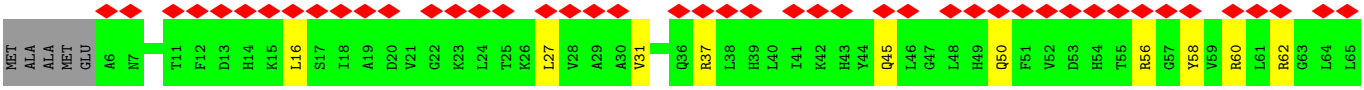
• Molecule 7: Triplex capsid protein 2

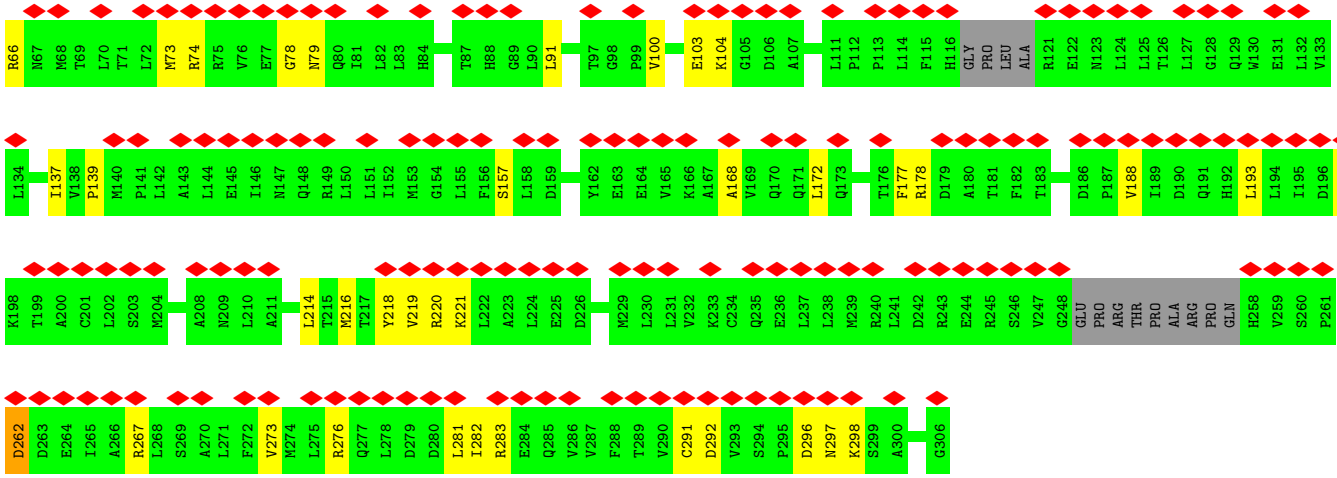
Chain U:



• Molecule 7: Triplex capsid protein 2

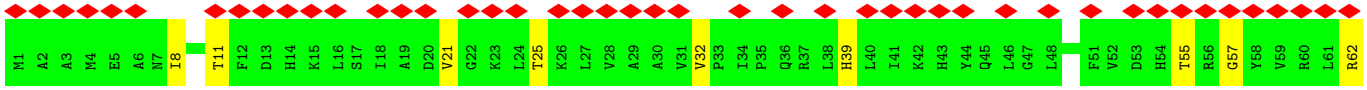
Chain V:

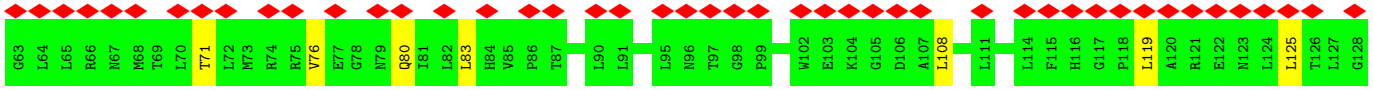


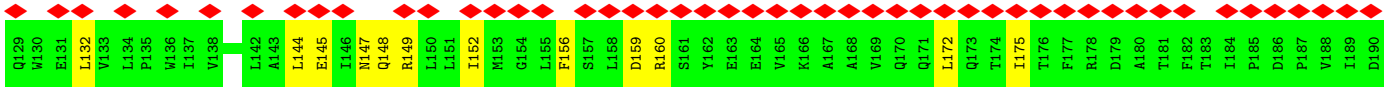


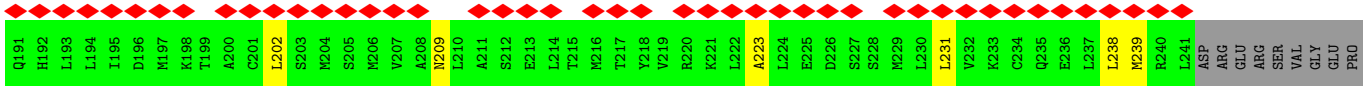
• Molecule 7: Triplex capsid protein 2

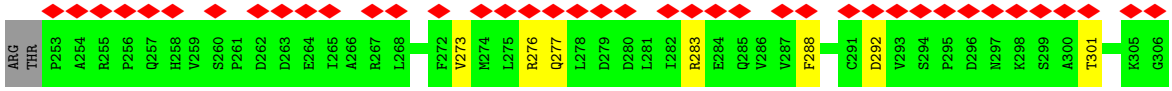
Chain X:





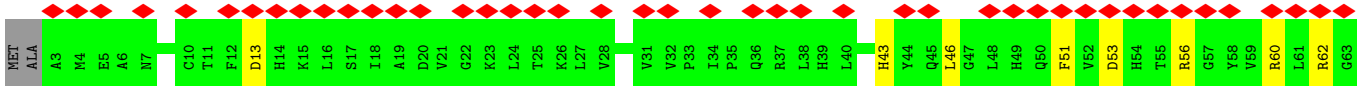


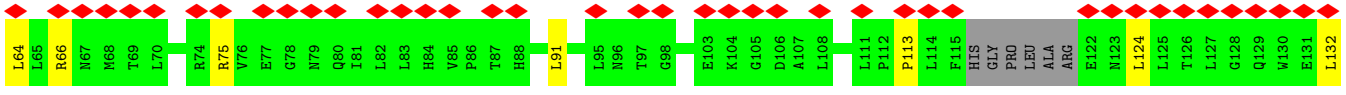


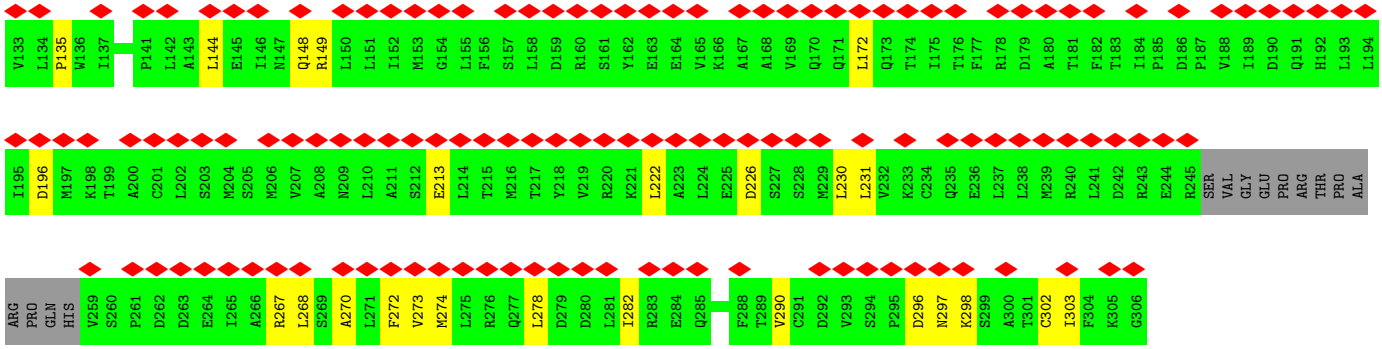


• Molecule 7: Triplex capsid protein 2

Chain Y:

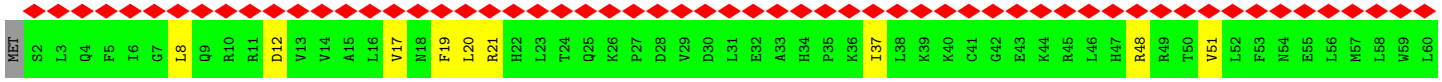


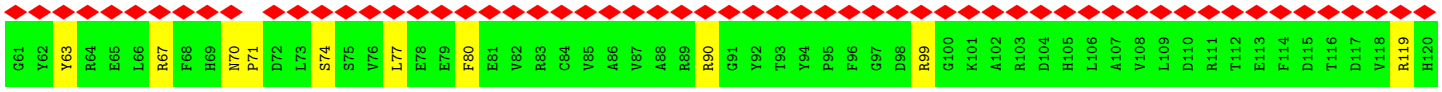


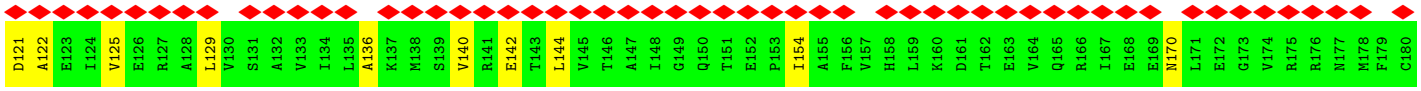


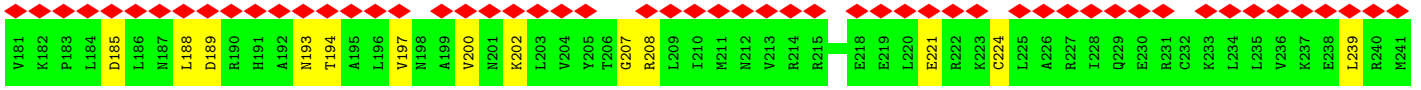
• Molecule 8: Large structural phosphoprotein

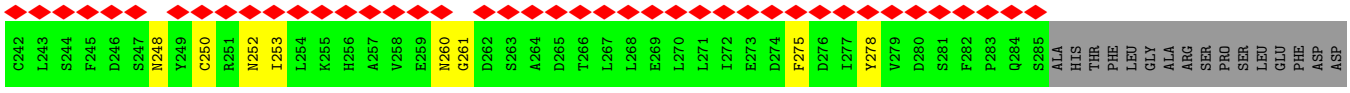
Chain Z:











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

VAL ALA THR PRO HIS ALA SER ALA ARG ALA GLN THR VAL THR SER THR PRO VAL GLN GLY ARG LEU GLU LYS GLN VAL SER GLY THR PRO SER THR VAL PRO ALA THR LEU LEU GLN PRO GLN PRO ALA SER SER LYS THR THR SER SER ARG ASN VAL THR SER GLY ALA GLY THR SER

SER ALA SER SER ALA ARG GLN PRO SER ALA SER ALA VAL SER PRO ALA THR SER PRO LEU SER MET LEU SER SER ALA SER PRO SER PRO ALA LYS SER ALA PRO PRO SER PRO VAL LYS GLY ARG GLY SER ARG VAL GLY VAL PRO SER

LEU LYS PRO THR LEU GLY GLY LYS ALA VAL VAL GLY ARG PRO PRO SER VAL PRO VAL SER GLY SER ALA PRO GLY ARG LEU SER GLY SER SER ARG ALA ALA SER THR THR PRO THR TYR PRO ALA VAL THR THR VAL TYR PRO PRO SER PRO GLN LYS SER SER THR ALA LYS SER SER VAL SER ASN ALA

PRO PRO VAL ALA SER PRO SER ILE LEU LYS PRO GLY ALA SER ALA ALA LEU GLN SER ARG ARG SER THR GLY THR ALA ALA VAL GLY SER PRO VAL LYS SER THR THR GLY MET LYS THR VAL ALA ALA PHE ASP LEU SER SER PRO GLN LYS SER GLY THR GLY PRO GLN PRO GLY SER ALA

GLY MET GLY GLY ALA LYS THR PRO SER ASP ALA VAL GLN ASN ILE LEU GLN LYS ILE GLU LYS ILE LYS ASN THR GLU GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	16225	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 ($e^-/Å^2$)	47.2	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	489.6, 489.6, 489.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.36, 1.36, 1.36	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/5969	0.53	0/8139
1	C	0.25	0/334	0.53	0/450
2	E	0.26	0/4094	0.53	1/5558 (0.0%)
2	F	0.25	0/721	0.58	0/969
3	G	0.24	0/3951	0.58	0/5357
4	H	0.25	0/10638	0.52	0/14487
4	I	0.25	0/10949	0.51	0/14916
4	J	0.24	0/10682	0.51	0/14553
4	K	0.25	0/10503	0.51	1/14307 (0.0%)
4	L	0.25	0/10949	0.51	0/14916
4	M	0.24	0/10949	0.50	0/14916
5	N	0.23	0/520	0.53	0/697
5	O	0.23	0/520	0.51	0/697
5	P	0.23	0/520	0.54	0/697
5	Q	0.24	0/520	0.54	0/697
5	R	0.24	0/520	0.55	0/697
5	S	0.23	0/520	0.53	0/697
6	T	0.25	0/1981	0.56	0/2687
6	W	0.25	0/2374	0.55	0/3221
7	U	0.24	0/2361	0.53	0/3206
7	V	0.26	0/2333	0.56	0/3164
7	X	0.24	0/2379	0.52	0/3230
7	Y	0.25	0/2305	0.52	0/3126
8	Z	0.25	0/2358	0.56	0/3182
All	All	0.25	0/98950	0.52	2/134566 (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
3	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	H	0	2
4	I	0	1
4	J	0	1
4	K	0	2
4	M	0	1
6	W	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	606	LEU	CA-CB-CG	5.55	128.06	115.30
4	K	753	ASP	CB-CG-OD2	5.13	122.92	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	G	312	SER	Peptide
4	H	1100	ASN	Peptide
4	H	265	SER	Peptide
4	I	1143	LEU	Peptide
4	J	794	ASN	Peptide
4	K	1100	ASN	Peptide
4	K	941	ARG	Peptide
4	M	1097	ALA	Peptide
6	W	136	LYS	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	5830	0	5830	158	0
1	C	332	0	358	14	0
2	E	3992	0	3913	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	710	0	711	12	0
3	G	3862	0	3779	43	0
4	H	10391	0	10342	127	0
4	I	10693	0	10635	149	0
4	J	10433	0	10379	102	0
4	K	10259	0	10216	98	0
4	L	10693	0	10635	127	0
4	M	10693	0	10635	119	0
5	N	513	0	539	7	0
5	O	513	0	539	3	0
5	P	513	0	539	5	0
5	Q	513	0	539	12	0
5	R	513	0	539	10	0
5	S	513	0	539	11	0
6	T	1939	0	1972	19	0
6	W	2325	0	2363	42	0
7	U	2317	0	2405	32	0
7	V	2292	0	2379	26	0
7	X	2334	0	2431	26	0
7	Y	2266	0	2355	23	0
8	Z	2320	0	2351	28	0
All	All	96759	0	96923	1238	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 6.

All (1238) 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:E:267:TYR:HE1	2:E:270:TYR:HB3	1.35	0.90
4:J:795:ASN:ND2	4:J:969:HIS:O	2.09	0.84
7:U:240:ARG:HB2	7:V:267:ARG:HH21	1.43	0.84
2:E:267:TYR:CE1	2:E:270:TYR:HB3	2.15	0.81
2:E:371:PHE:HB3	2:E:376:VAL:HB	1.64	0.80
4:M:575:THR:HG21	4:M:1007:THR:HA	1.63	0.78
3:G:53:ARG:NH2	3:G:58:ALA:O	2.17	0.77
4:L:1044:VAL:HG11	4:L:1096:VAL:HG13	1.68	0.76
2:E:337:TYR:HE2	2:E:431:ARG:HG3	1.51	0.75
6:W:290:VAL:HG22	7:X:277:GLN:HG3	1.70	0.74
4:L:432:ASN:OD1	4:L:438:GLN:NE2	2.21	0.74
4:L:600:THR:HG21	4:L:645:LEU:HD23	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:1038:ARG:HH22	4:L:1106:MET:HG2	1.54	0.73
4:L:1047:LEU:HD22	4:L:1097:ALA:HB2	1.69	0.73
1:A:1765:PRO:HG2	1:A:1768:MET:HB2	1.72	0.72
4:M:710:LEU:HD21	4:M:783:VAL:HG23	1.73	0.71
4:L:144:GLU:H	6:W:36:ARG:HH22	1.38	0.71
8:Z:136:ALA:HB2	8:Z:200:VAL:HG21	1.72	0.70
6:W:167:ILE:HD12	6:W:168:PRO:HD2	1.74	0.70
4:H:263:THR:HG22	4:H:296:VAL:HG22	1.74	0.70
4:H:553:THR:HG21	4:H:983:TYR:HB3	1.72	0.70
4:M:600:THR:HG22	4:M:644:LEU:HB2	1.74	0.70
3:G:432:LEU:O	3:G:556:ARG:NH1	2.25	0.69
2:F:35:LEU:HB2	3:G:402:VAL:HG23	1.75	0.69
4:M:433:ARG:HD2	4:M:1105:ASP:HA	1.72	0.69
2:E:339:TYR:HB2	2:E:364:ARG:HD2	1.75	0.69
1:A:1859:LEU:HB3	1:A:1877:VAL:HG21	1.74	0.69
2:E:263:ASN:HA	2:E:266:VAL:HG22	1.74	0.69
4:H:820:MET:HG3	4:H:877:ARG:HD3	1.74	0.69
4:M:230:LEU:H	4:M:1097:ALA:HB1	1.58	0.69
4:I:212:ARG:NH2	4:I:1203:ASP:OD1	2.25	0.68
4:I:484:GLN:NE2	4:I:486:GLU:OE2	2.26	0.68
1:A:1483:ARG:NH1	1:A:1526:GLU:OE1	2.27	0.68
4:L:450:CYS:O	4:L:1122:TYR:OH	2.11	0.68
1:A:2217:VAL:HG22	2:E:82:ARG:HD3	1.76	0.68
4:M:574:ARG:NH2	4:M:1023:GLN:OE1	2.27	0.68
4:H:272:VAL:HG12	4:H:368:ILE:HB	1.76	0.67
1:A:1520:ARG:NH2	1:A:1905:PRO:O	2.28	0.67
4:J:601:VAL:HG11	4:J:793:THR:HG22	1.76	0.67
1:A:1754:TYR:HB2	1:A:1757:TYR:CE2	2.30	0.67
2:E:423:PHE:HB2	2:E:426:GLU:HG2	1.74	0.67
4:K:420:VAL:HB	4:K:580:GLU:HG3	1.76	0.67
4:L:470:PRO:HB2	4:L:475:MET:HG3	1.78	0.66
4:M:753:ASP:OD1	5:S:66:ARG:NH1	2.29	0.66
2:E:263:ASN:O	2:E:587:HIS:NE2	2.28	0.66
4:J:757:LEU:HD11	5:P:62:LEU:HD12	1.77	0.66
4:I:274:VAL:HG13	4:I:370:GLU:HB3	1.78	0.66
4:K:927:PRO:HD2	4:K:952:LEU:HD21	1.78	0.66
4:K:399:LEU:HD23	4:K:1183:VAL:HG22	1.78	0.66
4:M:989:SER:OG	4:M:993:ARG:NH2	2.29	0.66
1:A:2211:LEU:HD23	1:A:2214:LEU:HD12	1.77	0.66
4:K:657:ILE:HG23	4:K:661:LEU:HD12	1.78	0.66
2:E:500:PHE:HD1	2:E:503:ARG:HH12	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1044:VAL:HG22	4:H:1099:VAL:HG22	1.78	0.66
2:E:268:PRO:HA	2:E:271:ASP:HA	1.78	0.65
4:H:248:GLU:OE2	4:H:365:LYS:NZ	2.21	0.65
4:M:759:ALA:O	4:M:761:ASP:N	2.29	0.65
4:K:553:THR:HG21	4:K:983:TYR:HB3	1.77	0.65
1:A:1476:LEU:HD22	1:A:1480:ARG:HH21	1.62	0.65
1:A:1867:LYS:HE3	1:A:1872:GLU:HA	1.77	0.64
7:Y:222:LEU:O	7:Y:226:ASP:N	2.31	0.64
1:A:1689:THR:OG1	1:A:2113:ARG:NH2	2.30	0.64
1:A:2206:ASN:OD1	2:E:93:GLN:NE2	2.31	0.64
4:K:709:ALA:HB3	4:K:1012:LEU:HD23	1.78	0.64
4:L:124:PRO:HG3	7:X:11:THR:HG21	1.79	0.64
4:H:1285:TYR:HA	4:H:1289:ALA:HB3	1.80	0.64
4:J:212:ARG:NH2	4:J:1203:ASP:OD1	2.30	0.64
2:E:268:PRO:C	2:E:271:ASP:H	2.02	0.63
4:H:87:THR:HG23	7:V:79:ASN:HA	1.80	0.63
4:L:139:LEU:HD22	4:L:160:VAL:HG21	1.79	0.63
4:L:596:LEU:O	4:L:600:THR:HG23	1.99	0.63
2:E:407:TRP:O	2:E:411:LEU:HD12	1.98	0.63
6:W:168:PRO:HA	6:W:273:VAL:HA	1.79	0.63
1:A:2221:LEU:HD23	1:A:2224:LEU:HD21	1.81	0.63
4:H:888:GLU:O	4:H:919:ASN:ND2	2.32	0.63
1:A:1984:ARG:HD2	2:E:493:GLY:HA3	1.79	0.63
4:K:694:ASN:HD22	4:K:704:SER:HB3	1.64	0.63
1:A:2228:VAL:HG11	2:F:72:VAL:HG11	1.81	0.63
2:E:365:HIS:O	2:E:368:VAL:HG12	1.99	0.63
3:G:146:THR:HA	3:G:164:LEU:HA	1.81	0.63
4:I:1235:GLN:HB2	4:I:1238:CYS:HB3	1.81	0.63
1:A:1527:ARG:HH11	1:A:1531:LEU:HD12	1.63	0.62
1:C:2211:LEU:O	1:C:2214:LEU:HG	1.99	0.62
4:L:315:ALA:HB2	4:L:321:ILE:HD11	1.80	0.62
7:U:290:VAL:HG12	7:U:302:CYS:SG	2.39	0.62
4:I:390:ASP:OD1	4:I:1039:THR:OG1	2.18	0.62
5:Q:28:LEU:HD12	5:Q:29:PRO:HD2	1.81	0.62
3:G:374:GLU:O	3:G:378:VAL:HG12	1.99	0.62
4:I:1272:ILE:O	4:I:1275:ASN:ND2	2.33	0.62
4:K:101:ALA:HB3	4:L:174:GLY:HA3	1.82	0.62
6:W:61:ALA:HA	6:W:138:VAL:HG21	1.80	0.62
2:F:60:TYR:O	2:F:64:GLU:HG2	2.00	0.62
4:J:821:PRO:HD3	4:J:877:ARG:HH21	1.65	0.62
4:L:615:VAL:HG11	4:L:802:LEU:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:280:MET:O	4:K:284:MET:HG2	2.00	0.61
4:L:574:ARG:O	4:L:578:ILE:HG13	2.00	0.61
1:A:1806:ILE:HD12	1:A:1975:VAL:HG21	1.80	0.61
2:E:499:GLU:O	2:E:503:ARG:NH1	2.33	0.61
4:H:437:VAL:HG21	4:I:1184:ASN:HD22	1.64	0.61
1:A:1453:ALA:HA	1:A:1456:TYR:CD2	2.36	0.61
1:A:2051:ARG:HD2	1:A:2052:VAL:H	1.66	0.61
2:E:509:TRP:HE1	2:E:516:VAL:HG21	1.65	0.61
4:H:1161:ALA:O	4:I:209:ARG:NH2	2.34	0.61
4:H:1336:LYS:NZ	4:H:1346:THR:OG1	2.33	0.61
4:M:1297:THR:HG21	4:M:1301:TYR:HD2	1.64	0.61
7:U:74:ARG:HB2	7:U:82:LEU:O	2.01	0.61
2:E:230:TYR:HB2	2:E:241:LEU:HD23	1.83	0.61
2:E:539:ASP:HB3	2:E:542:ARG:HG3	1.80	0.61
4:J:705:ALA:HB1	4:J:712:ASP:HB3	1.82	0.61
4:M:672:PHE:HA	4:M:675:ARG:HG2	1.83	0.61
1:A:1476:LEU:O	1:A:1480:ARG:HG2	2.01	0.61
1:A:1486:PHE:CE2	1:A:1519:THR:HG22	2.36	0.61
2:E:367:LEU:O	2:E:371:PHE:HD1	1.83	0.61
7:Y:290:VAL:HG22	7:Y:302:CYS:SG	2.41	0.61
1:A:1473:ARG:HA	1:A:1476:LEU:HD12	1.81	0.61
1:A:1971:GLN:HG3	1:A:1972:ARG:HG3	1.83	0.61
1:A:1573:ARG:NH1	1:A:1619:ALA:O	2.33	0.60
4:H:688:SER:OG	4:H:711:HIS:NE2	2.31	0.60
4:L:1175:ILE:HG22	4:L:1244:TYR:HE2	1.66	0.60
2:E:576:LYS:HE3	2:E:576:LYS:HA	1.82	0.60
1:C:2236:ARG:HA	1:C:2240:LEU:HD12	1.84	0.60
4:I:1047:LEU:HD22	4:I:1097:ALA:HB2	1.83	0.60
4:J:697:GLN:NE2	4:J:699:ALA:O	2.35	0.60
2:E:286:ALA:HB2	2:E:404:LEU:HD13	1.83	0.60
7:V:100:VAL:HG11	7:V:139:PRO:HD3	1.84	0.60
4:J:804:LEU:HA	4:J:807:LEU:HB3	1.84	0.60
4:M:757:LEU:HA	4:M:760:MET:HG2	1.83	0.60
6:W:102:LEU:HA	6:W:105:VAL:HG12	1.84	0.60
3:G:566:LEU:HD12	7:U:165:VAL:HG21	1.84	0.59
4:L:949:CYS:SG	4:L:956:ILE:HG21	2.42	0.59
7:X:25:THR:HA	7:X:76:VAL:HG11	1.82	0.59
4:M:657:ILE:HG12	4:M:661:LEU:HD12	1.84	0.59
1:A:1786:VAL:O	1:A:1972:ARG:NH1	2.35	0.59
1:A:1817:ASN:OD1	1:A:1818:LYS:N	2.35	0.59
4:H:856:MET:O	4:H:860:LEU:HG	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1612:ASN:HB2	1:A:1615:PHE:HB2	1.84	0.59
2:E:355:ARG:O	2:E:355:ARG:NH1	2.32	0.59
4:K:1128:ASP:O	4:K:1132:ARG:HG2	2.03	0.59
5:P:18:HIS:HA	5:P:48:THR:HG21	1.85	0.59
4:M:120:SER:HB3	4:M:1084:VAL:HG12	1.83	0.59
4:M:430:LEU:HD12	4:M:1108:VAL:HG12	1.84	0.59
4:I:804:LEU:HA	4:I:807:LEU:HB3	1.84	0.59
1:A:1481:ASP:O	1:A:1485:ARG:HG2	2.02	0.59
7:V:104:LYS:HG3	7:V:291:CYS:HA	1.85	0.59
4:I:662:ALA:HA	4:I:671:LEU:HD11	1.85	0.58
4:M:250:ALA:HB3	4:M:1049:TYR:HE2	1.67	0.58
7:Y:144:LEU:O	7:Y:148:GLN:HG2	2.03	0.58
2:E:349:MET:HB3	2:E:428:GLN:NE2	2.18	0.58
2:E:350:PRO:HD2	2:E:428:GLN:HG3	1.84	0.58
4:M:1217:HIS:NE2	4:M:1235:GLN:HG3	2.18	0.58
4:K:866:THR:HG22	4:K:872:LEU:HA	1.85	0.58
2:E:243:GLN:HE21	2:E:246:ASN:HB3	1.68	0.58
4:L:303:GLY:HA3	4:L:348:GLY:HA2	1.86	0.58
4:K:904:ARG:NH1	4:K:908:PRO:O	2.36	0.58
4:M:806:THR:HA	4:M:809:VAL:HG12	1.85	0.58
1:A:1779:GLN:OE1	1:A:2065:ARG:NH1	2.37	0.58
2:E:205:ASN:HA	2:E:208:PHE:CE1	2.37	0.58
4:I:65:TYR:HA	4:I:172:GLU:HG2	1.85	0.58
4:L:459:PRO:HB3	4:L:1248:HIS:CE1	2.38	0.58
4:M:75:ALA:HB2	4:M:179:PHE:CZ	2.38	0.58
4:M:617:VAL:HG13	4:M:619:GLY:H	1.69	0.58
4:M:785:TYR:O	4:M:943:TYR:OH	2.21	0.58
6:T:46:LEU:HD22	7:V:91:LEU:HD23	1.84	0.58
2:E:287:TYR:HB2	2:E:371:PHE:HE2	1.68	0.58
4:H:20:LEU:HD11	4:K:197:VAL:HG22	1.85	0.58
4:I:1336:LYS:NZ	4:I:1346:THR:OG1	2.37	0.58
7:U:122:GLU:O	7:U:124:LEU:N	2.37	0.58
4:M:895:VAL:HB	4:M:914:GLN:HB3	1.85	0.58
6:T:89:ILE:HG23	6:T:115:LEU:HD11	1.86	0.58
2:E:606:LEU:HB2	2:E:609:HIS:HB2	1.86	0.58
4:H:747:ARG:NH2	4:H:888:GLU:OE1	2.36	0.58
4:K:1043:GLU:OE1	4:K:1101:ARG:NH1	2.34	0.58
4:L:144:GLU:H	6:W:36:ARG:NH2	2.02	0.57
4:I:627:ILE:HG22	4:I:631:VAL:HG23	1.85	0.57
4:M:571:HIS:O	4:M:575:THR:HG23	2.04	0.57
1:A:1574:ARG:HE	1:A:1604:ILE:HG22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:VAL:O	2:E:207:MET:HG2	2.03	0.57
4:H:426:THR:HG23	4:H:427:THR:HG23	1.87	0.57
4:I:118:LYS:NZ	4:I:1087:GLY:O	2.31	0.57
2:E:32:ARG:O	2:E:36:GLU:HG3	2.04	0.57
1:A:1587:VAL:HG12	1:A:1910:VAL:HA	1.85	0.57
2:E:316:ALA:HB2	2:E:444:TRP:HZ3	1.67	0.57
4:K:214:ASN:HB3	4:L:1101:ARG:HD2	1.86	0.57
2:E:538:TRP:HE1	2:E:543:ARG:HA	1.69	0.57
4:L:101:ALA:HB3	4:M:174:GLY:HA3	1.87	0.57
4:I:633:ARG:NH1	4:I:867:ASP:OD2	2.36	0.57
4:L:1348:GLU:O	4:L:1355:VAL:N	2.34	0.57
4:L:1369:ASN:OD1	4:L:1370:SER:N	2.38	0.57
7:U:59:VAL:HG21	7:U:193:LEU:HD12	1.85	0.57
7:V:56:ARG:HD2	7:V:60:ARG:HD3	1.86	0.57
2:E:568:ASP:OD1	2:E:569:TYR:N	2.38	0.57
2:E:346:ARG:HH22	2:E:540:PRO:HB2	1.69	0.56
4:K:158:HIS:HB3	4:K:162:ARG:HH21	1.70	0.56
6:W:136:LYS:O	6:W:137:THR:HG23	2.05	0.56
4:H:652:ALA:O	4:H:656:LEU:HD12	2.04	0.56
4:I:265:SER:O	4:I:267:ALA:N	2.38	0.56
4:J:595:ARG:HA	4:J:598:LYS:HG2	1.87	0.56
4:J:970:ASP:HA	4:J:996:ALA:HB2	1.86	0.56
2:E:21:GLU:HB2	2:F:7:PHE:HB2	1.88	0.56
2:E:201:GLY:O	2:E:205:ASN:ND2	2.35	0.56
7:Y:226:ASP:HB2	7:Y:231:LEU:HD12	1.87	0.56
2:E:34:LEU:HD12	3:G:408:ARG:HD3	1.88	0.56
4:H:1068:GLU:HA	4:H:1073:THR:HG23	1.85	0.56
2:E:200:ARG:NH2	2:E:520:GLN:OE1	2.39	0.56
1:A:1452:LEU:HA	1:A:1455:GLU:HG2	1.88	0.56
3:G:132:LEU:HD11	3:G:149:LEU:HD13	1.88	0.56
4:I:623:ALA:O	4:I:627:ILE:HG12	2.05	0.56
4:J:625:LEU:HD13	4:J:628:ARG:HD2	1.87	0.56
4:J:635:ILE:HG22	4:J:670:LEU:HD13	1.87	0.56
7:Y:149:ARG:HD3	7:Y:172:LEU:O	2.06	0.56
2:E:500:PHE:HA	2:E:503:ARG:NH1	2.21	0.56
4:H:632:ALA:HB2	4:H:661:LEU:HD11	1.88	0.56
4:H:880:PHE:HZ	5:N:68:VAL:HG23	1.71	0.56
4:K:588:PRO:HD2	4:K:683:LEU:HD11	1.87	0.56
4:L:438:GLN:HE22	4:L:1107:GLY:HA2	1.71	0.56
4:I:633:ARG:NH1	4:I:865:ALA:O	2.39	0.55
1:A:1671:LEU:HD11	1:A:1694:LYS:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1098:TYR:OH	4:H:1369:ASN:OD1	2.17	0.55
4:I:531:THR:OG1	4:I:539:PHE:O	2.23	0.55
4:L:806:THR:HA	4:L:809:VAL:HG12	1.89	0.55
4:M:533:LEU:HG	4:M:1238:CYS:HA	1.88	0.55
1:A:1778:HIS:HB3	2:E:609:HIS:CE1	2.41	0.55
4:I:798:CYS:SG	4:I:799:GLY:N	2.79	0.55
4:J:1039:THR:HG23	4:J:1261:PRO:HB3	1.89	0.55
2:E:530:VAL:HG13	2:E:593:HIS:HE1	1.69	0.55
4:H:265:SER:O	4:H:267:ALA:N	2.39	0.55
4:I:1003:HIS:O	4:I:1007:THR:HG23	2.07	0.55
4:K:169:ASP:OD2	4:K:173:ARG:NH1	2.39	0.55
4:K:800:LEU:HD23	4:K:923:VAL:HG21	1.89	0.55
2:E:365:HIS:HE2	2:E:434:LEU:HB3	1.72	0.55
3:G:115:THR:HB	3:G:312:SER:HB3	1.88	0.55
4:I:535:PRO:HD3	4:I:1232:TRP:CG	2.41	0.55
4:M:1069:ARG:HH22	4:M:1074:THR:HB	1.71	0.55
7:U:142:LEU:O	7:U:146:ILE:HG12	2.06	0.55
7:U:158:LEU:HB2	7:V:221:LYS:HE3	1.89	0.55
1:A:1607:VAL:HG13	1:A:1608:THR:HG23	1.89	0.55
1:A:1851:THR:HG22	1:A:1877:VAL:HG12	1.89	0.55
4:H:448:THR:HG23	4:H:1113:LEU:HD22	1.88	0.55
5:O:62:LEU:O	5:O:66:ARG:HG2	2.07	0.55
4:I:426:THR:HG22	4:I:1029:HIS:HD2	1.72	0.55
4:K:1041:THR:HG23	4:K:1103:ARG:HB3	1.89	0.55
4:K:1332:LEU:HA	4:K:1335:THR:HG22	1.89	0.55
4:L:666:LEU:HD12	4:L:667:PRO:HD2	1.88	0.55
4:L:726:ASN:HB2	4:L:728:GLU:OE1	2.07	0.55
4:K:1124:HIS:HB3	4:K:1127:VAL:HG12	1.88	0.55
4:M:538:ASP:OD1	4:M:555:ARG:NE	2.38	0.55
4:J:588:PRO:HD2	4:J:683:LEU:HD11	1.90	0.54
4:K:638:MET:HG2	4:K:646:VAL:HG11	1.88	0.54
4:M:726:ASN:ND2	4:M:775:ASP:OD1	2.39	0.54
8:Z:260:ASN:OD1	8:Z:261:GLY:N	2.40	0.54
2:E:365:HIS:CE1	2:E:367:LEU:HB2	2.43	0.54
3:G:30:GLU:HG2	3:G:325:ARG:HB3	1.88	0.54
4:K:601:VAL:HG13	4:K:924:VAL:HG11	1.88	0.54
5:Q:62:LEU:O	5:Q:66:ARG:HG2	2.07	0.54
6:W:86:LEU:HD12	6:W:89:ILE:HD12	1.90	0.54
8:Z:119:ARG:H	8:Z:119:ARG:HD2	1.72	0.54
4:H:615:VAL:HG11	4:H:802:LEU:HD12	1.88	0.54
4:L:1336:LYS:NZ	4:L:1346:THR:OG1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:627:ILE:HG22	4:M:631:VAL:HG23	1.89	0.54
7:X:144:LEU:HD21	7:X:283:ARG:HE	1.71	0.54
7:V:66:ARG:NH1	7:V:283:ARG:O	2.35	0.54
1:A:1834:PRO:HG2	1:A:1838:THR:HG21	1.90	0.54
4:I:388:ASN:HB2	4:I:1311:ILE:HG12	1.89	0.54
4:I:1124:HIS:ND1	4:I:1127:VAL:HG23	2.23	0.54
4:L:440:ILE:HD12	4:L:1108:VAL:HB	1.89	0.54
2:E:259:ASN:OD1	2:E:260:ALA:N	2.41	0.54
2:E:337:TYR:CE2	2:E:431:ARG:HG3	2.39	0.54
4:I:164:LEU:HD21	6:W:20:LEU:HD22	1.90	0.54
4:I:1211:THR:HA	4:I:1214:ILE:HG22	1.88	0.54
4:J:624:PHE:HA	4:J:627:ILE:HG22	1.87	0.54
4:M:263:THR:HB	4:M:296:VAL:HG12	1.90	0.54
7:U:140:MET:HG3	7:U:144:LEU:HD23	1.88	0.54
1:A:1856:GLN:H	1:A:2181:ASP:HB3	1.73	0.54
1:A:2037:ILE:N	1:A:2038:PRO:HD3	2.22	0.54
3:G:355:ASP:OD1	3:G:356:ALA:N	2.40	0.54
4:I:575:THR:HA	4:I:578:ILE:HD12	1.89	0.54
4:J:1331:ALA:O	4:J:1335:THR:HG23	2.06	0.54
1:A:1527:ARG:NH1	1:A:1531:LEU:HD12	2.23	0.54
3:G:311:VAL:HG23	3:G:330:TRP:O	2.08	0.54
4:H:276:THR:HG21	4:H:386:GLU:HG2	1.90	0.54
4:J:1144:ASP:OD1	4:J:1144:ASP:N	2.37	0.54
4:M:545:ASN:O	4:M:545:ASN:ND2	2.40	0.54
4:J:631:VAL:HG13	4:J:647:PHE:CE2	2.43	0.54
5:R:19:ARG:HA	5:R:22:VAL:HG22	1.88	0.54
7:U:228:SER:O	7:U:232:VAL:N	2.36	0.54
1:A:1783:HIS:HA	1:A:1786:VAL:HG12	1.90	0.54
1:A:1786:VAL:HG11	1:A:2066:LEU:HD11	1.89	0.54
1:A:2051:ARG:HD2	1:A:2052:VAL:N	2.23	0.54
2:E:270:TYR:CZ	2:E:273:VAL:HB	2.43	0.54
4:L:1109:ARG:O	4:L:1171:ALA:HA	2.08	0.54
4:M:565:LEU:HG	4:M:1178:PRO:HB3	1.89	0.54
2:E:287:TYR:HB2	2:E:371:PHE:CE2	2.42	0.53
4:K:712:ASP:O	4:K:782:LYS:NZ	2.40	0.53
7:X:223:ALA:HA	7:X:231:LEU:HD21	1.90	0.53
8:Z:140:VAL:HG13	8:Z:142:GLU:H	1.73	0.53
1:A:1486:PHE:HE2	1:A:1519:THR:HG22	1.73	0.53
4:J:133:ALA:HB3	4:J:1071:ILE:HD12	1.90	0.53
5:S:17:LYS:O	5:S:21:VAL:HG23	2.07	0.53
1:A:1689:THR:HG23	1:A:2112:LEU:HD22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:451:HIS:HB3	4:K:1113:LEU:HD23	1.91	0.53
1:A:1653:VAL:HG21	1:A:1962:VAL:HG11	1.90	0.53
1:A:1969:LYS:O	1:A:1969:LYS:HD3	2.09	0.53
1:A:2211:LEU:HD21	2:F:90:LEU:HD12	1.91	0.53
2:E:428:GLN:O	2:E:430:LEU:N	2.41	0.53
4:H:215:ILE:HG21	4:H:1278:LEU:HD11	1.90	0.53
4:K:698:LEU:HD21	4:K:1127:VAL:HG23	1.90	0.53
4:K:1348:GLU:H	4:K:1355:VAL:HG13	1.74	0.53
4:L:201:THR:HG23	4:L:202:LEU:HD22	1.91	0.53
4:M:689:ALA:HB2	4:M:711:HIS:CE1	2.43	0.53
5:O:19:ARG:O	5:O:23:ASN:ND2	2.42	0.53
1:A:1548:ARG:NH2	1:A:1550:GLU:HB3	2.23	0.53
4:H:811:LEU:HD22	4:H:857:LEU:HD13	1.89	0.53
4:I:661:LEU:HB3	4:I:666:LEU:HD12	1.91	0.53
4:J:203:ALA:HB2	4:J:211:GLN:HE22	1.73	0.53
4:L:517:VAL:HG13	4:L:519:THR:H	1.74	0.53
3:G:566:LEU:HD13	7:U:157:SER:HB3	1.91	0.53
4:K:1362:LEU:O	4:K:1366:MET:HG3	2.08	0.53
6:T:76:SER:HB2	6:T:77:PRO:HD3	1.91	0.53
6:T:231:VAL:O	6:T:235:ILE:HG22	2.09	0.53
6:W:80:LEU:HD12	6:W:117:TRP:HZ3	1.74	0.53
7:Y:62:ARG:O	7:Y:66:ARG:HG2	2.08	0.53
1:A:1982:THR:HG22	1:A:1984:ARG:H	1.74	0.53
2:E:284:LEU:HD13	2:E:315:LEU:HD22	1.90	0.53
4:H:567:PRO:HB2	4:H:569:PRO:HD2	1.90	0.53
4:J:148:LEU:HA	4:J:151:ILE:HD12	1.90	0.53
4:K:80:PHE:CZ	4:K:82:ASP:HB2	2.44	0.53
6:W:179:ARG:HB3	6:W:183:GLN:HE22	1.74	0.53
4:I:677:LEU:O	4:I:680:VAL:HG12	2.08	0.53
4:J:138:TYR:O	4:J:153:ASN:ND2	2.35	0.53
5:Q:25:VAL:HA	5:Q:57:LYS:HE2	1.89	0.53
4:I:1147:THR:O	4:I:1151:LEU:HG	2.09	0.53
4:L:624:PHE:HB2	4:L:656:LEU:HD23	1.91	0.53
4:L:1246:THR:HA	4:L:1249:ARG:HB3	1.90	0.53
5:Q:18:HIS:O	5:Q:22:VAL:HG23	2.08	0.53
4:J:794:ASN:OD1	4:J:1000:ASN:ND2	2.35	0.52
2:E:403:VAL:HG22	2:E:407:TRP:CD1	2.44	0.52
4:I:672:PHE:CZ	4:J:643:GLN:HB2	2.44	0.52
4:L:1070:ASP:OD2	6:W:155:TYR:OH	2.17	0.52
4:H:508:THR:HG23	4:H:511:GLU:H	1.75	0.52
8:Z:129:LEU:HD21	8:Z:207:GLY:HA3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:981:HIS:O	4:I:985:ASN:ND2	2.41	0.52
7:U:32:VAL:HG23	7:U:71:THR:HG23	1.91	0.52
2:E:270:TYR:HE2	2:E:274:LEU:H	1.57	0.52
4:M:592:GLU:O	4:M:595:ARG:HG2	2.09	0.52
3:G:41:ARG:HH21	3:G:567:ALA:HB3	1.73	0.52
4:M:1039:THR:HG23	4:M:1261:PRO:HB3	1.91	0.52
6:T:251:LEU:HA	6:T:282:GLU:O	2.10	0.52
1:A:1987:ASP:OD1	1:A:1988:PHE:N	2.43	0.52
1:C:2220:ASP:OD2	2:F:79:LEU:HD13	2.10	0.52
2:E:343:PRO:HG3	2:E:543:ARG:HD2	1.91	0.52
4:K:122:LYS:NZ	4:K:1080:ASN:OD1	2.32	0.52
5:N:37:HIS:ND1	5:N:40:LEU:HB2	2.24	0.52
5:S:33:SER:OG	5:S:34:GLU:N	2.42	0.52
1:A:1602:GLU:HB3	1:A:1607:VAL:HB	1.91	0.52
1:A:1857:ASP:H	1:A:2181:ASP:HB2	1.74	0.52
2:E:280:ALA:HB2	2:E:436:CYS:SG	2.50	0.52
3:G:26:VAL:HG23	3:G:327:ARG:HB2	1.91	0.52
4:I:1034:LEU:HD21	4:I:1174:LEU:HD22	1.92	0.52
4:J:1327:THR:HG22	4:J:1355:VAL:HG13	1.92	0.52
4:L:446:LEU:HD13	4:L:1021:VAL:HG23	1.92	0.52
2:E:580:ASP:OD1	2:E:581:LEU:N	2.42	0.52
4:I:1164:THR:H	4:J:1201:ALA:HB1	1.75	0.52
4:K:940:HIS:O	4:K:944:SER:OG	2.23	0.52
4:L:1069:ARG:HH22	4:L:1074:THR:HG22	1.75	0.52
7:Y:296:ASP:O	7:Y:298:LYS:N	2.43	0.52
1:A:1570:ASP:OD2	1:A:1574:ARG:NH1	2.42	0.52
1:A:1699:LEU:HD21	1:A:1766:VAL:HG13	1.92	0.52
2:E:530:VAL:HG13	2:E:593:HIS:CE1	2.44	0.52
4:H:9:LEU:HD13	4:L:155:GLU:HG3	1.91	0.52
4:K:1297:THR:HG21	4:K:1301:TYR:HD2	1.75	0.52
6:W:288:GLU:OE2	7:X:276:ARG:NH2	2.36	0.52
7:Y:91:LEU:HA	7:Y:303:ILE:HA	1.92	0.52
1:A:2099:PRO:HB3	2:E:605:THR:HG22	1.91	0.51
4:H:810:ASP:O	4:H:814:ARG:NH1	2.43	0.51
4:K:223:MET:O	4:K:227:LEU:HG	2.09	0.51
4:K:1114:PHE:CD1	4:K:1137:VAL:HG11	2.44	0.51
7:Y:43:HIS:HA	7:Y:46:LEU:HD23	1.92	0.51
1:A:1767:GLN:NE2	1:A:2080:GLN:OE1	2.35	0.51
4:L:710:LEU:HD21	4:L:783:VAL:HG22	1.90	0.51
6:W:155:TYR:CG	6:W:159:LYS:HG2	2.44	0.51
3:G:362:ALA:O	3:G:366:VAL:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:7:LEU:HD13	4:K:92:LEU:HG	1.92	0.51
4:H:414:VAL:HG12	4:I:409:THR:HG22	1.93	0.51
4:J:295:THR:HA	4:J:356:SER:HA	1.93	0.51
4:J:1124:HIS:CD2	4:J:1126:GLU:HB3	2.45	0.51
4:J:1128:ASP:O	4:J:1132:ARG:HG2	2.11	0.51
4:L:75:ALA:HB2	4:L:179:PHE:CE2	2.45	0.51
4:L:78:ILE:HB	4:L:1058:ILE:HG22	1.91	0.51
4:L:363:GLY:O	4:L:364:GLU:HG2	2.11	0.51
5:R:21:VAL:HA	5:R:25:VAL:HG22	1.93	0.51
7:V:27:LEU:HD23	7:V:27:LEU:H	1.75	0.51
3:G:86:ARG:NH1	3:G:563:GLU:OE1	2.33	0.51
1:A:1915:ARG:NH1	1:A:1916:VAL:O	2.44	0.51
2:E:635:PHE:HD2	2:E:637:PRO:HD3	1.76	0.51
4:I:1065:THR:N	4:I:1076:HIS:O	2.37	0.51
4:J:138:TYR:CZ	4:J:152:LEU:HD13	2.45	0.51
7:V:177:PHE:CD2	7:V:178:ARG:HG2	2.46	0.51
1:A:1480:ARG:O	1:A:1484:THR:HG23	2.10	0.51
3:G:18:ASP:OD1	3:G:19:GLU:N	2.44	0.51
4:H:1327:THR:HG21	4:H:1333:MET:HB2	1.91	0.51
6:W:67:LEU:C	6:W:68:ILE:HD13	2.31	0.51
1:A:1888:PHE:HA	1:A:1891:GLN:NE2	2.26	0.51
2:E:594:TYR:CZ	2:E:598:LEU:HD11	2.45	0.51
4:H:1362:LEU:HG	4:H:1366:MET:SD	2.49	0.51
4:I:638:MET:HG3	4:I:646:VAL:HG11	1.93	0.51
4:J:985:ASN:O	4:J:988:ARG:NH1	2.44	0.51
4:L:475:MET:O	4:L:479:LEU:HG	2.10	0.51
4:L:1349:THR:HA	4:L:1354:TYR:HA	1.93	0.51
4:I:954:ASP:N	4:I:954:ASP:OD1	2.44	0.51
4:K:451:HIS:CE1	4:K:1117:PHE:HB2	2.45	0.51
4:M:534:HIS:HD2	4:M:536:PHE:H	1.58	0.51
4:M:861:VAL:HG21	4:M:876:CYS:SG	2.51	0.51
5:Q:42:THR:O	5:Q:45:SER:OG	2.21	0.51
7:U:63:GLY:HA2	7:U:66:ARG:HE	1.75	0.51
3:G:411:LEU:O	3:G:415:MET:HG2	2.11	0.51
4:J:775:ASP:O	4:J:779:THR:HG23	2.11	0.51
4:L:805:LYS:HE2	5:R:58:CYS:HB2	1.93	0.51
6:W:53:PRO:HG2	6:W:56:LEU:HD12	1.92	0.51
1:A:1645:ARG:HA	1:A:2163:PHE:HE1	1.76	0.51
4:I:735:ASP:OD1	4:I:736:ARG:N	2.38	0.51
4:K:747:ARG:NH1	4:K:888:GLU:OE2	2.32	0.51
7:X:11:THR:HG22	7:X:80:GLN:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:291:ILE:HG12	4:I:360:ILE:HG22	1.91	0.50
4:I:862:GLU:O	4:I:866:THR:OG1	2.23	0.50
4:J:798:CYS:SG	4:J:799:GLY:N	2.84	0.50
4:M:690:LEU:HD12	4:M:707:VAL:HG21	1.92	0.50
1:A:1663:TRP:CE2	1:A:1744:GLN:HB3	2.46	0.50
2:E:337:TYR:CG	2:E:365:HIS:HD2	2.30	0.50
2:E:350:PRO:HG2	2:E:354:GLY:HA2	1.93	0.50
4:L:400:TYR:HB2	4:L:1179:VAL:HG12	1.93	0.50
4:M:1350:HIS:CD2	4:M:1351:PHE:H	2.29	0.50
4:M:1332:LEU:O	4:M:1336:LYS:HG2	2.12	0.50
1:A:1855:PRO:HB3	1:A:2181:ASP:HA	1.93	0.50
4:I:1121:VAL:HG12	4:I:1132:ARG:HH21	1.76	0.50
4:J:488:MET:HG3	4:J:894:GLU:HB2	1.92	0.50
4:K:291:ILE:HA	4:K:360:ILE:HG22	1.93	0.50
4:L:404:ASP:OD1	4:L:405:ARG:N	2.44	0.50
4:L:1113:LEU:HA	4:L:1116:VAL:HG12	1.93	0.50
1:A:1853:VAL:HG12	1:A:1995:ARG:HB2	1.94	0.50
4:M:138:TYR:O	4:M:153:ASN:ND2	2.44	0.50
7:Y:213:GLU:OE1	7:Y:267:ARG:NH1	2.44	0.50
1:A:2149:ASP:OD1	1:A:2150:THR:N	2.45	0.50
4:I:1175:ILE:HG22	4:I:1244:TYR:CE2	2.47	0.50
1:C:2228:VAL:HG11	2:E:72:VAL:HG11	1.93	0.50
3:G:27:LEU:HB3	3:G:31:VAL:HG11	1.93	0.50
4:L:190:TYR:CD1	4:L:226:THR:HG21	2.47	0.50
4:L:518:VAL:HG22	4:L:1180:THR:HG21	1.93	0.50
4:M:1122:TYR:HB2	4:M:1128:ASP:HB2	1.94	0.50
5:N:39:VAL:HG11	5:N:71:SER:HB3	1.94	0.50
7:Y:53:ASP:OD2	7:Y:60:ARG:NH1	2.44	0.50
2:E:263:ASN:HA	2:E:266:VAL:CG2	2.40	0.50
4:I:785:TYR:O	4:I:943:TYR:OH	2.28	0.50
4:K:681:LEU:O	4:K:685:THR:HG23	2.11	0.50
6:T:136:LYS:O	6:T:137:THR:HG23	2.12	0.50
1:A:1572:LEU:HA	1:A:1575:LEU:HD12	1.93	0.49
1:A:1651:VAL:HG22	1:A:2109:ILE:HD11	1.92	0.49
4:I:450:CYS:O	4:I:1122:TYR:OH	2.25	0.49
4:L:440:ILE:HB	4:L:1108:VAL:HG21	1.94	0.49
4:M:1175:ILE:HG22	4:M:1244:TYR:CE2	2.47	0.49
1:A:1552:ILE:HA	1:A:2022:ARG:HH22	1.76	0.49
2:E:428:GLN:CD	2:E:428:GLN:H	2.15	0.49
4:K:1290:LYS:HE2	4:K:1310:LEU:HB3	1.95	0.49
4:L:538:ASP:OD1	4:L:538:ASP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:941:ARG:HG2	4:L:992:SER:HB3	1.94	0.49
4:M:517:VAL:HG22	4:M:518:VAL:H	1.77	0.49
4:M:857:LEU:O	4:M:861:VAL:HG22	2.11	0.49
1:A:1850:ALA:HB1	1:A:1949:LEU:HD22	1.94	0.49
1:A:1958:VAL:H	1:A:1981:TYR:HB3	1.76	0.49
2:E:337:TYR:HB2	2:E:365:HIS:HD2	1.77	0.49
2:E:502:VAL:O	2:E:506:ILE:HB	2.12	0.49
4:L:886:VAL:HG11	5:R:62:LEU:HD21	1.93	0.49
4:L:1175:ILE:HG22	4:L:1244:TYR:CE2	2.47	0.49
6:T:116:GLN:O	6:T:120:LEU:HB2	2.13	0.49
1:A:1943:THR:HB	1:A:2047:HIS:CE1	2.47	0.49
2:E:349:MET:HB3	2:E:428:GLN:HE21	1.76	0.49
4:J:61:LEU:HD12	4:J:61:LEU:H	1.76	0.49
4:J:1044:VAL:HG21	4:J:1096:VAL:HG13	1.94	0.49
4:L:126:THR:HG21	7:X:39:HIS:HD2	1.76	0.49
5:S:47:TYR:OH	5:S:63:ASP:OD2	2.23	0.49
4:H:941:ARG:NH1	4:H:982:GLU:OE2	2.46	0.49
4:I:596:LEU:HD21	4:I:645:LEU:HB2	1.95	0.49
4:L:448:THR:HG23	4:L:1113:LEU:HD22	1.95	0.49
4:L:1122:TYR:HB2	4:L:1128:ASP:HB2	1.93	0.49
4:L:1285:TYR:HA	4:L:1289:ALA:HB3	1.93	0.49
4:M:495:ILE:HG22	4:M:496:PRO:HD3	1.93	0.49
4:M:534:HIS:CE1	4:M:1239:LEU:HD12	2.47	0.49
1:C:2214:LEU:HD23	2:E:87:GLU:HG3	1.95	0.49
4:I:682:ARG:HA	4:I:685:THR:HG22	1.95	0.49
4:K:77:ALA:HB1	4:K:302:TYR:CD2	2.48	0.49
4:L:400:TYR:OH	4:L:403:GLU:OE2	2.23	0.49
8:Z:19:PHE:CE2	8:Z:37:ILE:HG13	2.48	0.49
1:A:1684:PRO:O	1:A:1687:THR:OG1	2.29	0.49
2:E:460:PHE:CE1	2:E:465:LEU:HD11	2.47	0.49
4:H:498:PHE:O	4:H:501:VAL:HG22	2.12	0.49
4:H:1291:ASP:OD1	4:H:1316:ARG:NH2	2.40	0.49
4:I:426:THR:HG22	4:I:1029:HIS:CD2	2.47	0.49
4:J:689:ALA:HB2	4:J:711:HIS:NE2	2.28	0.49
5:R:64:LEU:O	5:R:68:VAL:HG23	2.12	0.49
7:V:193:LEU:HD11	7:V:197:MET:HB3	1.95	0.49
1:A:1474:SER:O	1:A:1478:LYS:HG2	2.13	0.49
4:H:638:MET:SD	4:H:864:VAL:HG23	2.53	0.49
4:J:592:GLU:O	4:J:595:ARG:HG2	2.13	0.49
4:K:641:THR:HG23	4:K:642:ARG:HG3	1.94	0.49
1:A:1839:PRO:HG3	1:A:1939:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:260:ALA:O	2:E:264:VAL:HG23	2.13	0.49
3:G:85:GLU:HG3	3:G:556:ARG:HG3	1.94	0.49
4:H:211:GLN:O	4:H:215:ILE:HG12	2.13	0.49
4:I:273:MET:N	4:I:368:ILE:O	2.40	0.49
4:J:1124:HIS:O	4:J:1127:VAL:HG12	2.13	0.49
4:L:750:GLY:HA2	5:R:70:VAL:HG11	1.94	0.49
7:X:149:ARG:HH21	7:X:172:LEU:HA	1.77	0.49
1:A:1613:VAL:HG21	1:A:2021:ILE:HD11	1.95	0.48
1:A:1693:LEU:O	1:A:1696:PHE:HB3	2.13	0.48
2:E:337:TYR:HB2	2:E:365:HIS:CD2	2.48	0.48
4:H:438:GLN:HE22	4:H:1107:GLY:HA2	1.78	0.48
4:H:941:ARG:HG2	4:H:992:SER:HB3	1.95	0.48
4:K:1359:ILE:HG23	4:K:1360:ILE:HG13	1.95	0.48
4:L:1034:LEU:HD12	4:L:1174:LEU:HD13	1.95	0.48
1:A:1526:GLU:HB2	1:A:1530:GLN:NE2	2.28	0.48
1:A:1589:ASP:OD1	1:A:1593:MET:N	2.32	0.48
2:E:276:ASP:O	2:E:279:ALA:N	2.46	0.48
4:I:862:GLU:HA	4:I:872:LEU:HG	1.94	0.48
7:U:212:SER:O	7:U:215:THR:HG22	2.13	0.48
1:A:1526:GLU:HB2	1:A:1530:GLN:HE22	1.77	0.48
4:L:262:THR:HG22	4:L:268:LYS:HD3	1.95	0.48
4:M:594:LEU:HD21	4:M:680:VAL:HG21	1.95	0.48
1:C:2215:ARG:HA	1:C:2215:ARG:HE	1.78	0.48
2:E:300:SER:O	2:E:303:THR:OG1	2.31	0.48
2:E:365:HIS:HB3	2:E:368:VAL:HG12	1.95	0.48
2:E:425:HIS:NE2	2:E:426:GLU:OE2	2.46	0.48
4:L:1050:SER:HG	4:L:1054:CYS:HG	1.61	0.48
8:Z:189:ASP:OD1	8:Z:189:ASP:N	2.41	0.48
2:E:460:PHE:CE1	2:E:465:LEU:HD21	2.49	0.48
4:H:82:ASP:OD1	4:H:82:ASP:N	2.35	0.48
4:H:588:PRO:HD2	4:H:683:LEU:HD21	1.96	0.48
4:H:753:ASP:OD2	4:H:756:ARG:HD3	2.13	0.48
4:I:514:GLN:HE21	4:I:563:ASP:HB2	1.78	0.48
4:M:626:LEU:HD21	4:M:881:LEU:HB2	1.96	0.48
5:Q:63:ASP:OD1	5:Q:66:ARG:NH1	2.47	0.48
5:R:14:ARG:HH12	5:R:48:THR:HG21	1.78	0.48
6:W:59:PHE:CE2	6:W:105:VAL:HG11	2.48	0.48
2:E:219:GLY:HA3	2:E:619:PHE:HA	1.96	0.48
4:L:499:TYR:OH	4:L:974:PRO:O	2.18	0.48
4:M:535:PRO:HG3	4:M:1232:TRP:CD2	2.49	0.48
1:A:2106:PRO:HA	1:A:2157:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2230:ASP:O	1:C:2233:GLN:HG3	2.13	0.48
4:H:627:ILE:HG22	4:H:631:VAL:HG23	1.95	0.48
4:K:585:ARG:O	4:K:587:PRO:HD3	2.13	0.48
4:L:77:ALA:HB1	4:L:302:TYR:CD1	2.47	0.48
1:A:1491:LYS:HE2	1:A:1491:LYS:HA	1.95	0.48
1:A:1790:HIS:CD2	1:A:2056:PRO:HG2	2.48	0.48
1:A:1934:LEU:O	1:A:1938:PHE:HB2	2.13	0.48
1:A:2019:ALA:O	1:A:2023:ARG:HG2	2.14	0.48
4:J:1116:VAL:HG13	4:J:1117:PHE:CD2	2.49	0.48
7:U:49:HIS:HA	7:U:52:VAL:HG12	1.94	0.48
1:A:1663:TRP:CD1	1:A:1744:GLN:HB3	2.48	0.48
4:H:1332:LEU:HD13	4:H:1355:VAL:HG13	1.96	0.48
4:I:355:LEU:HD12	4:I:356:SER:H	1.78	0.48
4:I:698:LEU:HD21	4:I:1127:VAL:HG22	1.96	0.48
4:I:730:VAL:HG13	4:I:895:VAL:HG13	1.96	0.48
4:I:1331:ALA:O	4:I:1335:THR:HG23	2.14	0.48
4:J:886:VAL:HG11	5:P:62:LEU:HD11	1.96	0.48
4:J:1109:ARG:HG2	4:J:1169:LYS:HE3	1.96	0.48
4:M:542:CYS:SG	4:M:543:GLN:N	2.87	0.48
3:G:455:GLN:HE21	4:I:1253:GLY:N	2.12	0.48
4:K:280:MET:O	4:K:284:MET:HE3	2.14	0.48
5:S:40:LEU:HD21	5:S:64:LEU:HD11	1.95	0.48
7:U:203:SER:O	7:U:207:VAL:HG13	2.14	0.48
4:H:77:ALA:HB1	4:H:302:TYR:HD2	1.79	0.47
2:E:249:ILE:HG23	2:E:253:LEU:HD23	1.96	0.47
4:I:558:ILE:HD11	4:I:1031:GLY:HA3	1.96	0.47
4:J:1211:THR:HA	4:J:1214:ILE:HG22	1.96	0.47
1:C:2224:LEU:HD11	2:F:79:LEU:HD22	1.97	0.47
2:E:28:GLU:O	2:E:32:ARG:HG2	2.15	0.47
3:G:41:ARG:HG2	3:G:154:PRO:HD3	1.95	0.47
4:M:1038:ARG:NH1	4:M:1040:ASP:OD2	2.46	0.47
8:Z:63:TYR:HE1	8:Z:221:GLU:HG2	1.79	0.47
2:E:525:LEU:HD13	2:E:598:LEU:HD21	1.95	0.47
4:I:1156:MET:HG3	4:I:1301:TYR:CZ	2.49	0.47
4:L:927:PRO:HD2	4:L:952:LEU:HD21	1.96	0.47
1:A:1875:ALA:N	1:A:1879:GLU:OE1	2.40	0.47
4:I:1139:ARG:HD2	4:I:1140:PRO:HD2	1.97	0.47
4:J:194:GLN:NE2	4:J:245:ARG:HD2	2.29	0.47
4:M:652:ALA:O	4:M:656:LEU:HG	2.15	0.47
5:P:21:VAL:HG23	5:P:25:VAL:HB	1.97	0.47
4:H:1267:ASN:O	4:H:1271:ILE:HG12	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:284:MET:HA	4:I:291:ILE:CD1	2.44	0.47
4:I:726:ASN:ND2	4:I:728:GLU:OE1	2.47	0.47
4:K:451:HIS:CE1	4:K:453:VAL:HG23	2.50	0.47
4:K:905:GLN:O	4:K:1123:ARG:NH1	2.48	0.47
4:M:1331:ALA:O	4:M:1335:THR:HG23	2.15	0.47
7:U:33:PRO:HB2	7:U:68:MET:SD	2.54	0.47
3:G:53:ARG:HH11	3:G:553:ARG:HH12	1.62	0.47
4:I:71:LEU:N	4:I:370:GLU:OE2	2.47	0.47
4:J:655:THR:O	4:J:659:GLU:HG2	2.14	0.47
4:J:747:ARG:HG2	4:J:767:PHE:HB3	1.95	0.47
4:L:424:LEU:HD12	4:L:425:PRO:HD2	1.95	0.47
4:L:556:ILE:HG21	4:L:986:TRP:CE2	2.50	0.47
4:L:712:ASP:O	4:L:782:LYS:NZ	2.47	0.47
4:M:460:CYS:HB3	4:M:533:LEU:HD23	1.97	0.47
4:M:862:GLU:HG2	4:M:863:ASP:H	1.79	0.47
3:G:364:GLU:OE1	3:G:558:ARG:NH1	2.48	0.47
4:H:611:TYR:CD1	4:H:923:VAL:HG22	2.50	0.47
4:I:263:THR:HB	4:I:296:VAL:HG12	1.96	0.47
4:I:718:PRO:HG2	4:I:943:TYR:HE2	1.79	0.47
4:J:75:ALA:HB2	4:J:179:PHE:CE2	2.50	0.47
4:L:77:ALA:HB1	4:L:302:TYR:HD1	1.80	0.47
4:L:813:TYR:HA	5:R:65:LEU:HD21	1.97	0.47
6:T:185:VAL:HG12	6:T:206:THR:HG22	1.96	0.47
6:T:251:LEU:HD12	6:T:251:LEU:O	2.15	0.47
7:X:273:VAL:O	7:X:277:GLN:HG2	2.15	0.47
8:Z:248:ASN:O	8:Z:252:ASN:ND2	2.47	0.47
2:E:323:ILE:HD12	2:E:335:ASN:ND2	2.30	0.47
4:I:310:GLU:O	4:I:314:THR:HG23	2.15	0.47
4:I:1350:HIS:CG	4:I:1351:PHE:H	2.32	0.47
6:W:112:ARG:O	6:W:116:GLN:HG2	2.15	0.47
1:A:1645:ARG:HA	1:A:2163:PHE:CE1	2.50	0.47
1:A:1795:ASP:HB3	2:E:453:PHE:HB2	1.96	0.47
4:I:263:THR:OG1	4:I:264:SER:N	2.47	0.47
4:J:669:GLN:O	4:J:673:HIS:ND1	2.46	0.47
4:K:685:THR:HG22	4:K:783:VAL:HG21	1.97	0.47
4:M:790:PRO:HA	4:M:793:THR:HG22	1.96	0.47
1:A:1549:LEU:O	1:A:1552:ILE:HG12	2.14	0.46
1:A:1754:TYR:HE1	1:A:1800:GLN:O	1.97	0.46
2:E:460:PHE:CZ	2:E:465:LEU:HD11	2.50	0.46
2:E:635:PHE:CD2	2:E:637:PRO:HD3	2.50	0.46
1:A:1504:PRO:HD3	1:A:1517:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:92:LEU:HB3	4:L:7:LEU:HD22	1.96	0.46
4:J:715:LEU:HG	4:J:782:LYS:HD3	1.97	0.46
4:K:389:VAL:HG12	4:K:1044:VAL:HG11	1.95	0.46
5:Q:37:HIS:CD2	5:Q:40:LEU:HB2	2.50	0.46
4:K:287:LEU:O	4:K:291:ILE:HG23	2.15	0.46
4:L:451:HIS:ND1	4:L:453:VAL:HG12	2.30	0.46
4:L:1090:TYR:CZ	4:L:1282:ILE:HD11	2.50	0.46
2:E:352:SER:HB2	2:E:356:HIS:ND1	2.31	0.46
4:H:452:PRO:HB3	4:H:905:GLN:HE22	1.80	0.46
4:H:473:PRO:HA	4:H:476:GLN:HG2	1.97	0.46
4:H:1234:SER:OG	4:H:1235:GLN:OE1	2.32	0.46
4:I:1095:CYS:SG	4:I:1096:VAL:N	2.88	0.46
4:J:861:VAL:HG13	4:J:865:ALA:HB3	1.96	0.46
1:A:1979:LEU:HD11	1:A:1988:PHE:HZ	1.80	0.46
4:H:472:GLU:OE1	4:H:1218:ARG:NH1	2.48	0.46
4:H:639:PHE:CD2	4:H:670:LEU:HD21	2.51	0.46
4:H:686:ARG:NH2	4:I:997:THR:HA	2.30	0.46
4:H:1166:HIS:CD2	4:I:1223:GLN:HA	2.51	0.46
4:I:1238:CYS:O	4:I:1242:VAL:HG12	2.16	0.46
4:J:499:TYR:O	4:J:502:ARG:NH2	2.48	0.46
4:K:804:LEU:HD21	4:K:886:VAL:HG22	1.97	0.46
4:L:871:PRO:HD2	4:L:874:GLN:HE22	1.81	0.46
4:L:941:ARG:HD3	4:L:989:SER:HA	1.97	0.46
4:M:534:HIS:CD2	4:M:536:PHE:H	2.32	0.46
1:A:1585:LEU:HA	1:A:1913:MET:HA	1.98	0.46
2:E:350:PRO:HD2	2:E:428:GLN:HE21	1.80	0.46
2:E:606:LEU:HD12	2:E:606:LEU:O	2.14	0.46
4:H:597:PHE:CD2	4:H:792:MET:HG2	2.50	0.46
4:H:601:VAL:HG13	4:H:924:VAL:HG11	1.98	0.46
4:H:1039:THR:OG1	4:H:1261:PRO:HB3	2.16	0.46
4:I:542:CYS:SG	4:I:543:GLN:N	2.89	0.46
4:I:770:ASP:OD1	4:I:770:ASP:N	2.48	0.46
4:I:917:LEU:HD21	4:I:937:VAL:HG21	1.98	0.46
4:L:810:ASP:O	4:L:814:ARG:NH1	2.48	0.46
4:M:156:ALA:O	4:M:160:VAL:HG23	2.15	0.46
4:M:1111:GLN:HB3	4:M:1171:ALA:HB1	1.98	0.46
1:A:1957:PRO:O	1:A:2038:PRO:HG2	2.15	0.46
2:E:326:TRP:HE1	2:E:332:ALA:HB1	1.81	0.46
2:E:524:GLY:HA3	2:E:631:LEU:HA	1.97	0.46
4:H:662:ALA:HB1	4:I:605:ASN:HD22	1.81	0.46
4:H:1067:GLU:HB3	4:H:1074:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1215:TYR:CE2	4:H:1268:THR:HG21	2.51	0.46
5:R:49:ARG:HA	5:R:49:ARG:NE	2.30	0.46
7:U:60:ARG:O	7:U:64:LEU:HG	2.16	0.46
7:Y:270:ALA:O	7:Y:274:MET:HG2	2.16	0.46
2:E:442:LEU:HD21	2:E:601:LEU:HB2	1.98	0.46
4:H:174:GLY:HA3	4:I:101:ALA:HB3	1.97	0.46
4:I:968:ARG:NH2	4:I:970:ASP:OD2	2.49	0.46
4:J:420:VAL:HG22	4:J:577:GLU:HG2	1.98	0.46
4:J:446:LEU:HD13	4:J:1021:VAL:HG23	1.96	0.46
4:J:651:TYR:HB2	4:J:784:PHE:CD2	2.51	0.46
4:J:867:ASP:HB2	4:J:870:THR:HG22	1.98	0.46
4:J:1332:LEU:HD13	4:J:1355:VAL:HG23	1.98	0.46
4:K:1315:CYS:HA	4:K:1318:THR:HG22	1.98	0.46
6:W:245:THR:HG22	6:W:290:VAL:HG12	1.97	0.46
4:J:787:CYS:HB3	4:J:1005:VAL:HG13	1.98	0.46
4:L:1211:THR:HA	4:L:1214:ILE:HG22	1.97	0.46
4:L:1350:HIS:N	4:L:1353:ASN:O	2.37	0.46
5:S:37:HIS:ND1	5:S:40:LEU:HD23	2.31	0.46
7:U:153:MET:SD	7:U:169:VAL:HG12	2.56	0.46
7:U:175:ILE:HD11	7:U:184:ILE:HD11	1.97	0.46
1:A:1663:TRP:HA	1:A:1666:ILE:HG22	1.97	0.46
1:A:1839:PRO:HG3	1:A:1939:ILE:HD13	1.97	0.46
1:A:2103:ASN:ND2	2:E:317:ASP:HA	2.31	0.46
4:I:1064:VAL:HG22	4:I:1077:VAL:HG12	1.98	0.46
1:A:1981:TYR:CZ	1:A:1988:PHE:HB3	2.51	0.45
1:A:2001:GLN:N	1:A:2001:GLN:OE1	2.47	0.45
1:C:2235:MET:HA	1:C:2239:TYR:HD1	1.81	0.45
1:C:2239:TYR:HB3	2:F:57:ARG:HH22	1.81	0.45
2:E:226:LYS:NZ	2:E:243:GLN:O	2.44	0.45
4:H:194:GLN:HA	4:H:197:VAL:HG12	1.98	0.45
4:I:522:TYR:HB3	4:I:1228:THR:O	2.16	0.45
4:J:420:VAL:HG11	4:J:577:GLU:HA	1.97	0.45
4:K:895:VAL:N	4:K:914:GLN:O	2.32	0.45
1:A:1516:GLY:HA2	1:A:1519:THR:HG23	1.98	0.45
1:A:1643:THR:HG22	1:A:2186:VAL:HG11	1.98	0.45
4:K:473:PRO:HA	4:K:476:GLN:HG2	1.98	0.45
4:L:1114:PHE:CD2	4:L:1137:VAL:HG21	2.51	0.45
7:X:238:LEU:HG	7:X:239:MET:H	1.82	0.45
1:A:1799:GLU:HG3	1:A:2164:GLY:HA3	1.99	0.45
1:A:1867:LYS:NZ	1:A:1874:TYR:O	2.40	0.45
1:C:2238:LEU:HD23	1:C:2239:TYR:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:318:ASP:HA	2:E:321:ARG:HG2	1.97	0.45
4:H:1239:LEU:O	4:H:1243:LEU:HD23	2.16	0.45
4:K:983:TYR:O	4:K:988:ARG:NH2	2.49	0.45
6:W:67:LEU:O	6:W:68:ILE:HD13	2.17	0.45
6:W:234:ARG:NH2	7:X:209:ASN:OD1	2.49	0.45
8:Z:48:ARG:O	8:Z:51:VAL:HG12	2.17	0.45
8:Z:67:ARG:HG2	8:Z:67:ARG:HH11	1.81	0.45
1:A:1456:TYR:CD1	1:A:1482:LEU:HD11	2.51	0.45
4:H:274:VAL:HG12	4:H:370:GLU:HB3	1.97	0.45
4:J:600:THR:HG23	4:J:644:LEU:HG	1.99	0.45
4:J:988:ARG:HB2	4:J:990:PRO:HD2	1.98	0.45
6:T:244:CYS:HB3	7:U:273:VAL:HG11	1.97	0.45
7:X:152:ILE:HD12	7:Y:268:LEU:HD23	1.97	0.45
7:X:202:LEU:HD22	7:Y:230:LEU:HD13	1.97	0.45
1:A:2236:ARG:HH12	2:F:66:ARG:HB2	1.81	0.45
4:H:178:SER:O	4:H:182:THR:HG23	2.17	0.45
4:J:315:ALA:HB2	4:J:321:ILE:HG22	1.98	0.45
4:K:178:SER:O	4:K:182:THR:HG23	2.16	0.45
4:M:1046:MET:SD	4:M:1096:VAL:HG22	2.57	0.45
5:R:63:ASP:HA	5:R:66:ARG:HG2	1.98	0.45
4:H:785:TYR:O	4:H:943:TYR:OH	2.33	0.45
4:I:662:ALA:HB1	4:J:605:ASN:HB3	1.98	0.45
4:M:575:THR:HG22	4:M:1010:ALA:HB3	1.98	0.45
8:Z:80:PHE:CZ	8:Z:125:VAL:HG23	2.51	0.45
1:A:2019:ALA:HA	1:A:2022:ARG:CZ	2.47	0.45
4:H:93:PHE:HE2	4:H:118:LYS:HG3	1.82	0.45
4:H:189:PRO:HD3	4:H:1286:LEU:HD21	1.97	0.45
4:H:1044:VAL:HG11	4:H:1096:VAL:HG13	1.98	0.45
4:K:400:TYR:HB3	4:K:1179:VAL:HG12	1.97	0.45
4:K:409:THR:HG23	4:K:410:VAL:HG13	1.99	0.45
4:M:315:ALA:HB2	4:M:321:ILE:HD11	1.99	0.45
4:M:811:LEU:HD23	4:M:812:PHE:CE2	2.52	0.45
4:M:1029:HIS:ND1	4:M:1030:PRO:O	2.44	0.45
5:P:62:LEU:O	5:P:66:ARG:HG2	2.17	0.45
6:W:252:GLY:HA3	6:W:279:PHE:CE1	2.52	0.45
2:E:442:LEU:HB2	2:E:602:LEU:HD22	1.99	0.45
2:E:529:ALA:O	2:E:597:GLY:HA3	2.17	0.45
4:H:478:LEU:HD11	4:H:509:VAL:HG23	1.98	0.45
4:H:597:PHE:HA	4:H:600:THR:HG22	1.98	0.45
6:T:290:VAL:OXT	7:U:277:GLN:NE2	2.50	0.45
4:I:339:LEU:HB2	4:L:13:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:633:ARG:HD3	4:J:870:THR:HG21	1.98	0.45
4:J:1142:LEU:HD12	4:J:1143:LEU:O	2.17	0.45
4:M:280:MET:O	4:M:284:MET:HG2	2.17	0.45
7:V:214:LEU:HB3	7:V:218:TYR:CE2	2.52	0.45
7:Y:113:PRO:HG3	7:Y:135:PRO:HA	1.99	0.45
2:E:533:SER:HB3	2:E:597:GLY:CA	2.46	0.45
4:J:684:VAL:HG21	4:J:1005:VAL:HG12	1.99	0.45
4:J:706:TYR:CE1	4:J:900:ASP:HB2	2.52	0.45
4:J:874:GLN:HA	4:J:877:ARG:HB2	1.99	0.45
4:L:241:LYS:O	4:L:244:THR:HG22	2.16	0.45
5:S:63:ASP:HA	5:S:66:ARG:HD2	1.99	0.45
7:U:34:ILE:O	7:U:69:THR:HG22	2.17	0.45
1:A:1456:TYR:CE1	1:A:1482:LEU:HD11	2.52	0.44
1:A:1526:GLU:O	1:A:1529:VAL:HG12	2.17	0.44
2:E:31:LEU:HD22	2:E:32:ARG:NH2	2.32	0.44
2:E:217:SER:N	2:E:638:SER:O	2.48	0.44
3:G:115:THR:HG22	3:G:115:THR:O	2.17	0.44
4:J:895:VAL:HB	4:J:914:GLN:HB2	1.99	0.44
4:K:1155:SER:OG	4:K:1255:ASN:ND2	2.49	0.44
4:M:1121:VAL:HG12	4:M:1132:ARG:HH21	1.81	0.44
5:S:22:VAL:HA	5:S:26:LEU:HD12	1.99	0.44
6:W:250:LYS:O	6:W:284:GLY:N	2.48	0.44
4:I:92:LEU:HB3	4:L:7:LEU:HD13	1.99	0.44
4:K:426:THR:HG23	4:K:427:THR:HG23	2.00	0.44
4:K:1177:THR:OG1	4:K:1181:MET:SD	2.70	0.44
4:L:441:ASP:OD1	4:L:441:ASP:N	2.49	0.44
4:M:388:ASN:HB2	4:M:1311:ILE:HD12	1.98	0.44
4:M:424:LEU:HD12	4:M:425:PRO:HD2	1.99	0.44
4:M:1034:LEU:HD13	4:M:1174:LEU:HD22	1.99	0.44
5:Q:31:GLU:HG2	5:Q:32:ILE:HD12	1.99	0.44
6:T:134:CYS:O	6:T:149:VAL:HG22	2.18	0.44
6:T:252:GLY:HA3	6:T:279:PHE:CE2	2.53	0.44
8:Z:17:VAL:O	8:Z:21:ARG:HG3	2.17	0.44
8:Z:90:ARG:HH11	8:Z:90:ARG:HG2	1.81	0.44
4:H:459:PRO:HA	4:H:462:GLN:HG2	1.99	0.44
4:I:127:ILE:HD13	4:I:170:ALA:HB1	1.99	0.44
4:I:1349:THR:HA	4:I:1354:TYR:HA	1.98	0.44
4:I:1365:SER:O	4:I:1369:ASN:OD1	2.35	0.44
4:M:228:PHE:O	4:M:232:ARG:HG3	2.18	0.44
4:M:1113:LEU:HA	4:M:1116:VAL:HG12	1.99	0.44
5:N:34:GLU:H	5:N:34:GLU:CD	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:63:GLY:HA2	7:U:66:ARG:NE	2.32	0.44
8:Z:74:SER:HA	8:Z:77:LEU:HB3	2.00	0.44
4:H:93:PHE:CE2	4:H:118:LYS:HG3	2.52	0.44
4:J:601:VAL:HG13	4:J:924:VAL:HG11	2.00	0.44
4:L:73:ALA:HA	4:L:261:TYR:CZ	2.52	0.44
4:M:451:HIS:CE1	4:M:453:VAL:HG23	2.52	0.44
4:M:970:ASP:O	4:M:993:ARG:NH1	2.50	0.44
6:W:76:SER:OG	6:W:77:PRO:HD3	2.17	0.44
1:A:1657:GLN:OE1	1:A:2045:GLN:NE2	2.40	0.44
1:A:1756:GLU:HG2	1:A:2104:ARG:H	1.83	0.44
2:E:53:MET:HA	2:E:56:VAL:HG12	2.00	0.44
2:E:622:ASN:HB2	2:E:626:GLU:OE1	2.18	0.44
4:H:891:LYS:HB3	4:H:891:LYS:HE2	1.78	0.44
4:I:73:ALA:HA	4:I:261:TYR:CE2	2.52	0.44
4:I:96:GLN:HB3	4:I:113:THR:HG22	1.99	0.44
4:I:1254:TYR:CZ	4:I:1256:SER:HA	2.52	0.44
4:L:300:ALA:HB2	4:L:353:THR:HG23	2.00	0.44
4:L:805:LYS:HB2	4:L:889:HIS:NE2	2.31	0.44
4:M:898:PRO:HB2	4:M:904:ARG:NH2	2.32	0.44
7:V:157:SER:OG	7:V:188:VAL:HG11	2.18	0.44
2:E:336:TYR:O	2:E:365:HIS:HA	2.17	0.44
4:H:188:PRO:HD2	4:H:1092:SER:O	2.17	0.44
4:H:430:LEU:O	4:H:438:GLN:N	2.51	0.44
4:K:752:SER:O	5:Q:66:ARG:NH1	2.51	0.44
4:L:631:VAL:O	4:L:635:ILE:HG12	2.17	0.44
4:M:763:ASP:OD1	4:M:763:ASP:N	2.50	0.44
4:M:1332:LEU:HD13	4:M:1355:VAL:HG23	1.99	0.44
7:Y:124:LEU:HD23	7:Y:124:LEU:H	1.83	0.44
1:A:1753:LEU:HD21	1:A:1785:VAL:HG11	2.00	0.44
2:E:322:GLU:OE1	2:E:366:VAL:HG22	2.18	0.44
2:E:623:ASP:OD1	2:E:624:ILE:N	2.50	0.44
3:G:391:ALA:HB3	3:G:503:ILE:HD11	2.00	0.44
4:I:433:ARG:HB2	4:I:1102:VAL:HG21	2.00	0.44
4:I:611:TYR:CZ	4:I:923:VAL:HG23	2.53	0.44
4:I:927:PRO:HB2	4:I:930:LEU:HB3	1.99	0.44
4:I:1121:VAL:HG12	4:I:1132:ARG:NH2	2.33	0.44
4:I:1231:PRO:O	4:I:1235:GLN:HG2	2.18	0.44
4:K:682:ARG:NH2	4:K:776:ASP:OD2	2.44	0.44
4:K:880:PHE:O	4:K:883:VAL:HG12	2.17	0.44
4:L:71:LEU:HD13	4:L:372:LEU:HD11	1.99	0.44
4:M:862:GLU:O	4:M:864:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:18:HIS:CE1	5:N:44:LEU:HB3	2.53	0.44
5:S:33:SER:OG	5:S:34:GLU:OE1	2.35	0.44
6:W:167:ILE:O	6:W:274:VAL:N	2.37	0.44
6:W:227:ARG:O	6:W:231:VAL:HG23	2.17	0.44
4:I:801:GLY:HA3	4:I:890:VAL:HB	2.00	0.44
4:K:108:THR:O	4:K:110:ARG:NH1	2.51	0.44
4:K:651:TYR:HB2	4:K:784:PHE:CD1	2.52	0.44
7:X:145:GLU:OE1	7:X:175:ILE:HG23	2.18	0.44
7:Y:270:ALA:HA	7:Y:273:VAL:HG12	2.00	0.44
1:A:1486:PHE:CZ	1:A:1515:LEU:HG	2.53	0.44
1:C:2203:LEU:HD23	1:C:2203:LEU:HA	1.81	0.44
4:H:216:LEU:O	4:H:220:LYS:HG3	2.18	0.44
4:H:628:ARG:HG3	4:H:661:LEU:HD13	2.00	0.44
4:H:664:GLY:O	4:H:666:LEU:N	2.50	0.44
4:H:1282:ILE:O	4:H:1286:LEU:HG	2.18	0.44
4:I:309:PRO:O	4:I:313:VAL:HG23	2.18	0.44
4:I:456:GLU:OE2	4:I:905:GLN:NE2	2.51	0.44
4:I:459:PRO:HB2	4:I:1242:VAL:HG21	2.00	0.44
4:L:427:THR:HG22	4:L:441:ASP:HB3	1.99	0.44
4:L:574:ARG:O	4:L:577:GLU:HG2	2.18	0.44
7:U:31:VAL:HG21	7:U:137:ILE:HG13	2.00	0.44
7:V:273:VAL:HA	7:V:276:ARG:HD3	1.98	0.44
6:W:137:THR:HG1	6:W:147:THR:HG1	1.66	0.44
1:A:1698:TYR:HD1	1:A:1699:LEU:HD12	1.82	0.43
2:E:330:VAL:HG11	2:E:364:ARG:HG2	2.00	0.43
2:E:428:GLN:C	2:E:430:LEU:N	2.70	0.43
2:E:531:THR:O	2:E:535:ARG:HG2	2.18	0.43
3:G:46:ARG:NH2	3:G:557:ASP:OD1	2.49	0.43
3:G:388:GLN:HA	3:G:539:PHE:HA	2.00	0.43
4:H:631:VAL:O	4:H:635:ILE:HG22	2.18	0.43
4:H:651:TYR:HB2	4:H:784:PHE:CD1	2.53	0.43
4:I:9:LEU:HD13	4:J:316:ILE:HD11	1.99	0.43
4:I:80:PHE:N	4:I:1059:ILE:O	2.43	0.43
4:I:419:THR:HG22	4:I:421:ARG:H	1.82	0.43
4:K:1043:GLU:OE1	4:K:1101:ARG:HD2	2.18	0.43
5:Q:43:MET:HB3	5:Q:47:TYR:CZ	2.52	0.43
7:X:8:ILE:HB	7:X:83:LEU:HB2	2.00	0.43
8:Z:63:TYR:HB2	8:Z:224:CYS:SG	2.58	0.43
1:A:1548:ARG:HG3	1:A:1551:ASP:OD2	2.18	0.43
3:G:453:LYS:HB3	3:G:455:GLN:OE1	2.17	0.43
4:I:600:THR:HG21	4:I:645:LEU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:807:LEU:HD23	4:I:808:LEU:HD22	1.99	0.43
8:Z:239:LEU:HD21	8:Z:250:CYS:HB3	1.99	0.43
4:H:192:VAL:O	4:H:196:LEU:HG	2.18	0.43
4:H:1166:HIS:NE2	4:I:1223:GLN:HA	2.33	0.43
4:J:900:ASP:OD1	4:J:1014:LYS:NZ	2.37	0.43
4:M:1066:LYS:NZ	4:M:1068:GLU:OE2	2.34	0.43
4:M:1297:THR:HG21	4:M:1301:TYR:CD2	2.51	0.43
6:T:252:GLY:HA3	6:T:279:PHE:HE2	1.83	0.43
8:Z:188:LEU:HD22	8:Z:202:LYS:HG3	2.00	0.43
1:A:2065:ARG:HD3	1:A:2065:ARG:HA	1.88	0.43
1:C:2235:MET:HA	1:C:2239:TYR:CD1	2.53	0.43
4:H:173:ARG:NH1	4:H:375:VAL:O	2.48	0.43
4:H:449:LEU:HD21	4:H:1034:LEU:HD21	1.99	0.43
4:I:528:THR:O	4:I:531:THR:HG22	2.17	0.43
4:I:1109:ARG:CZ	4:I:1169:LYS:HG3	2.48	0.43
4:M:1327:THR:HG22	4:M:1355:VAL:HG13	2.01	0.43
6:W:164:ALA:HB2	6:W:277:ASP:HA	1.98	0.43
1:A:1765:PRO:HB3	1:A:2118:PRO:O	2.19	0.43
2:E:350:PRO:HD2	2:E:428:GLN:CG	2.48	0.43
2:E:428:GLN:O	2:E:429:TYR:C	2.55	0.43
4:H:399:LEU:HD23	4:H:1183:VAL:HG22	2.01	0.43
4:I:271:GLY:C	4:I:367:VAL:HG23	2.38	0.43
4:J:461:LEU:O	4:J:465:THR:HG23	2.18	0.43
4:L:472:GLU:HB2	4:L:475:MET:HG2	2.01	0.43
4:L:595:ARG:O	4:L:599:THR:HG23	2.18	0.43
4:M:701:GLU:OE1	4:M:714:ARG:NH2	2.42	0.43
4:M:1235:GLN:N	4:M:1235:GLN:OE1	2.51	0.43
7:X:32:VAL:O	7:X:71:THR:OG1	2.34	0.43
1:A:1503:LEU:HD13	1:A:1590:VAL:HB	1.99	0.43
1:A:1609:ASP:O	1:A:1832:VAL:HG11	2.19	0.43
4:I:192:VAL:O	4:I:196:LEU:HG	2.19	0.43
4:I:209:ARG:HG2	4:I:212:ARG:HH22	1.84	0.43
4:I:718:PRO:HD2	4:I:785:TYR:HB3	2.01	0.43
4:K:535:PRO:HB3	4:K:1232:TRP:CZ2	2.53	0.43
7:X:62:ARG:NH1	7:X:147:ASN:OD1	2.52	0.43
7:Y:278:LEU:O	7:Y:282:ILE:HG12	2.18	0.43
1:A:1814:MET:HG2	1:A:2054:ARG:HB2	2.01	0.43
1:A:1957:PRO:HG3	1:A:2036:PHE:HA	1.99	0.43
2:E:223:TYR:OH	2:E:245:ASP:O	2.25	0.43
4:H:1361:PRO:O	4:H:1365:SER:OG	2.29	0.43
4:I:565:LEU:HD23	4:I:1232:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:565:LEU:HG	4:K:1178:PRO:HB3	2.00	0.43
4:K:1116:VAL:HG13	4:K:1117:PHE:CD2	2.52	0.43
4:L:1121:VAL:HG12	4:L:1132:ARG:NH2	2.33	0.43
1:A:1526:GLU:HA	1:A:1529:VAL:HG12	2.01	0.43
1:A:1939:ILE:HG13	1:A:1940:GLN:N	2.34	0.43
4:J:600:THR:HA	4:J:644:LEU:HD12	2.00	0.43
4:L:950:ALA:HA	4:L:956:ILE:HB	2.00	0.43
7:V:31:VAL:HG12	7:V:137:ILE:HD11	2.01	0.43
7:V:62:ARG:O	7:V:66:ARG:HG3	2.18	0.43
7:Y:222:LEU:HB3	7:Y:231:LEU:HD13	2.00	0.43
1:A:1705:HIS:HE2	1:A:2070:GLU:CD	2.21	0.43
1:A:1796:HIS:HA	2:E:451:SER:HB2	2.00	0.43
1:A:2104:ARG:NE	1:A:2153:THR:HB	2.33	0.43
1:A:2236:ARG:HH22	2:F:66:ARG:HB2	1.84	0.43
4:H:12:LYS:HG2	4:L:56:THR:HB	2.00	0.43
4:L:627:ILE:O	4:L:627:ILE:HG22	2.19	0.43
4:L:815:PRO:HA	4:L:818:LEU:HG	2.01	0.43
1:A:1813:ALA:HB2	1:A:2051:ARG:HH12	1.84	0.43
1:A:1863:TRP:HH2	1:A:1880:LEU:HG	1.84	0.43
2:E:207:MET:HE1	2:E:465:LEU:HD13	2.01	0.43
3:G:85:GLU:O	3:G:88:THR:HG22	2.18	0.43
4:H:410:VAL:CG1	4:H:414:VAL:HG22	2.49	0.43
4:H:1220:ALA:HB1	4:H:1225:PHE:HA	2.01	0.43
4:I:147:ILE:O	4:I:151:ILE:HG12	2.19	0.43
4:J:661:LEU:HD13	4:J:666:LEU:HD11	2.00	0.43
4:K:614:ASP:HA	4:K:653:LEU:HD21	2.00	0.43
6:W:173:LEU:HD21	6:W:175:TRP:NE1	2.34	0.43
7:X:21:VAL:O	7:X:25:THR:HG23	2.18	0.43
8:Z:250:CYS:O	8:Z:253:ILE:HG12	2.19	0.43
1:A:1835:GLN:HG2	1:A:1838:THR:HG23	2.00	0.42
4:H:87:THR:HG21	7:V:16:LEU:HD12	2.00	0.42
4:H:1175:ILE:HG22	4:H:1244:TYR:CE2	2.55	0.42
4:J:1098:TYR:HD2	4:J:1100:ASN:HD22	1.67	0.42
4:K:459:PRO:O	4:K:463:THR:HG23	2.18	0.42
4:L:495:ILE:HB	4:L:496:PRO:HD3	2.01	0.42
4:M:556:ILE:HD12	4:M:899:LEU:HD11	2.01	0.42
6:W:58:GLU:HB2	6:W:106:TYR:CE1	2.54	0.42
8:Z:275:PHE:HA	8:Z:278:TYR:CE2	2.54	0.42
1:A:1596:ILE:O	1:A:1604:ILE:HG12	2.18	0.42
2:E:301:VAL:O	2:E:305:LEU:HG	2.18	0.42
2:E:339:TYR:CB	2:E:364:ARG:HD2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:355:ARG:HH11	2:E:355:ARG:C	2.22	0.42
2:E:604:VAL:HG22	2:E:606:LEU:H	1.84	0.42
4:H:774:THR:OG1	4:H:777:GLU:OE1	2.31	0.42
4:I:638:MET:SD	4:I:864:VAL:HG13	2.59	0.42
4:I:752:SER:HA	5:O:63:ASP:OD1	2.19	0.42
4:K:310:GLU:H	4:K:310:GLU:HG2	1.64	0.42
4:L:449:LEU:HD21	4:L:1032:PHE:CE1	2.54	0.42
4:L:1180:THR:O	4:L:1180:THR:HG22	2.19	0.42
4:M:594:LEU:HD13	4:M:594:LEU:HA	1.93	0.42
4:M:646:VAL:HG23	4:M:647:PHE:CD2	2.54	0.42
6:T:227:ARG:O	6:T:231:VAL:HG23	2.19	0.42
7:V:216:MET:O	7:V:219:VAL:HG12	2.18	0.42
6:W:184:TYR:CE1	6:W:210:ALA:HB2	2.53	0.42
1:A:1800:GLN:NE2	2:E:450:ASP:HA	2.34	0.42
1:A:1999:LEU:HB2	1:A:2021:ILE:CG2	2.50	0.42
2:E:450:ASP:OD1	2:E:451:SER:N	2.52	0.42
3:G:417:TRP:HE3	3:G:485:VAL:HG13	1.85	0.42
3:G:517:GLN:HA	3:G:518:PRO:HD3	1.93	0.42
4:I:489:GLY:HA2	4:I:735:ASP:HA	2.01	0.42
4:J:495:ILE:HG21	4:J:938:PRO:HD2	2.01	0.42
4:K:75:ALA:HB2	4:K:179:PHE:CE2	2.54	0.42
4:L:21:THR:OG1	4:L:22:HIS:N	2.48	0.42
4:M:698:LEU:HD11	4:M:1130:TRP:CG	2.54	0.42
6:W:243:LEU:HD12	6:W:244:CYS:SG	2.60	0.42
1:A:1604:ILE:O	1:A:1608:THR:OG1	2.27	0.42
1:A:1794:PRO:HG2	1:A:1977:ARG:NH2	2.35	0.42
4:H:645:LEU:HD12	4:H:648:ALA:HB2	2.01	0.42
4:J:706:TYR:O	4:J:1019:SER:HB2	2.19	0.42
4:J:1208:GLU:O	4:J:1211:THR:HG22	2.19	0.42
4:K:329:LYS:O	4:K:333:THR:HG23	2.19	0.42
4:K:763:ASP:OD1	4:K:763:ASP:N	2.51	0.42
1:A:1793:PRO:HG2	2:E:494:ARG:NH1	2.33	0.42
1:A:1863:TRP:CE3	1:A:1877:VAL:HA	2.55	0.42
2:E:224:ARG:HH22	2:E:618:LEU:HD22	1.83	0.42
2:E:226:LYS:HE3	2:E:246:ASN:O	2.18	0.42
2:E:258:VAL:HG12	2:E:262:GLU:OE2	2.18	0.42
4:I:776:ASP:OD1	4:I:776:ASP:N	2.50	0.42
4:I:917:LEU:HD23	4:I:917:LEU:HA	1.91	0.42
4:J:276:THR:HG21	4:J:386:GLU:HG2	2.00	0.42
4:L:222:LYS:O	4:L:226:THR:HG22	2.20	0.42
4:L:804:LEU:O	4:L:808:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:1221:ASP:OD1	4:M:1222:ALA:N	2.52	0.42
5:S:28:LEU:HG	5:S:29:PRO:HD2	2.01	0.42
1:A:1552:ILE:HA	1:A:2022:ARG:NH2	2.34	0.42
1:A:1579:ARG:HG3	1:A:1580:HIS:CE1	2.55	0.42
4:I:657:ILE:O	4:I:661:LEU:HB2	2.20	0.42
4:J:611:TYR:CZ	4:J:923:VAL:HG23	2.55	0.42
4:K:80:PHE:CE1	4:K:82:ASP:HB2	2.55	0.42
6:T:49:ARG:O	7:V:104:LYS:NZ	2.42	0.42
7:U:109:CYS:N	7:U:138:VAL:O	2.47	0.42
1:A:1698:TYR:HE2	1:A:2074:THR:HA	1.85	0.42
3:G:6:TYR:OH	7:V:220:ARG:HA	2.20	0.42
3:G:457:LEU:HD23	6:W:116:GLN:OE1	2.20	0.42
4:H:156:ALA:O	4:H:159:THR:HG22	2.20	0.42
4:J:478:LEU:HB2	4:J:509:VAL:HG22	2.02	0.42
4:L:455:HIS:CD2	4:L:1017:PRO:HG3	2.53	0.42
4:L:461:LEU:HD13	4:L:552:CYS:HB2	2.02	0.42
4:M:849:GLN:OE1	4:M:871:PRO:HB2	2.20	0.42
1:A:1806:ILE:HG21	1:A:2053:LEU:HD13	2.00	0.42
1:A:1995:ARG:HE	1:A:1997:LEU:HD21	1.84	0.42
2:E:35:LEU:HD13	3:G:380:ARG:NH1	2.35	0.42
2:E:316:ALA:HA	2:E:319:VAL:HG22	2.02	0.42
3:G:531:PHE:CZ	3:G:543:SER:HB3	2.55	0.42
4:J:147:ILE:O	4:J:151:ILE:HG13	2.20	0.42
4:J:657:ILE:HG12	4:J:661:LEU:HD12	2.01	0.42
4:K:1210:ALA:O	4:K:1214:ILE:HG23	2.19	0.42
4:L:1059:ILE:HG22	4:L:1081:ILE:HG22	2.02	0.42
4:M:611:TYR:CZ	4:M:923:VAL:HG23	2.55	0.42
5:Q:57:LYS:H	5:Q:57:LYS:HG2	1.62	0.42
6:T:61:ALA:HB3	6:T:266:HIS:NE2	2.34	0.42
1:A:1959:CYS:O	1:A:2040:VAL:N	2.49	0.42
2:E:366:VAL:HG13	2:E:367:LEU:HD13	2.02	0.42
4:H:438:GLN:NE2	4:H:1108:VAL:HG13	2.34	0.42
4:H:453:VAL:HG13	4:H:1243:LEU:HD11	2.02	0.42
4:I:988:ARG:HB2	4:I:990:PRO:HD2	2.02	0.42
4:J:597:PHE:CE1	4:J:648:ALA:HB1	2.54	0.42
4:J:723:LEU:HD13	4:J:768:VAL:HG11	2.02	0.42
4:K:263:THR:HB	4:K:267:ALA:HB3	2.02	0.42
5:N:44:LEU:O	5:N:48:THR:HG23	2.20	0.42
6:W:133:GLY:HA3	6:W:149:VAL:O	2.19	0.42
7:X:108:LEU:HD12	7:X:288:PHE:HB2	2.01	0.42
7:X:152:ILE:HD11	7:Y:272:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:19:PHE:CD2	8:Z:20:LEU:HD22	2.55	0.42
2:E:271:ASP:O	2:E:272:CYS:C	2.57	0.42
3:G:311:VAL:HB	3:G:331:TYR:CD1	2.55	0.42
4:H:360:ILE:HG23	4:H:362:LEU:HD22	2.00	0.42
4:I:1222:ALA:C	4:I:1224:THR:H	2.24	0.42
4:K:438:GLN:OE1	4:K:1108:VAL:HG22	2.20	0.42
4:M:212:ARG:NH2	4:M:1203:ASP:OD1	2.50	0.42
4:M:731:GLN:HB3	4:M:738:PRO:HB3	2.02	0.42
4:M:754:VAL:HG21	5:S:50:MET:HE1	2.02	0.42
7:V:45:GLN:O	7:V:50:GLN:NE2	2.49	0.42
7:V:168:ALA:O	7:V:172:LEU:HD23	2.20	0.42
7:V:281:LEU:HD12	7:V:282:ILE:HG23	2.02	0.42
1:A:1675:LEU:HD21	1:A:2078:TYR:CD1	2.54	0.41
2:E:337:TYR:HD1	2:E:365:HIS:HB2	1.85	0.41
4:H:491:ALA:O	4:H:495:ILE:HG13	2.20	0.41
4:H:1144:ASP:H	4:H:1147:THR:HG22	1.85	0.41
4:I:469:PRO:HA	4:I:470:PRO:HD3	1.96	0.41
4:J:798:CYS:HA	4:J:943:TYR:HB3	2.01	0.41
7:Y:13:ASP:H	7:Y:43:HIS:CD2	2.38	0.41
1:A:1880:LEU:HD23	1:A:1880:LEU:HA	1.92	0.41
1:A:2207:VAL:O	1:A:2211:LEU:HG	2.19	0.41
4:I:632:ALA:HB2	4:I:661:LEU:HD11	2.02	0.41
4:M:647:PHE:CD1	4:M:653:LEU:HD13	2.55	0.41
4:M:1040:ASP:OD1	4:M:1106:MET:HG2	2.19	0.41
7:U:88:HIS:CE1	7:U:306:GLY:H	2.38	0.41
7:Y:51:PHE:CG	7:Y:64:LEU:HD13	2.54	0.41
2:E:365:HIS:ND1	2:E:368:VAL:N	2.68	0.41
4:I:607:PRO:HG2	4:I:610:CYS:SG	2.60	0.41
4:I:1065:THR:HB	4:I:1076:HIS:HB2	2.02	0.41
4:I:1124:HIS:CE1	4:I:1126:GLU:HB2	2.55	0.41
4:L:622:ASP:HA	4:L:625:LEU:HD23	2.03	0.41
4:L:968:ARG:NH2	4:M:691:PRO:O	2.52	0.41
4:M:426:THR:HG23	4:M:427:THR:HG23	2.01	0.41
4:M:651:TYR:CZ	4:M:655:THR:HG21	2.55	0.41
4:M:1043:GLU:OE2	4:M:1101:ARG:HB2	2.19	0.41
6:W:18:ASN:O	6:W:22:THR:HG23	2.20	0.41
7:X:55:THR:HG22	7:X:57:GLY:H	1.85	0.41
1:A:1456:TYR:OH	1:A:1486:PHE:HD1	2.04	0.41
1:A:1663:TRP:NE1	1:A:1744:GLN:HB3	2.36	0.41
1:A:1685:ALA:HA	1:A:1688:HIS:CE1	2.55	0.41
2:E:538:TRP:CH2	2:E:540:PRO:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:473:TRP:CZ2	3:G:526:THR:HG22	2.55	0.41
4:I:4:TRP:CD1	4:I:36:ARG:HG3	2.55	0.41
4:I:59:ASN:HB2	4:J:95:VAL:HA	2.02	0.41
4:I:534:HIS:ND1	4:I:535:PRO:HD2	2.35	0.41
4:J:133:ALA:N	4:J:1071:ILE:O	2.43	0.41
4:K:637:ASN:O	4:K:641:THR:HG22	2.21	0.41
4:L:495:ILE:HD12	4:L:937:VAL:HG12	2.01	0.41
4:M:230:LEU:HD12	4:M:1097:ALA:O	2.20	0.41
4:M:798:CYS:SG	4:M:799:GLY:N	2.93	0.41
4:M:817:PHE:O	4:M:820:MET:HG2	2.19	0.41
7:V:296:ASP:O	7:V:298:LYS:N	2.54	0.41
1:A:2101:PRO:HB3	2:E:320:SER:HB2	2.02	0.41
1:A:2181:ASP:OD1	1:A:2182:GLU:N	2.54	0.41
2:E:270:TYR:C	2:E:272:CYS:N	2.72	0.41
4:H:1334:GLU:O	4:H:1338:LYS:HG3	2.20	0.41
4:I:1285:TYR:HA	4:I:1289:ALA:HB2	2.03	0.41
4:J:178:SER:O	4:J:182:THR:HG23	2.20	0.41
4:K:734:ALA:HB2	4:K:739:LEU:HD11	2.02	0.41
4:K:1133:HIS:HD1	4:K:1133:HIS:C	2.24	0.41
7:U:268:LEU:HD23	7:U:271:LEU:HD23	2.02	0.41
7:X:148:GLN:O	7:X:152:ILE:HG12	2.21	0.41
1:A:2019:ALA:HA	1:A:2022:ARG:NE	2.36	0.41
2:F:91:ASN:HB3	2:F:93:GLN:HG3	2.03	0.41
3:G:41:ARG:NH2	3:G:567:ALA:HB3	2.36	0.41
3:G:388:GLN:NE2	3:G:537:GLY:O	2.53	0.41
4:J:1243:LEU:HD23	4:J:1244:TYR:CE2	2.55	0.41
4:K:449:LEU:HD21	4:K:1034:LEU:HD21	2.02	0.41
4:L:263:THR:HG23	4:L:266:GLY:H	1.85	0.41
4:L:1090:TYR:CE2	4:L:1282:ILE:HD11	2.56	0.41
4:M:71:LEU:HD22	4:M:372:LEU:HD11	2.02	0.41
4:M:704:SER:HA	4:M:707:VAL:HG12	2.02	0.41
7:X:156:PHE:CE1	7:X:160:ARG:HG3	2.55	0.41
1:A:1880:LEU:O	1:A:1884:LEU:HG	2.21	0.41
2:E:319:VAL:O	2:E:323:ILE:HG12	2.21	0.41
2:E:371:PHE:O	2:E:375:GLY:N	2.54	0.41
4:H:13:VAL:HG23	4:K:339:LEU:O	2.21	0.41
4:H:1232:TRP:O	4:H:1238:CYS:HB3	2.21	0.41
4:H:1315:CYS:O	4:H:1319:GLN:N	2.48	0.41
4:I:473:PRO:HA	4:I:476:GLN:HB3	2.03	0.41
4:J:344:LEU:H	4:J:344:LEU:HD22	1.85	0.41
4:J:1121:VAL:HG23	4:J:1128:ASP:OD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:61:LEU:H	4:K:61:LEU:HD12	1.86	0.41
4:K:708:ASN:OD1	4:K:709:ALA:N	2.52	0.41
4:M:710:LEU:HD12	4:M:1012:LEU:HD12	2.02	0.41
4:M:1190:ASN:OD1	4:M:1223:GLN:NE2	2.53	0.41
7:U:96:ASN:ND2	7:U:297:ASN:O	2.45	0.41
8:Z:119:ARG:HD2	8:Z:119:ARG:N	2.35	0.41
8:Z:154:ILE:HG21	8:Z:208:ARG:HD3	2.03	0.41
1:A:1585:LEU:HD11	1:A:1904:LEU:HD11	2.02	0.41
1:A:1960:LEU:HB2	1:A:1978:HIS:HD2	1.85	0.41
2:E:270:TYR:O	2:E:273:VAL:HG23	2.21	0.41
2:E:340:ARG:HB3	2:E:361:THR:HA	2.03	0.41
2:E:499:GLU:O	2:E:502:VAL:HG12	2.21	0.41
3:G:5:LEU:HD13	3:G:306:TRP:CD2	2.55	0.41
4:H:647:PHE:HB3	4:H:653:LEU:HB3	2.03	0.41
4:H:714:ARG:NH1	4:H:898:PRO:O	2.52	0.41
4:H:1032:PHE:HA	4:H:1179:VAL:HG22	2.02	0.41
4:I:1119:MET:HG2	4:I:1148:ILE:HD12	2.03	0.41
4:I:1149:SER:OG	6:W:117:TRP:NE1	2.41	0.41
4:J:1175:ILE:HG22	4:J:1244:TYR:CE2	2.56	0.41
4:M:610:CYS:SG	4:M:646:VAL:HB	2.61	0.41
4:M:970:ASP:HB2	4:M:993:ARG:HD3	2.01	0.41
4:M:1121:VAL:HG12	4:M:1132:ARG:NH2	2.36	0.41
8:Z:194:THR:HG23	8:Z:197:VAL:H	1.86	0.41
1:A:1574:ARG:NE	1:A:1604:ILE:HG22	2.34	0.41
2:E:354:GLY:O	2:E:427:GLN:HA	2.20	0.41
2:F:41:THR:HA	4:K:500:ARG:HH22	1.86	0.41
3:G:70:ASP:OD1	3:G:547:LEU:N	2.54	0.41
4:H:434:ASP:OD1	4:H:435:ARG:N	2.54	0.41
4:H:455:HIS:NE2	4:H:1017:PRO:HG3	2.36	0.41
4:H:556:ILE:H	4:H:556:ILE:HG12	1.69	0.41
4:H:633:ARG:NH1	4:H:867:ASP:OD2	2.51	0.41
4:H:1291:ASP:O	4:H:1311:ILE:N	2.48	0.41
4:I:75:ALA:HB2	4:I:179:PHE:CZ	2.56	0.41
4:I:558:ILE:HD12	4:I:1015:ILE:HD11	2.03	0.41
4:I:998:CYS:SG	4:I:1004:SER:HB2	2.61	0.41
4:K:694:ASN:ND2	4:K:704:SER:HB3	2.32	0.41
4:K:989:SER:N	4:K:990:PRO:HD2	2.36	0.41
4:K:997:THR:HG23	4:L:583:ARG:HD3	2.02	0.41
4:L:539:PHE:O	4:L:540:THR:OG1	2.39	0.41
4:L:1104:THR:HB	4:L:1170:ALA:HB2	2.03	0.41
4:L:1231:PRO:O	4:L:1235:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:47:THR:HG22	6:T:149:VAL:HG12	2.03	0.41
6:T:69:ARG:HH21	6:T:79:HIS:CE1	2.38	0.41
7:U:115:PHE:HB2	7:U:183:THR:HG23	2.03	0.41
7:U:291:CYS:SG	7:V:37:ARG:HD3	2.61	0.41
6:W:108:ALA:O	6:W:112:ARG:HG2	2.21	0.41
6:W:127:ARG:HH22	6:W:243:LEU:HD11	1.85	0.41
6:W:285:ASP:OD1	6:W:285:ASP:N	2.47	0.41
7:X:292:ASP:HB3	7:X:301:THR:OG1	2.19	0.41
1:A:2220:ASP:O	1:A:2223:GLN:HG3	2.21	0.41
2:E:524:GLY:HA2	2:E:634:GLY:HA2	2.03	0.41
4:H:386:GLU:HA	4:H:1045:ASP:HA	2.03	0.41
4:H:504:GLU:HG3	4:H:966:TYR:OH	2.21	0.41
4:I:174:GLY:HA3	4:J:101:ALA:HB3	2.02	0.41
4:I:790:PRO:HA	4:I:793:THR:HG22	2.02	0.41
4:I:1139:ARG:O	4:I:1141:GLN:N	2.53	0.41
4:I:1283:ASP:O	4:I:1287:LEU:HD23	2.21	0.41
4:J:1154:GLY:O	4:J:1255:ASN:ND2	2.53	0.41
4:K:83:LEU:HD23	4:K:83:LEU:HA	1.87	0.41
4:L:1021:VAL:HG21	4:L:1134:ALA:HB1	2.03	0.41
4:L:1102:VAL:HG12	4:L:1104:THR:H	1.86	0.41
4:M:807:LEU:O	4:M:811:LEU:HB2	2.21	0.41
1:A:1955:GLY:HA2	1:A:1992:GLN:HE22	1.86	0.40
4:H:1054:CYS:SG	4:H:1055:THR:HG22	2.60	0.40
4:I:179:PHE:CE2	4:I:183:LEU:HD11	2.56	0.40
4:I:495:ILE:HD12	4:I:976:PRO:HG2	2.04	0.40
4:J:224:LEU:HD23	4:J:224:LEU:HA	1.85	0.40
4:J:1260:SER:HB2	4:J:1263:ALA:HB2	2.02	0.40
4:L:624:PHE:CB	4:L:656:LEU:HD23	2.51	0.40
4:M:93:PHE:HB2	4:M:116:VAL:HG22	2.02	0.40
4:M:191:PHE:CE1	4:M:192:VAL:HG13	2.55	0.40
4:M:419:THR:HG23	4:M:580:GLU:OE2	2.21	0.40
7:V:262:ASP:N	7:V:262:ASP:OD1	2.54	0.40
8:Z:8:LEU:HD21	8:Z:12:ASP:HB2	2.02	0.40
8:Z:70:ASN:HA	8:Z:71:PRO:HD3	1.92	0.40
1:A:1473:ARG:O	1:A:1477:GLU:OE1	2.39	0.40
4:H:699:ALA:O	4:H:700:GLU:HB2	2.21	0.40
4:H:793:THR:O	4:H:796:ARG:HG2	2.21	0.40
4:I:200:ALA:HB1	4:L:20:LEU:O	2.21	0.40
4:I:811:LEU:HD21	4:I:857:LEU:HD21	2.03	0.40
4:I:817:PHE:HB3	4:I:880:PHE:CE2	2.55	0.40
4:J:118:LYS:HE2	4:J:118:LYS:HB2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:336:GLN:HA	4:K:337:PRO:HD3	1.93	0.40
5:N:21:VAL:O	5:N:25:VAL:HB	2.21	0.40
6:W:179:ARG:HB3	6:W:183:GLN:NE2	2.36	0.40
7:Y:46:LEU:HD11	7:Y:132:LEU:HD11	2.02	0.40
8:Z:122:ALA:HA	8:Z:125:VAL:HG12	2.03	0.40
1:A:1876:SER:OG	1:A:1879:GLU:HG3	2.21	0.40
1:C:2209:SER:O	1:C:2213:ILE:HG12	2.21	0.40
4:H:180:LEU:HD23	4:H:384:PRO:HG2	2.03	0.40
4:H:420:VAL:HG21	4:H:577:GLU:HA	2.04	0.40
4:H:873:LEU:HA	4:H:876:CYS:SG	2.61	0.40
4:H:1348:GLU:O	4:H:1355:VAL:HG22	2.21	0.40
4:I:970:ASP:OD1	4:I:970:ASP:N	2.40	0.40
4:I:1144:ASP:OD1	4:I:1144:ASP:N	2.53	0.40
4:J:704:SER:HA	4:J:707:VAL:HG12	2.03	0.40
4:J:760:MET:SD	4:J:888:GLU:HA	2.61	0.40
4:K:98:PRO:HD2	4:L:378:ASN:HB2	2.04	0.40
4:K:578:ILE:HG21	4:K:687:ILE:HG23	2.03	0.40
4:K:1217:HIS:NE2	4:K:1235:GLN:HB3	2.36	0.40
4:L:257:ASN:OD1	4:L:259:THR:HG22	2.22	0.40
4:M:709:ALA:HA	4:M:1014:LYS:HE3	2.01	0.40
4:M:1222:ALA:C	4:M:1224:THR:H	2.24	0.40
4:M:1268:THR:O	4:M:1272:ILE:HG12	2.22	0.40
6:W:47:THR:HG22	6:W:149:VAL:HG12	2.03	0.40
7:X:125:LEU:HD12	7:X:132:LEU:HB2	2.03	0.40
4:H:609:LEU:HD11	4:H:861:VAL:HG22	2.03	0.40
4:I:609:LEU:HD21	4:I:630:PHE:HE2	1.87	0.40
4:J:209:ARG:HA	4:J:212:ARG:HG2	2.03	0.40
4:K:724:PRO:HB3	4:K:778:TRP:CE2	2.57	0.40
4:L:85:LYS:HG2	4:M:48:ILE:O	2.21	0.40
4:L:146:THR:O	4:L:150:LYS:HG3	2.21	0.40
4:L:753:ASP:OD2	4:L:756:ARG:NH2	2.53	0.40
4:M:36:ARG:NH2	4:M:44:GLU:OE1	2.53	0.40
4:J:926:ALA:HB2	4:J:948:ILE:HG13	2.02	0.40
4:M:446:LEU:HD21	4:M:1021:VAL:HG13	2.04	0.40
5:Q:17:LYS:O	5:Q:21:VAL:HG12	2.21	0.40
7:U:114:LEU:HD23	7:U:185:PRO:HD3	2.02	0.40
8:Z:170:ASN:ND2	8:Z:185:ASP:OD1	2.38	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	710/2241 (32%)	695 (98%)	15 (2%)	0	100	100
1	C	38/2241 (2%)	38 (100%)	0	0	100	100
2	E	483/642 (75%)	459 (95%)	22 (5%)	2 (0%)	30	66
2	F	81/642 (13%)	80 (99%)	1 (1%)	0	100	100
3	G	467/594 (79%)	451 (97%)	16 (3%)	0	100	100
4	H	1303/1370 (95%)	1241 (95%)	61 (5%)	1 (0%)	48	81
4	I	1346/1370 (98%)	1281 (95%)	64 (5%)	1 (0%)	48	81
4	J	1313/1370 (96%)	1251 (95%)	61 (5%)	1 (0%)	48	81
4	K	1290/1370 (94%)	1235 (96%)	55 (4%)	0	100	100
4	L	1346/1370 (98%)	1290 (96%)	55 (4%)	1 (0%)	48	81
4	M	1346/1370 (98%)	1288 (96%)	55 (4%)	3 (0%)	44	76
5	N	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	O	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
5	P	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	Q	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
5	S	61/75 (81%)	61 (100%)	0	0	100	100
6	T	238/290 (82%)	228 (96%)	10 (4%)	0	100	100
6	W	288/290 (99%)	277 (96%)	11 (4%)	0	100	100
7	U	288/306 (94%)	270 (94%)	17 (6%)	1 (0%)	37	71
7	V	282/306 (92%)	265 (94%)	15 (5%)	2 (1%)	19	55
7	X	291/306 (95%)	275 (94%)	16 (6%)	0	100	100
7	Y	279/306 (91%)	268 (96%)	10 (4%)	1 (0%)	30	66
8	Z	282/1048 (27%)	275 (98%)	6 (2%)	1 (0%)	30	66
All	All	12037/17882 (67%)	11527 (96%)	496 (4%)	14 (0%)	50	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	266	GLY
4	I	266	GLY
4	M	760	MET
4	M	886	VAL
7	Y	297	ASN
2	E	336	TYR
2	E	429	TYR
7	U	75	ARG
4	L	1223	GLN
8	Z	193	ASN
7	V	297	ASN
4	J	795	ASN
4	M	268	LYS
7	V	78	GLY

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	647/1941 (33%)	643 (99%)	4 (1%)	84 88
1	C	38/1941 (2%)	38 (100%)	0	100 100
2	E	422/526 (80%)	414 (98%)	8 (2%)	52 70
2	F	76/526 (14%)	73 (96%)	3 (4%)	27 50
3	G	397/500 (79%)	388 (98%)	9 (2%)	45 64
4	H	1142/1192 (96%)	1132 (99%)	10 (1%)	75 83
4	I	1175/1192 (99%)	1169 (100%)	6 (0%)	86 90
4	J	1146/1192 (96%)	1138 (99%)	8 (1%)	81 86
4	K	1129/1192 (95%)	1121 (99%)	8 (1%)	81 86
4	L	1175/1192 (99%)	1165 (99%)	10 (1%)	75 83
4	M	1175/1192 (99%)	1167 (99%)	8 (1%)	81 86
5	N	59/68 (87%)	59 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	O	59/68 (87%)	59 (100%)	0	100 100
5	P	59/68 (87%)	58 (98%)	1 (2%)	56 73
5	Q	59/68 (87%)	59 (100%)	0	100 100
5	R	59/68 (87%)	58 (98%)	1 (2%)	56 73
5	S	59/68 (87%)	59 (100%)	0	100 100
6	T	211/252 (84%)	209 (99%)	2 (1%)	75 83
6	W	252/252 (100%)	246 (98%)	6 (2%)	44 63
7	U	262/273 (96%)	260 (99%)	2 (1%)	79 84
7	V	260/273 (95%)	254 (98%)	6 (2%)	45 64
7	X	263/273 (96%)	261 (99%)	2 (1%)	79 84
7	Y	257/273 (94%)	254 (99%)	3 (1%)	67 79
8	Z	255/883 (29%)	252 (99%)	3 (1%)	67 79
All	All	10636/15473 (69%)	10536 (99%)	100 (1%)	74 83

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1473	ARG
1	A	1548	ARG
1	A	1915	ARG
1	A	2206	ASN
2	E	73	GLN
2	E	95	GLU
2	E	271	ASP
2	E	272	CYS
2	E	274	LEU
2	E	275	SER
2	E	349	MET
2	E	503	ARG
2	F	15	PHE
2	F	57	ARG
2	F	63	GLN
3	G	79	ASP
3	G	82	PHE
3	G	160	ASP
3	G	447	ARG
3	G	484	GLN
3	G	514	TRP

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Mol	Chain	Res	Type
3	G	535	LEU
3	G	553	ARG
3	G	559	PHE
4	H	82	ASP
4	H	99	ARG
4	H	199	ASN
4	H	305	PHE
4	H	432	ASN
4	H	441	ASP
4	H	714	ARG
4	H	1208	GLU
4	H	1235	GLN
4	H	1368	PHE
4	I	62	GLU
4	I	80	PHE
4	I	441	ASP
4	I	477	ARG
4	I	511	GLU
4	I	1115	ARG
4	J	135	CYS
4	J	576	TRP
4	J	577	GLU
4	J	585	ARG
4	J	869	HIS
4	J	1045	ASP
4	J	1047	LEU
4	J	1316	ARG
4	K	208	ASN
4	K	502	ARG
4	K	672	PHE
4	K	769	ASP
4	K	988	ARG
4	K	1111	GLN
4	K	1153	PHE
4	K	1303	CYS
4	L	36	ARG
4	L	99	ARG
4	L	361	ARG
4	L	589	ASP
4	L	775	ASP
4	L	1101	ARG
4	L	1115	ARG

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Mol	Chain	Res	Type
4	L	1181	MET
4	L	1294	ARG
4	L	1368	PHE
4	M	186	LYS
4	M	357	MET
4	M	394	PHE
4	M	422	ASN
4	M	435	ARG
4	M	441	ASP
4	M	449	LEU
4	M	1101	ARG
5	P	75	ARG
5	R	19	ARG
6	T	100	CYS
6	T	278	ASN
7	U	60	ARG
7	U	214	LEU
7	V	58	TYR
7	V	73	MET
7	V	74	ARG
7	V	103	GLU
7	V	262	ASP
7	V	292	ASP
6	W	28	ARG
6	W	42	ASP
6	W	102	LEU
6	W	148	CYS
6	W	155	TYR
6	W	263	PHE
7	X	119	LEU
7	X	159	ASP
7	Y	56	ARG
7	Y	75	ARG
7	Y	196	ASP
8	Z	99	ARG
8	Z	121	ASP
8	Z	144	LEU

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

Mol	Chain	Res	Type
1	A	1796	HIS

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Mol	Chain	Res	Type
1	A	2206	ASN
2	E	93	GLN
2	E	335	ASN
4	I	432	ASN
4	I	1184	ASN
4	J	432	ASN
4	J	438	GLN
4	J	1166	HIS
4	K	451	HIS
4	L	1248	HIS
4	M	697	GLN
4	M	915	HIS
4	M	965	HIS
5	N	18	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

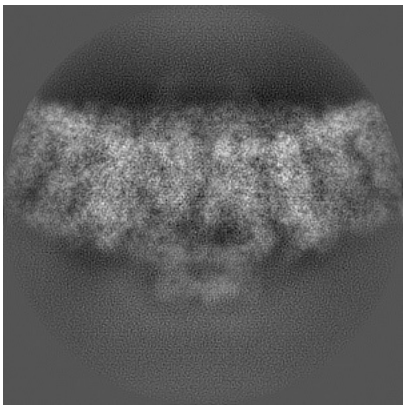
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41202. These allow visual inspection of the internal detail of the map and identification of artifacts.

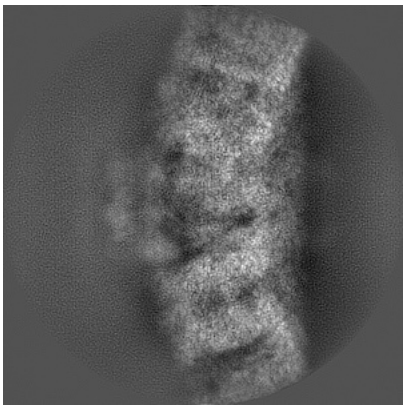
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

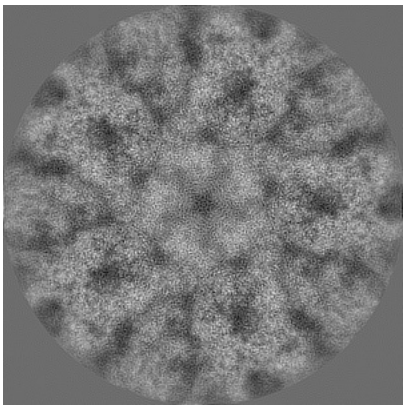
6.1.1 Primary map



X

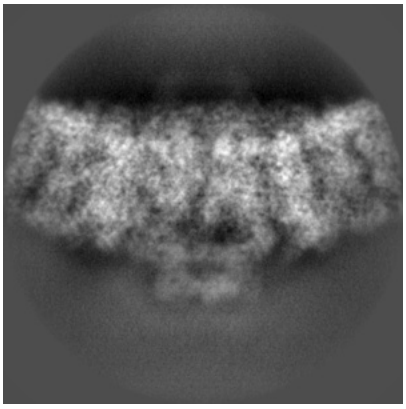


Y

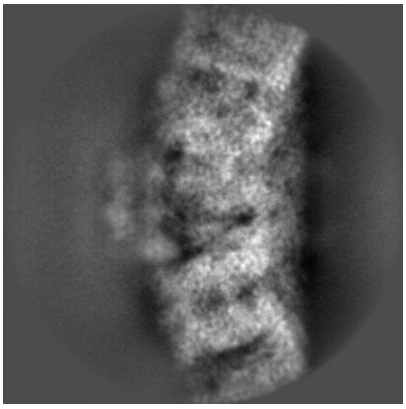


Z

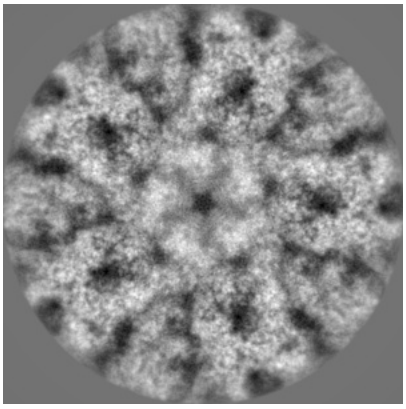
6.1.2 Raw map



X



Y

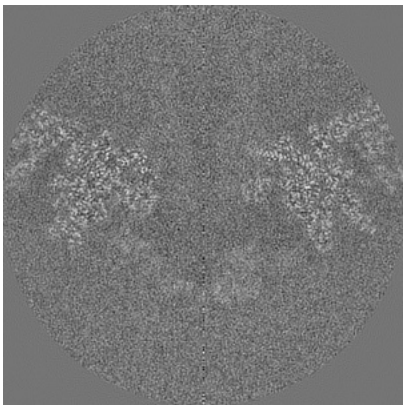


Z

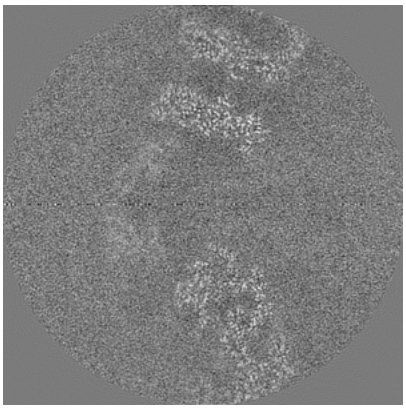
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

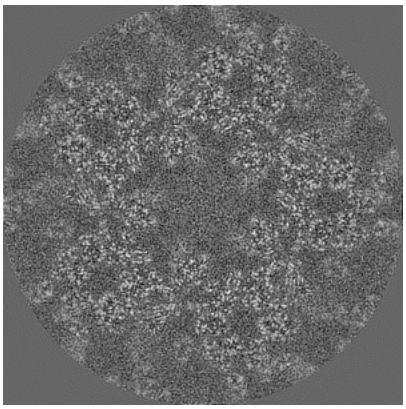
6.2.1 Primary map



X Index: 180

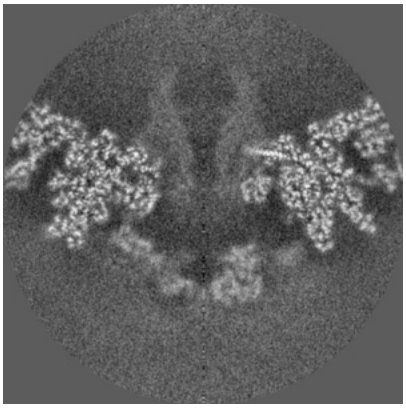


Y Index: 180

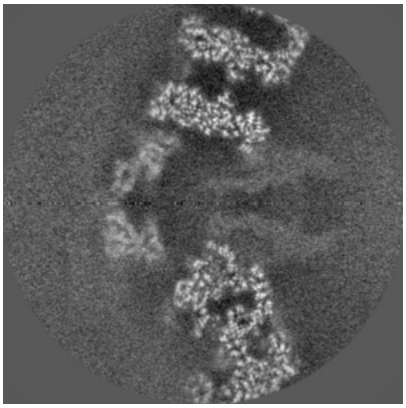


Z Index: 180

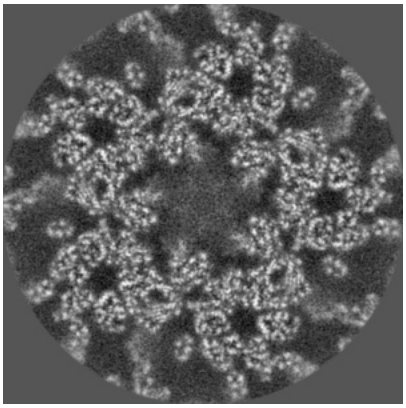
6.2.2 Raw map



X Index: 180



Y Index: 180

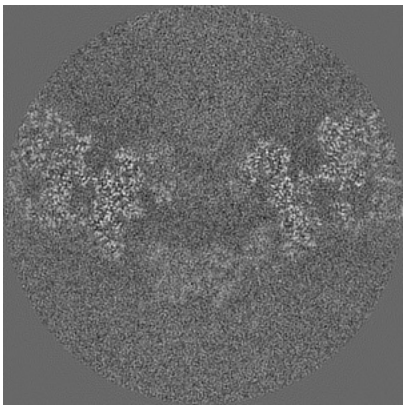


Z Index: 180

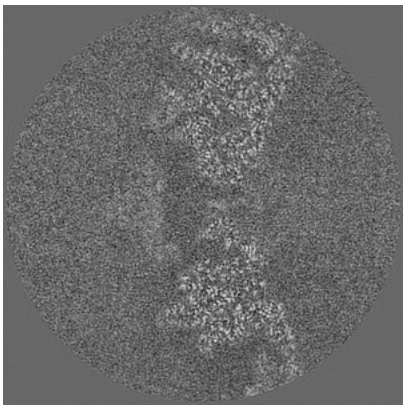
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

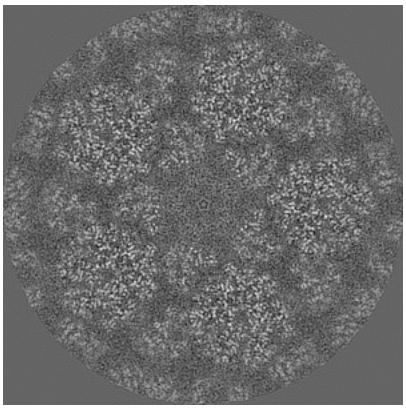
6.3.1 Primary map



X Index: 204

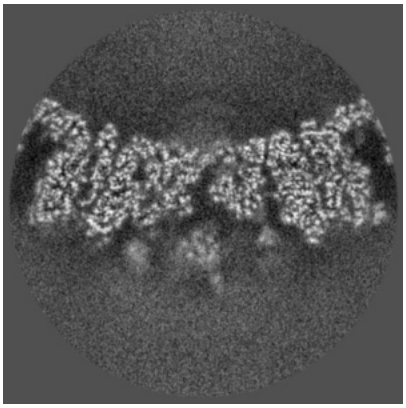


Y Index: 217

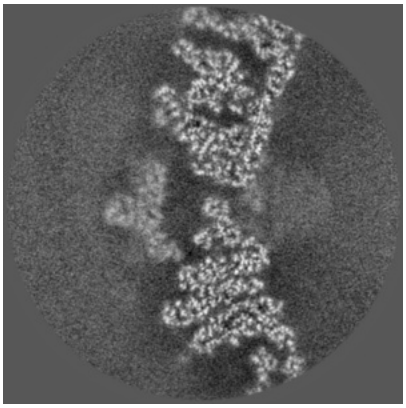


Z Index: 203

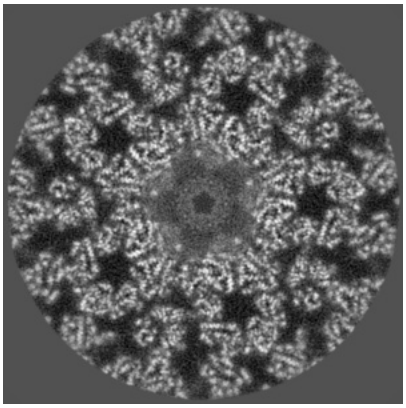
6.3.2 Raw map



X Index: 230



Y Index: 220

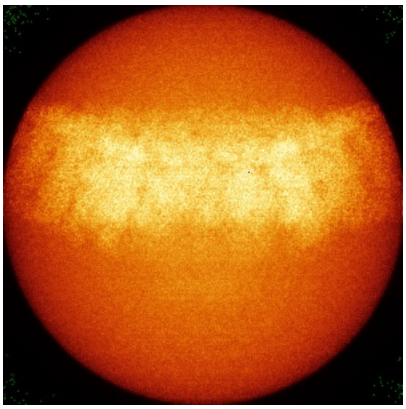


Z Index: 223

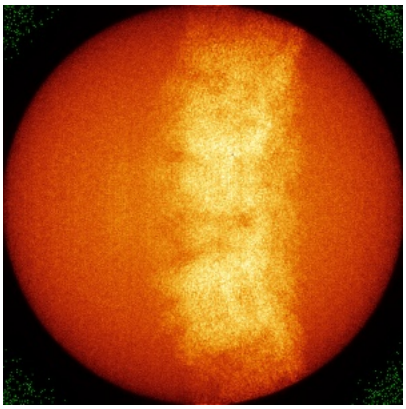
The images above show the largest variance slices of the map in three orthogonal directions.

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

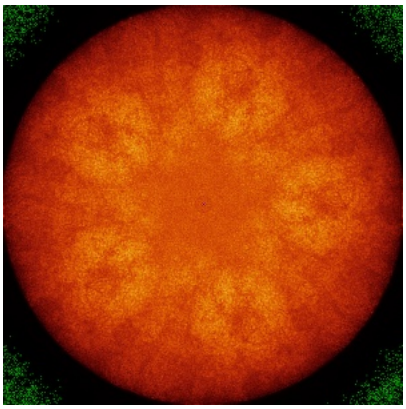
6.4.1 Primary map



X

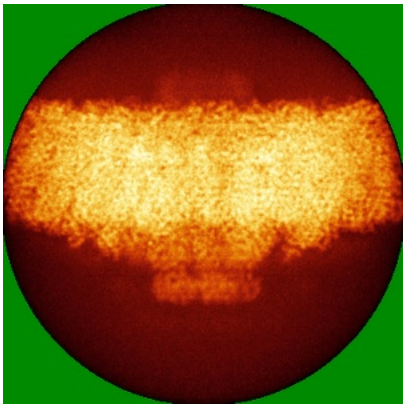


Y

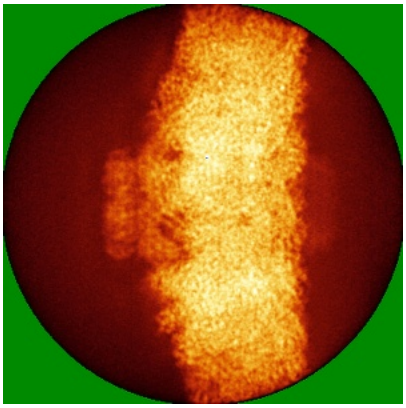


Z

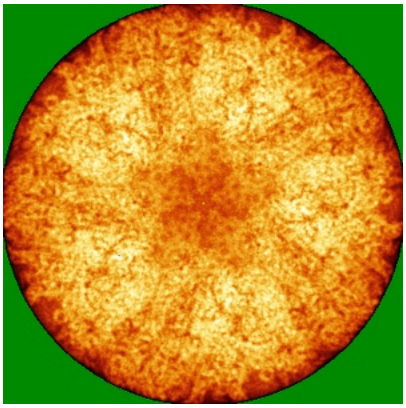
6.4.2 Raw map



X



Y

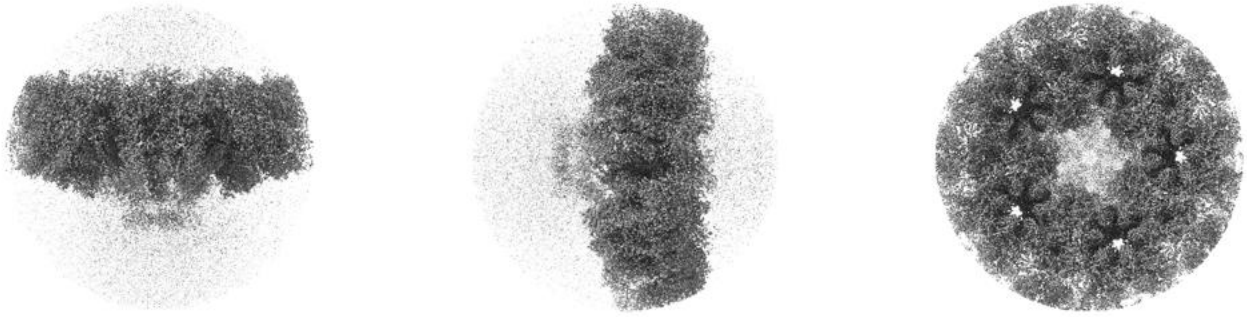


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

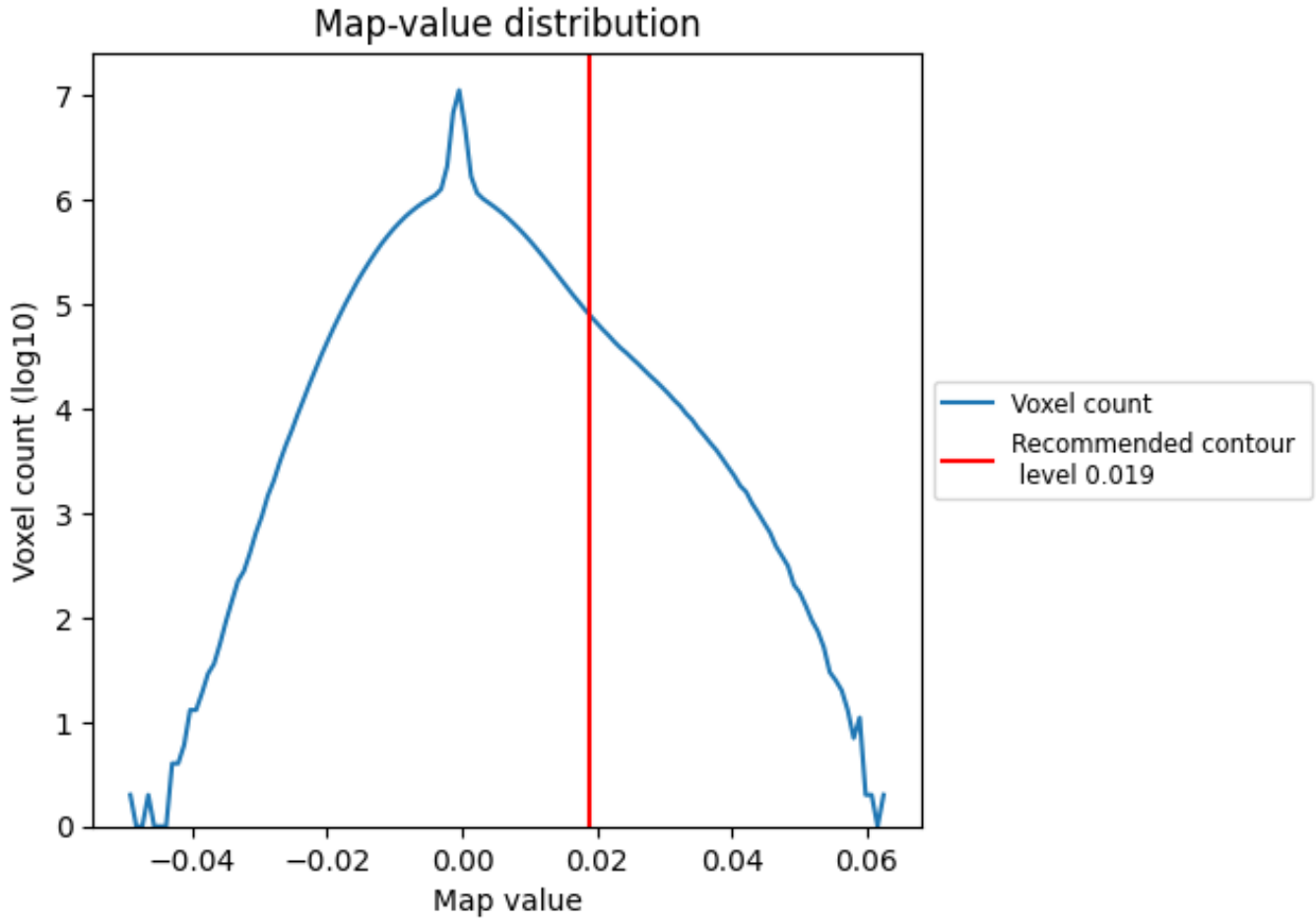
6.6 Mask visualisation (i)

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

7 Map analysis

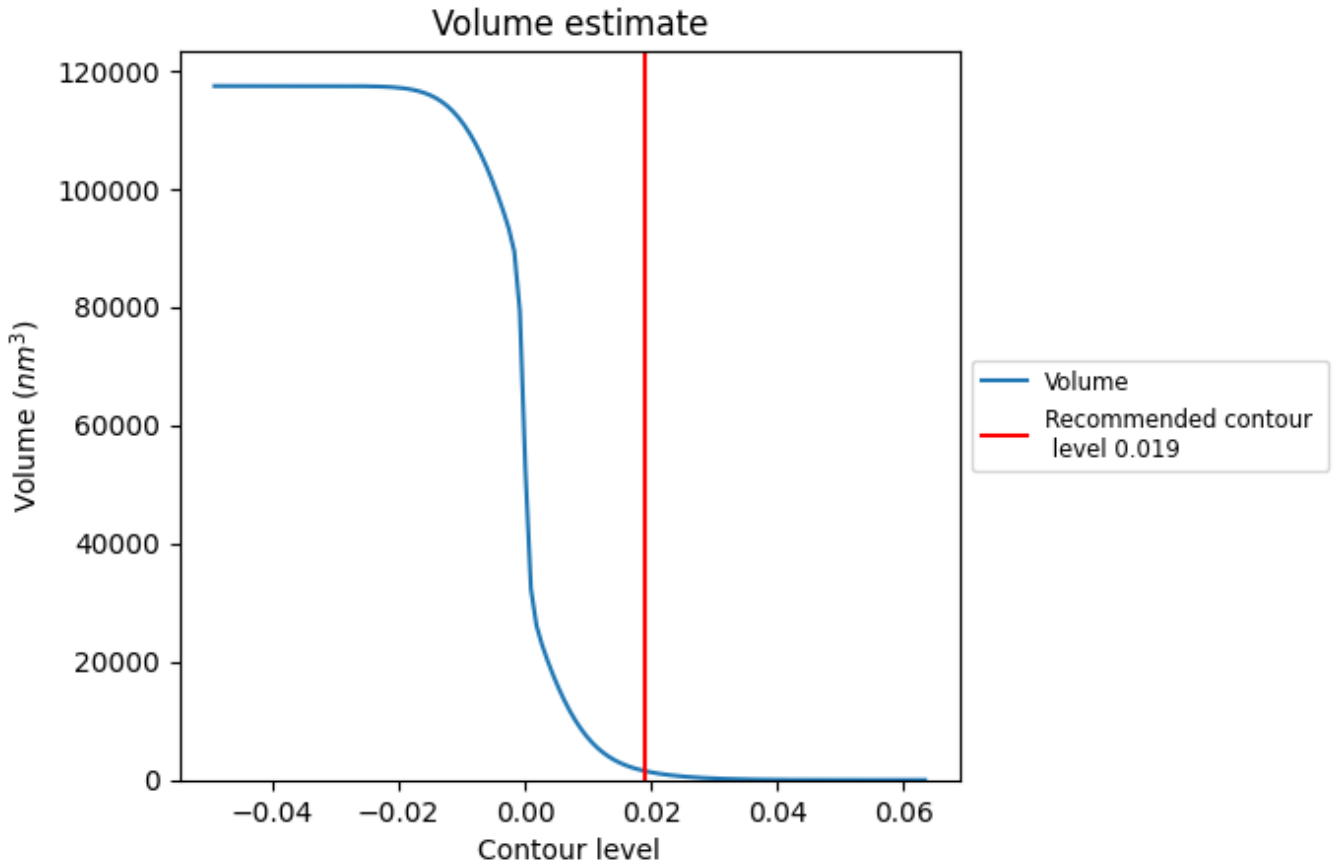
This section contains the results of statistical analysis of the map.

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.

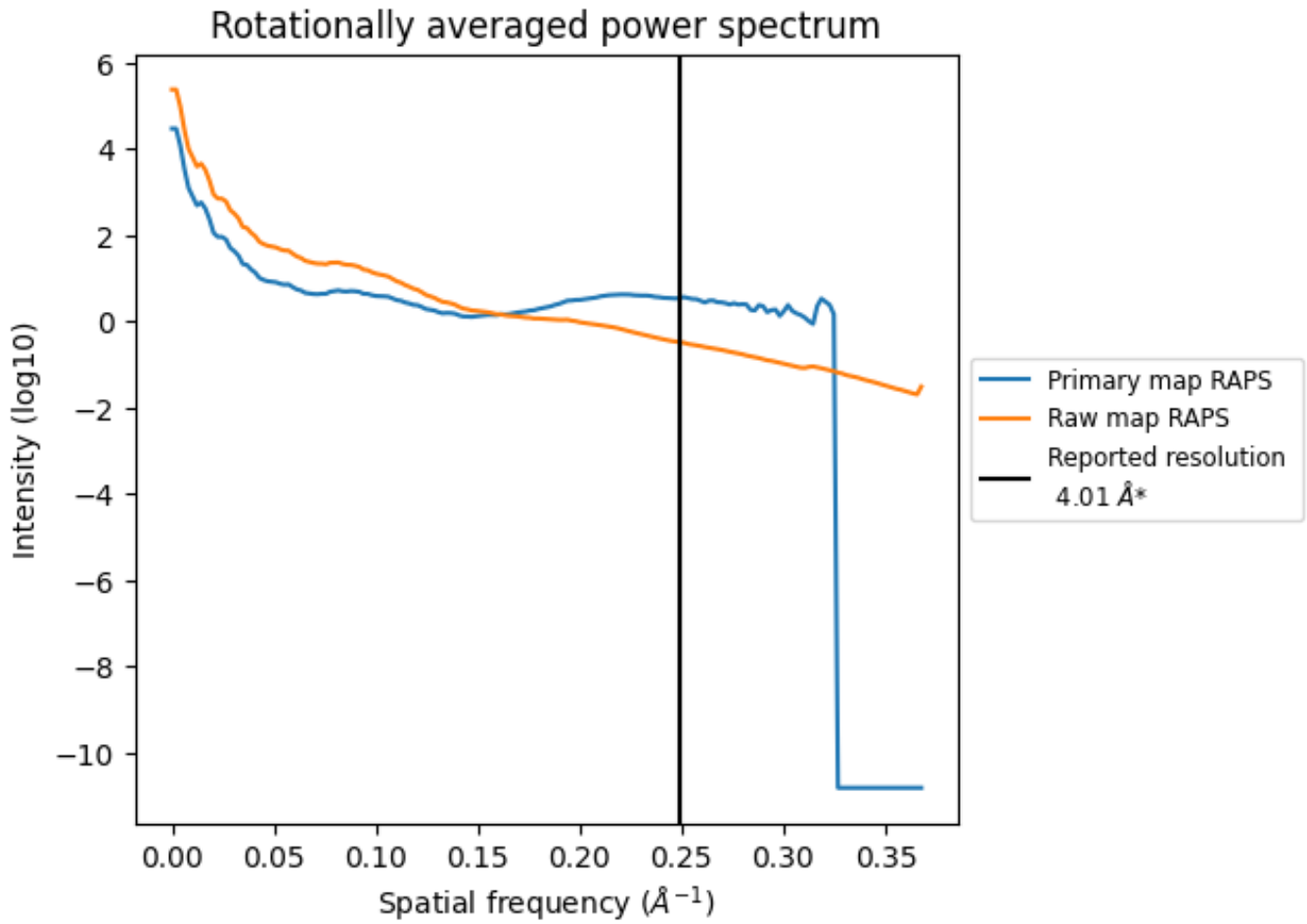
7.2 Volume estimate



The volume at the recommended contour level is 1523 nm^3; this corresponds to an approximate mass of 1376 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)

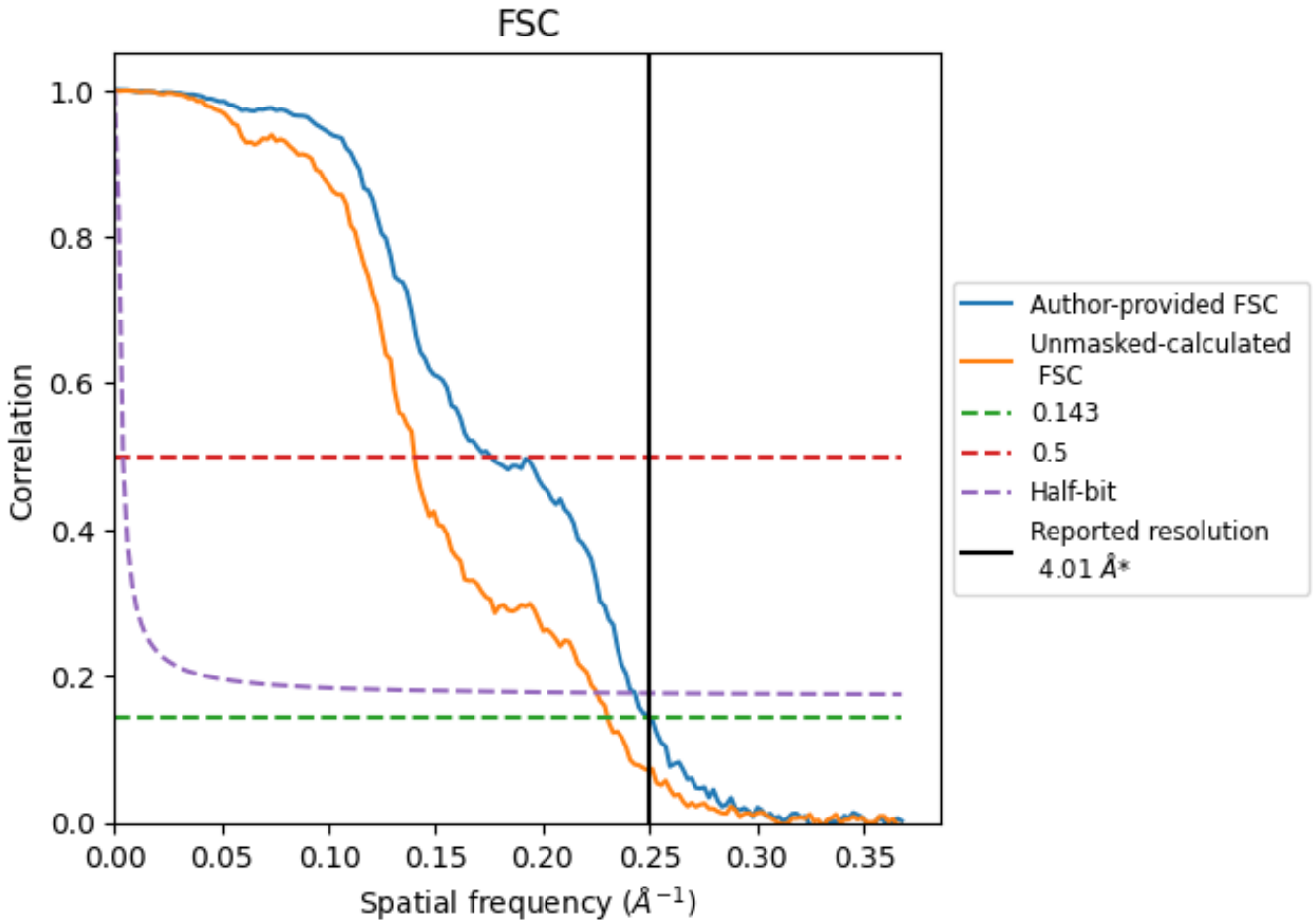


*Reported resolution corresponds to spatial frequency of 0.249 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.249 Å^{-1}

8.2 Resolution estimates (i)

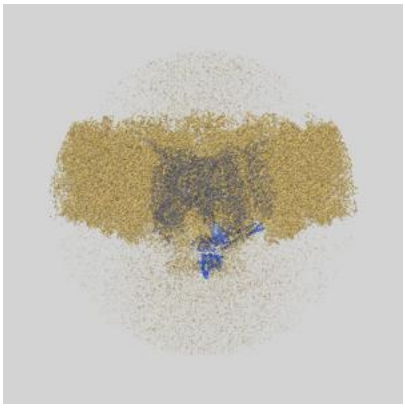
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.01	-	-
Author-provided FSC curve	3.99	5.69	4.11
Unmasked-calculated*	4.34	7.13	4.44

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

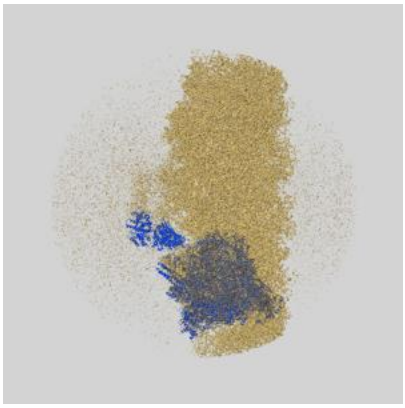
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41202 and PDB model 8TEU. Per-residue inclusion information can be found in section 3 on page 7.

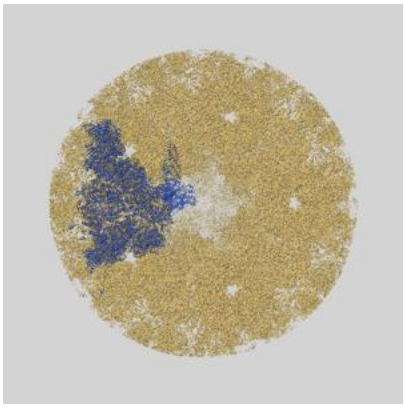
9.1 Map-model overlay



X



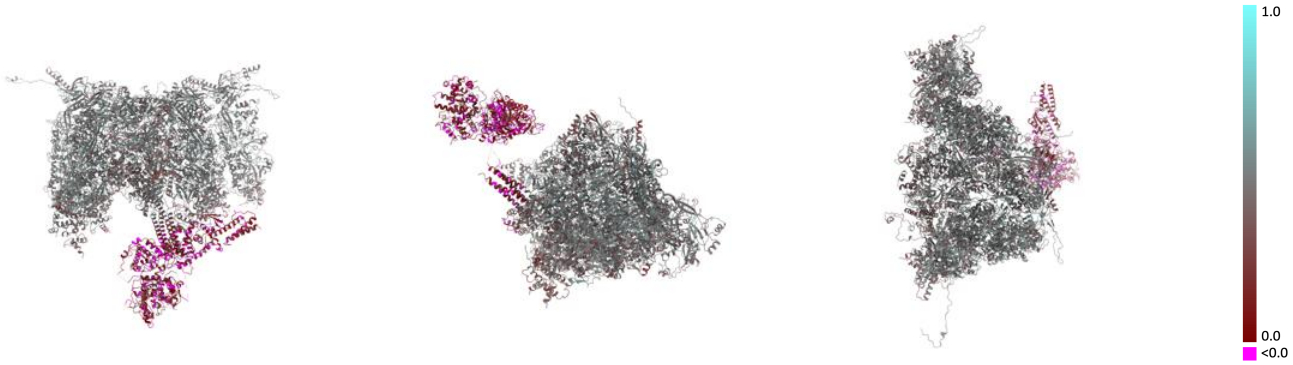
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

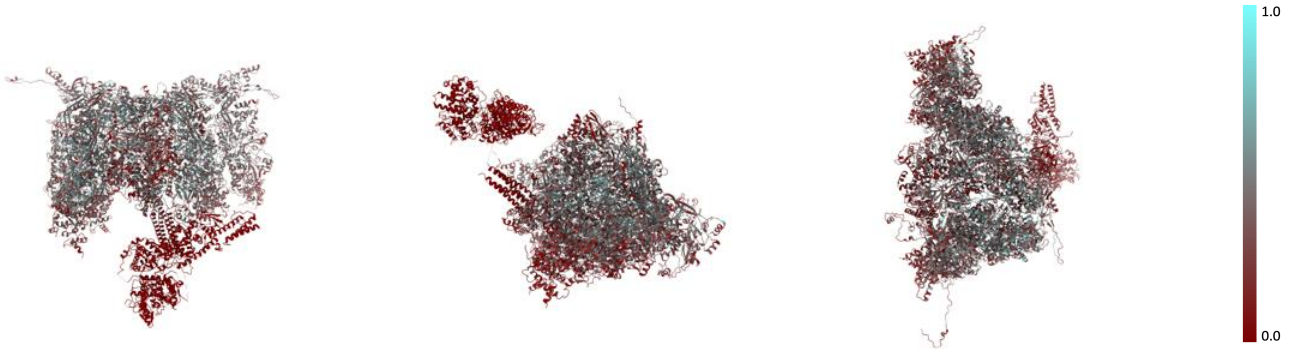
9.2 Q-score mapped to coordinate model (i)



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.

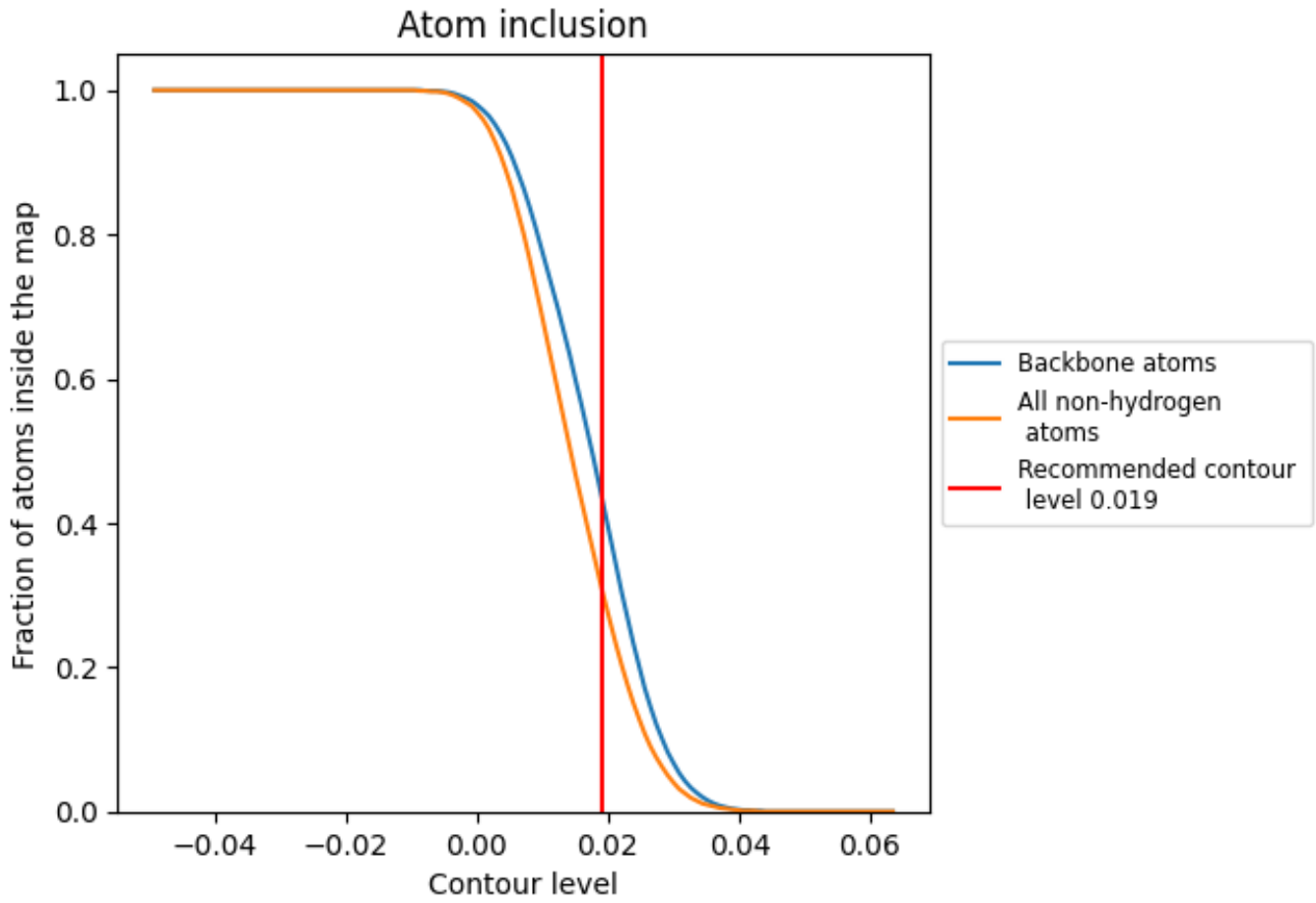
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 44% of all backbone atoms, 31% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3100	0.4300
A	0.0170	0.1030
C	0.0190	0.1850
E	0.0350	0.1650
F	0.1000	0.3010
G	0.3070	0.4630
H	0.4230	0.4860
I	0.4030	0.4820
J	0.3360	0.4690
K	0.4120	0.4810
L	0.3660	0.4750
M	0.3180	0.4690
N	0.1870	0.3950
O	0.1990	0.3710
P	0.1270	0.3470
Q	0.1950	0.3570
R	0.1290	0.3740
S	0.1120	0.3710
T	0.2090	0.4150
U	0.3140	0.4590
V	0.3100	0.4470
W	0.3340	0.4730
X	0.2610	0.4490
Y	0.2850	0.4550
Z	0.1620	0.4000