Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 04:49 pm GMT

PDB ID	:	5NUG
EMDB ID	:	EMD-3698
Title	:	Motor domains from human cytoplasmic dynein-1 in the phi-particle conformation
Authors	:	Zhang, K.; Foster, H.E.; Carter, A.P.
Deposited on	:	2017-04-30
Resolution	:	3.80 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:

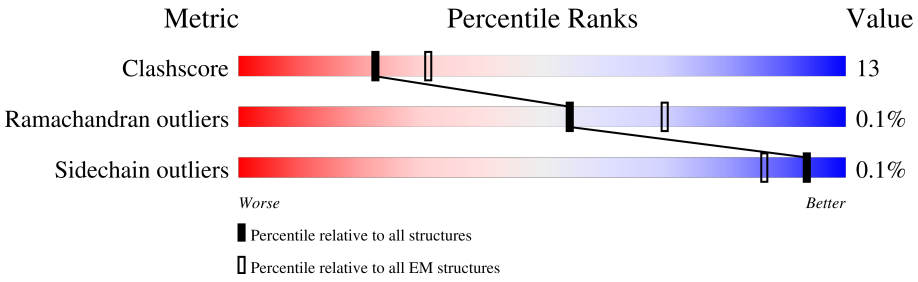
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4646	63% 52% 11% 37%
1	B	4646	63% 52% 11% 37%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	4801	-	-	X	-
2	ADP	B	4801	-	-	X	-

2 Entry composition (i)

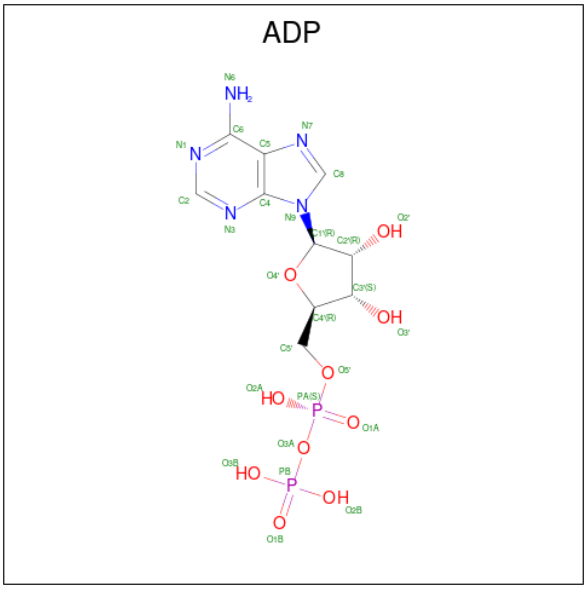
There are 4 unique types of molecules in this entry. The entry contains 46232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		
1	B	2920	Total	C	N	O	S	0	0
			23003	14686	3978	4227	112		

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	A	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

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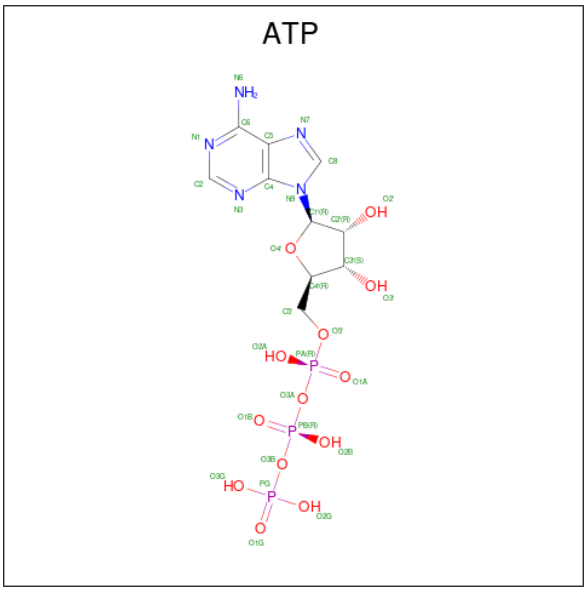
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	
2	B	1	Total	C	N	O	P	0
			81	30	15	30	6	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

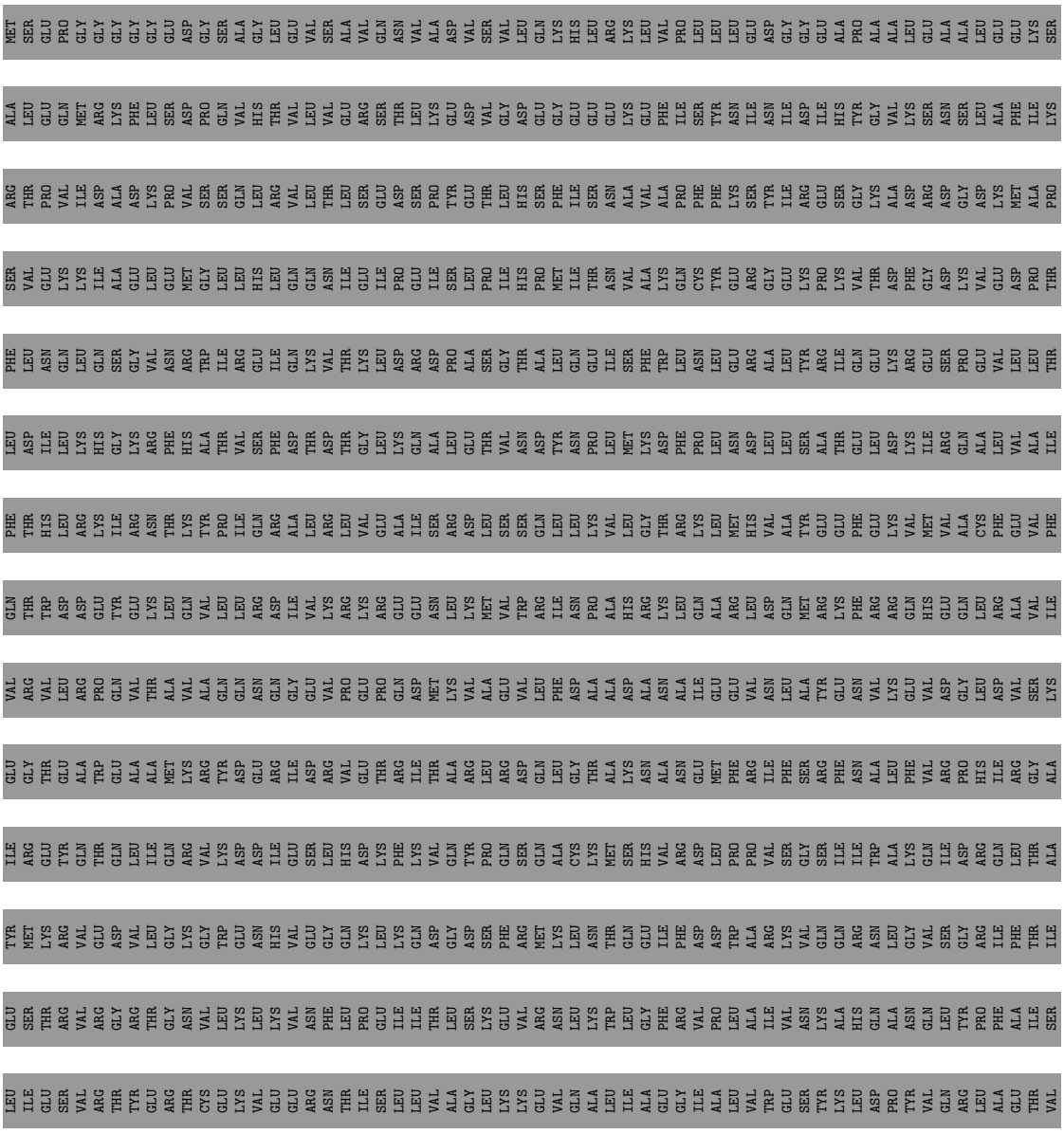
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

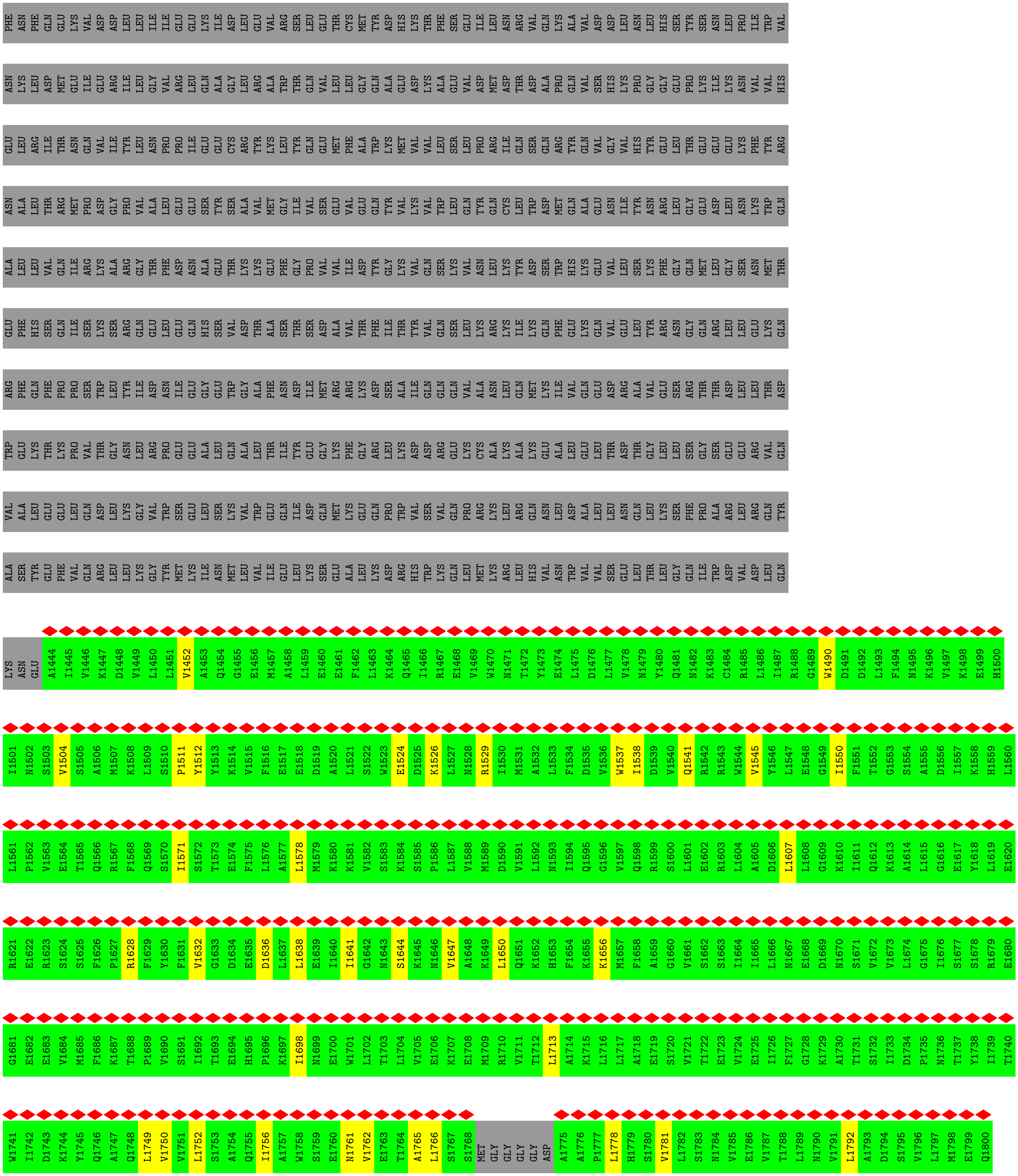
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain A:




PHE ASN PHE GLN GLU LYS VAL ASP ASP LEU LEU ILE ILE GLU GLU LYS ILE ASP LEU GLU VAL ARG SER LEU GLU THR CYS MET TYR ASP HIS LYS THR PHE SER GLU ILE LEU ASN ARG VAL GLN LYS ALA VAL ASP ASP LEU ASN LEU HIS SER TYR SER ASN LEU PRO ILE TRP VAL
ASN LYS LEU ASP MET GLU ILE GLU ARG ILE LEU GLY VAL ARG LEU GLN ALA GLY LEU ARG ALA TRP THR GLN VAL LEU LEU GLY GLN ALA GLU ASP LYS ALA GLU VAL ASP MET ASP THR ASP ALA PRO GLN VAL SER HIS LYS PRO GLY GLY GLU PRO LYS ILE LYS ASN VAL VAL HIS
GLU LEU ARG ILE THR ASN GLN VAL ILE TYR LEU ASN PRO PRO ILE GLU GLU CYS ARG TYR LYS LEU TYR GLN GLU MET PHE ALA TRP LYS MET VAL VAL LEU SER LEU PRO ARG ILE GLN SER GLN ARG TYR GLN VAL GLY VAL HIS TYR GLU LEU THR GLU GLU GLU LYS PHE TYR ARG
ASN ALA LEU THR ARG MET PRO ASP GLY PRO VAL ALA LEU GLU GLU SER TYR SER ALA VAL MET GLY ILE VAL SER GLU VAL GLU GLN TYR VAL LYS VAL TRP LEU GLN TYR GLN CYS LEU TRP ASP MET GLN ALA GLU ASN ILE TYR ASN ARG LEU GLY GLU ASP LEU ASN LYS GLN
ALA LEU LEU VAL GLN ILE ARG LYS ALA ARG GLY THR PHE ASP ASN ALA GLU THR LYS LYS GLU PHE GLY PRO VAL VAL ILE ASP TYR GLY LYS VAL GLN SER LYS VAL ASN LEU LYS TYR ASP SER TRP HIS LYS GLU VAL LEU SER LYS PHE GLY GLN MET LEU GLY SER ASN MET THR
GLU PHE HIS SER GLN ILE SER LYS SER ARG GLU GLN LEU GLU GLN HIS SER VAL ASP THR ALA SER THR SER ASP ALA VAL THR PHE ILE THR TYR VAL GLN SER LEU LYS ARG LYS ILE LYS GLN PHE GLU LYS GLN VAL GLU LEU TYR ARG ASN GLY GLN ARG LEU LEU GLU LYS GLN
ARG PHE GLN PHE PRO PRO SER TRP LEU TYR ILE ASP ASN ILE GLU GLY GLU TRP GLY ALA PHE ASN ASP ILE MET ARG ARG LYS ASP SER ALA ILE GLN GLN GLN VAL ALA ASN LEU GLN MET LYS ILE VAL GLN GLU ASP ARG ALA VAL GLU SER ARG THR THR ASP LEU LEU THR ASP
TRP GLU LYS THR LYS PRO VAL THR GLY ASN LEU ARG PRO GLU GLU ALA LEU GLN ALA LEU THR ILE TYR GLU GLY LYS PHE GLY ARG LEU LYS ASP ASP ARG GLU LYS CYS ALA LYS ALA LYS GLU ALA LEU GLU LEU THR ASP THR GLY LEU LEU SER GLY SER GLU GLU ARG VAL GLN
VAL ALA LEU GLU GLU LEU GLN ASP LEU LYS GLY VAL TRP SER GLU LEU SER LYS VAL TRP GLU GLN ILE ASP GLN MET LYS GLU GLN PRO TRP VAL SER VAL GLN PRO ARG LYS LEU ARG GLN ASN LEU ASP ALA LEU LEU ASN GLN LEU LYS SER PHE PRO ALA ARG LEU ARG GLN TYR
ALA SER TYR GLU PHE VAL GLN ARG LEU LEU LYS GLY TYR MET LYS ILE ASN MET LEU VAL ILE GLU LEU LYS SER GLU ALA LEU LYS ASP ARG HIS TRP LYS GLN LEU MET LYS ARG LEU HIS VAL ASN TRP VAL VAL SER GLU LEU THR LEU GLY GLN ILE TRP ASP VAL ASP LEU GLN
LYS ASN GLU A1444 I1445 V1446 K1447 D1448 V1449 L1450 L1451 V1452 A1453 Q1454 G1455 E1456 M1457 A1458 L1459 E1460 E1461 F1462 L1463 K1464 Q1465 I1466 R1467 E1468 V1469 W1470 N1471 T1472 Y1473 E1474 L1475 D1476 L1477 V1478 N1479 Y1480 Q1481 N1482 K1483 C1484 R1485 L1486 I1487 R1488 G1489 W1490 D1491 D1492 L1493 F1494 N1495 K1496 V1497 K1498 E1499 H1500
I1501 N1502 S1503 V1504 S1505 A1506 M1507 K1508 L1509 S1510 P1511 Y1512 Y1513 K1514 V1515 F1516 E1517 E1518 D1519 A1520 L1521 S1522 W1523 E1524 D1525 K1526 L1527 N1528 R1529 I1530 M1531 A1532 L1533 F1534 D1535 V1536 W1537 I1538 D1539 V1540 Q1541 R1542 R1543 W1544 V1545 Y1546 L1547 E1548 G1549 I1550 F1551 T1552 G1553 S1554 A1555 D1556 I1557 K1558 H1559 L1560
L1561 P1562 V1563 E1564 T1565 Q1566 R1567 F1568 Q1569 S1570 I1571 S1572 T1573 E1574 F1575 L1576 A1577 L1578 M1579 K1580 K1581 V1582 S1583 K1584 S1585 P1586 L1587 V1588 M1589 D1590 V1591 L1592 N1593 I1594 Q1595 G1596 V1597 Q1598 R1599 S1600 L1601 E1602 R1603 L1604 A1605 D1606 L1607 L1608 G1609 K1610 I1611 Q1612 K1613 A1614 L1615 G1616 E1617 Y1618 L1619 E1620
R1621 E1622 R1623 S1624 S1625 F1626 P1627 R1628 F1629 Y1630 F1631 V1632 G1633 D1634 E1635 D1636 L1637 L1638 E1639 I1640 I1641 G1642 N1643 S1644 K1645 N1646 V1647 A1648 K1649 L1650 Q1651 K1652 H1653 F1654 K1655 K1656 M1657 F1658 A1659 G1660 V1661 S1662 S1663 I1664 I1665 L1666 N1667 E1668 D1669 N1670 S1671 V1672 V1673 L1674 G1675 I1676 S1677 S1678 R1679 E1680
G1681 E1682 E1683 V1684 M1685 F1686 K1687 T1688 P1689 V1690 S1691 I1692 T1693 E1694 H1695 P1696 K1697 I1698 N1699 E1700 W1701 L1702 T1703 L1704 V1705 E1706 K1707 E1708 M1709 R1710 V1711 T1712 L1713 A1714 K1715 L1716 L1717 A1718 E1719 S1720 V1721 T1722 E1723 V1724 E1725 I1726 F1727 G1728 K1729 A1730 T1731 S1732 I1733 D1734 P1735 N1736 T1737 Y1738 I1739 T1740
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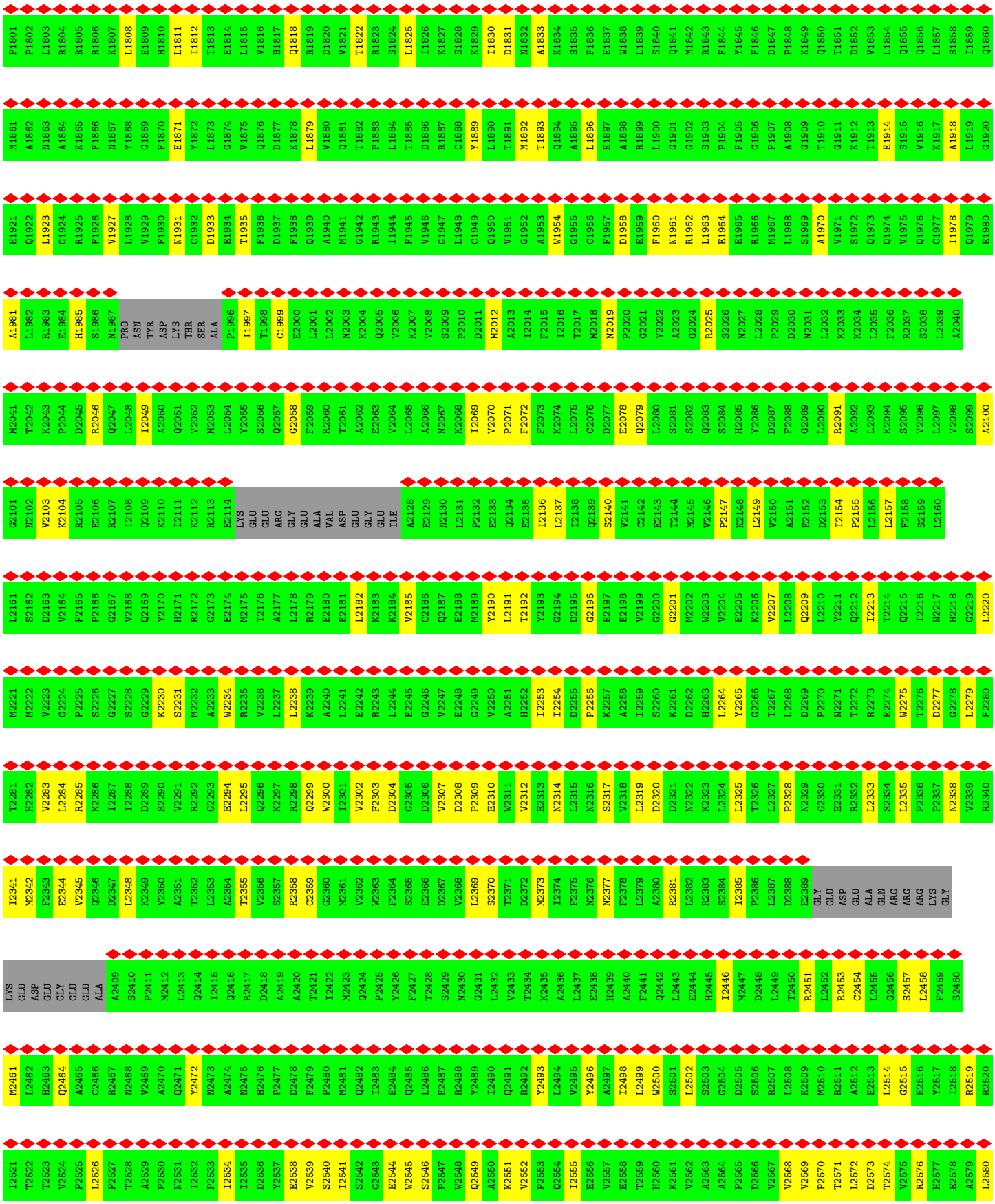
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I2341 M2342 F2343 E2344 V2345 Q2346 D2347 L2348 K2349 Y2350 A2351 T2352 L2353 A2354 T2355 V2356 S2357 R2358 C2359 G2360 M2361 V2362 W2363 F2364 S2365 E2366 D2367 V2368 L2369 S2370 T2371 D2372 M2373 I2374 F2375 N2376 N2377 F2378 L2379 A2380 R2381 L2382 R2383 S2384 I2385 P2386 L2387 D2388 E2389 GLY GLU ASP GLU ALA GLN ARG ARG ARG LYS GLY
LYS GLU ASP GLU GLY GLU GLU ALA A2409 S2410 P2411 M2412 L2413 Q2414 I2415 Q2416 R2417 D2418 A2419 A2420 T2421 I2422 M2423 Q2424 P2425 Y2426 F2427 T2428 S2429 N2430 G2431 L2432 V2433 T2434 K2435 A2436 L2437 E2438 H2439 A2440 F2441 Q2442 L2443 E2444 H2445 I2446 M2447 D2448 L2449 T2450 R2451 L2452 R2453 C2454 L2455 G2456 S2457 L2458 F2459 S2460
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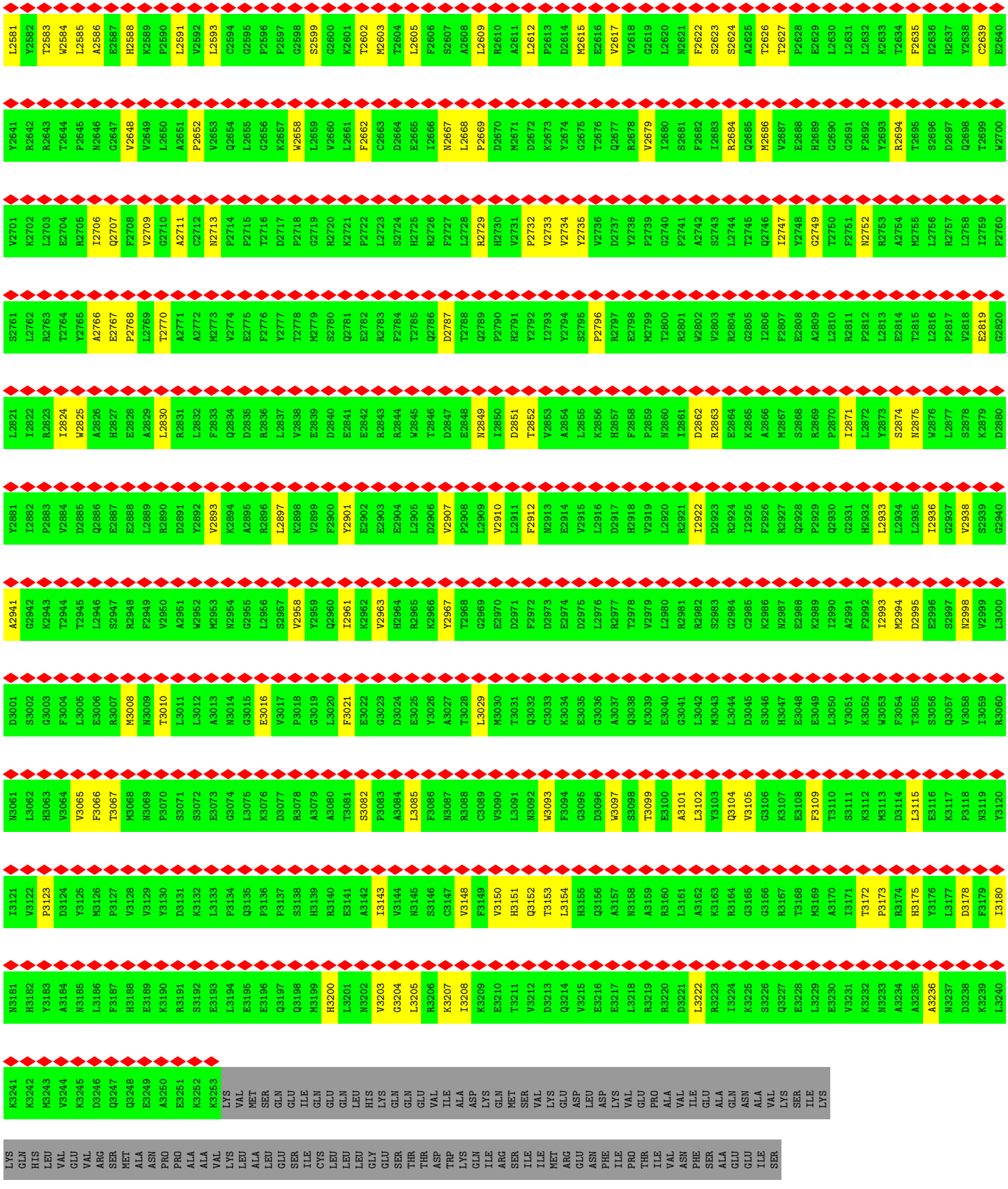
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S2761 L2762 R2763 T2764 Y2765 A2766 E2767 P2768 L2769 T2770 A2771 A2772 M2773 V2774 E2775 F2776 Y2777 T2778 M2779 S2780 Q2781 E2782 R2783 F2784 T2785 Q2786 D2787 T2788 Q2789 P2790 H2791 Y2792 I2793 Y2794 S2795 P2796 R2797 E2798 M2799 T2800 R2801 W2802 V2803 R2804 G2805 I2806 F2807 E2808 A2809 L2810 R2811 P2812 L2813 E2814 T2815 L2816 P2817 V2818 E2819 G2820
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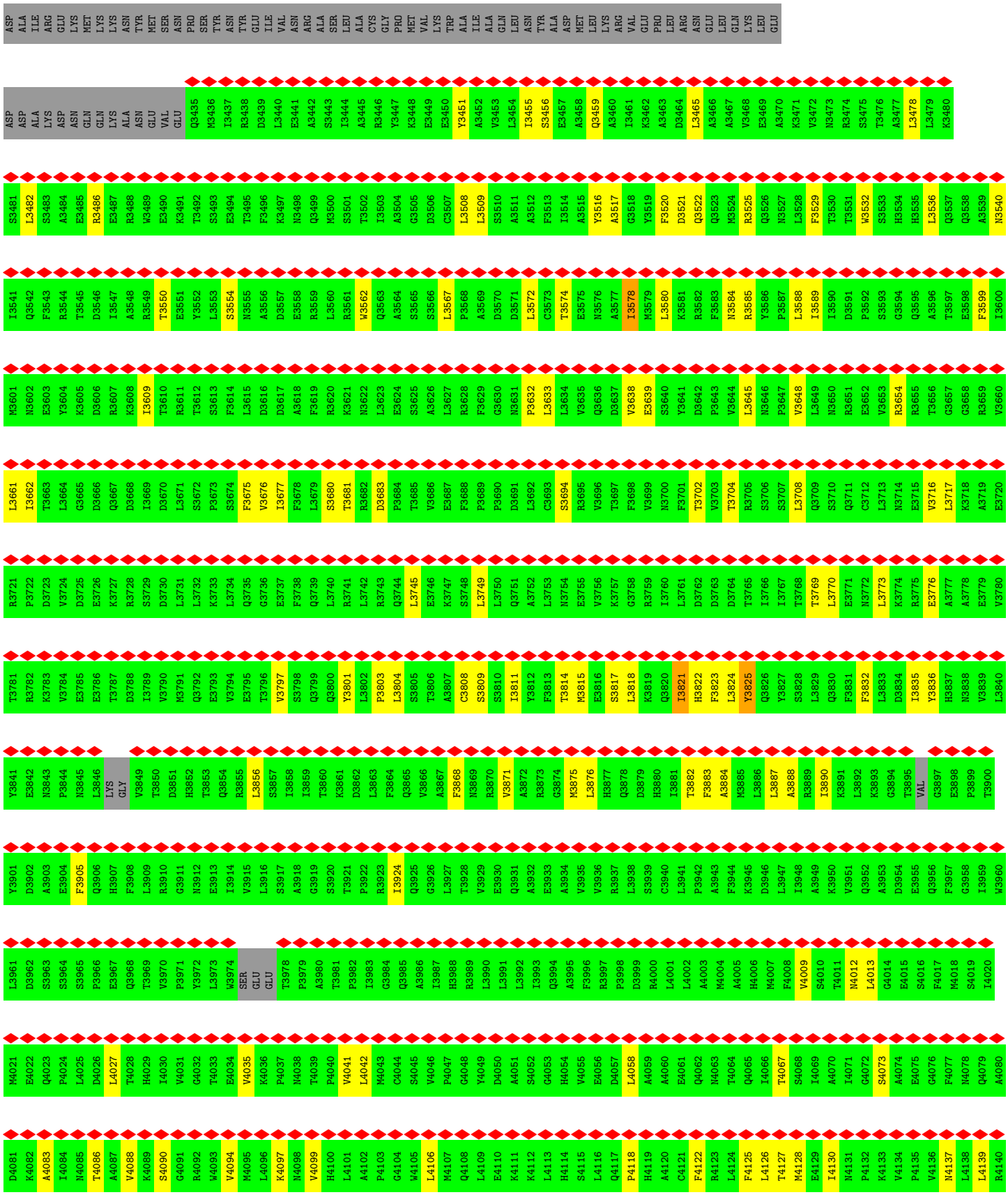
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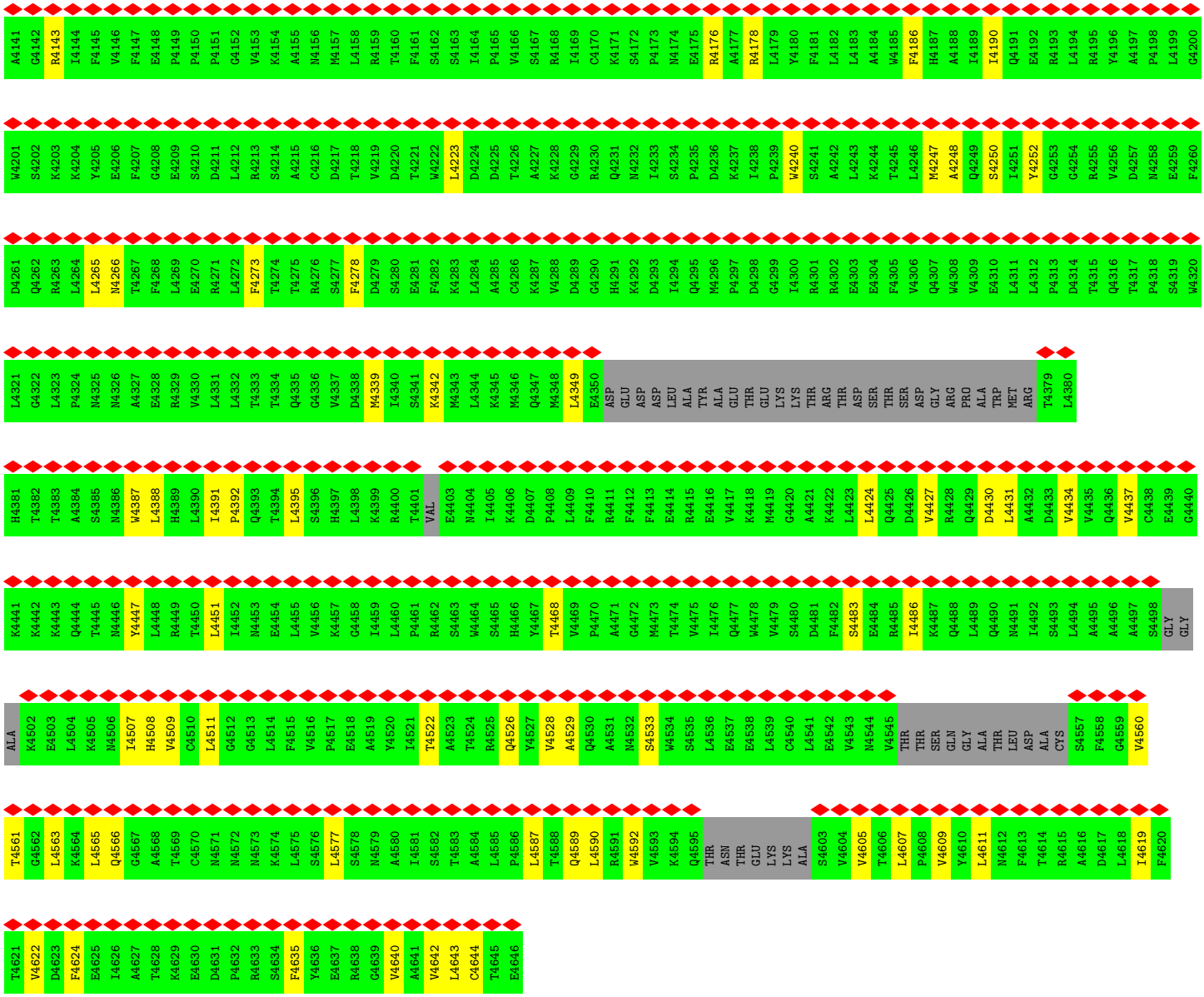
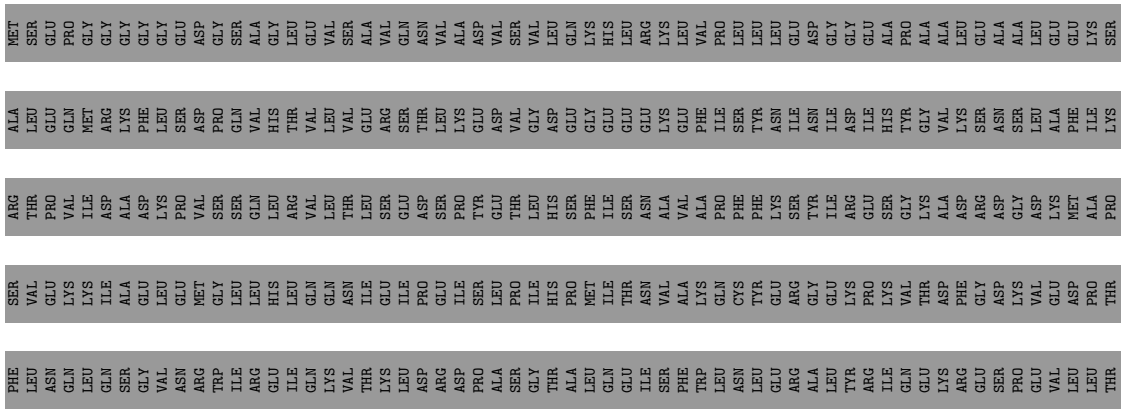
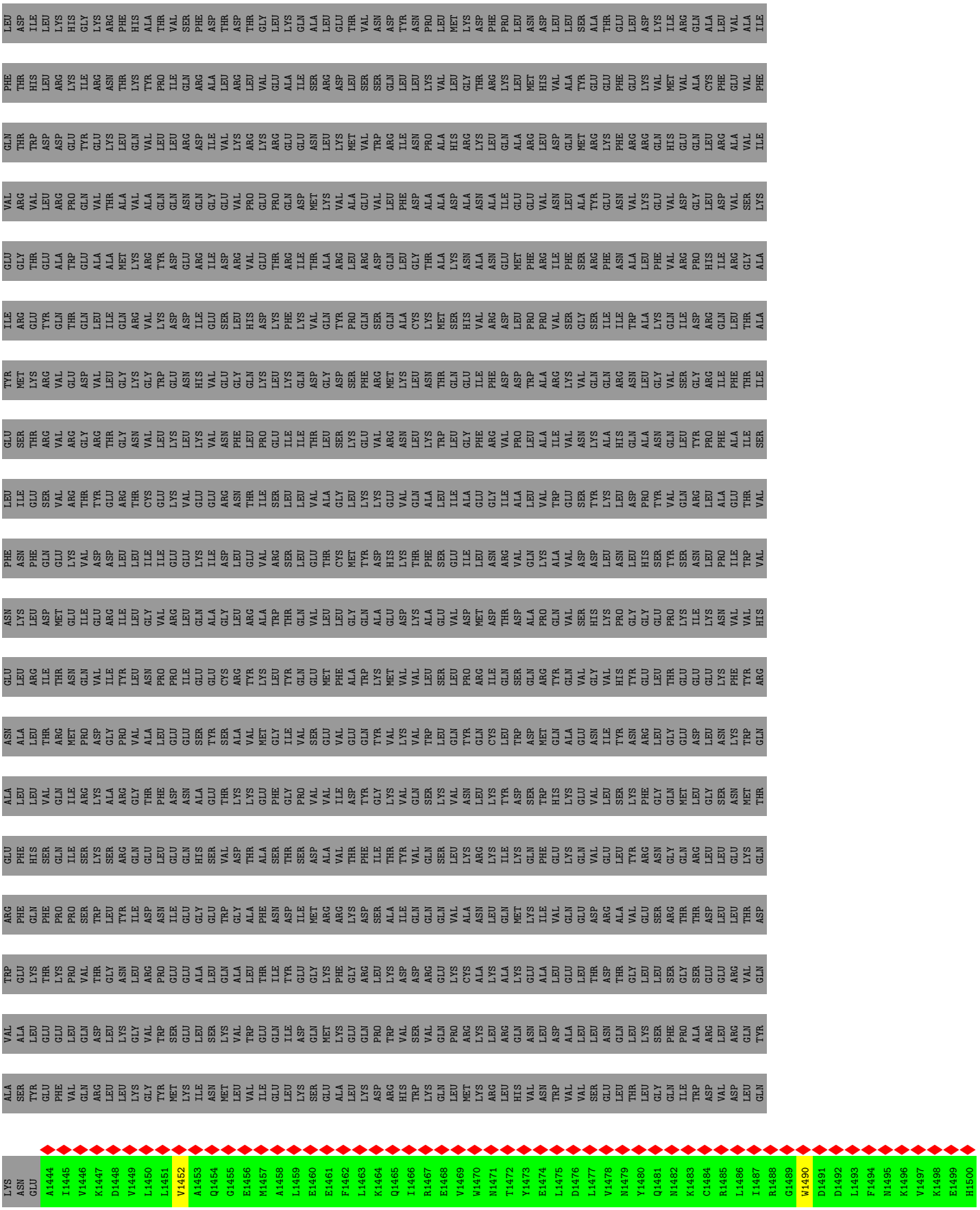


• Molecule 1: Cytoplasmic dynein 1 heavy chain 1

Chain B:

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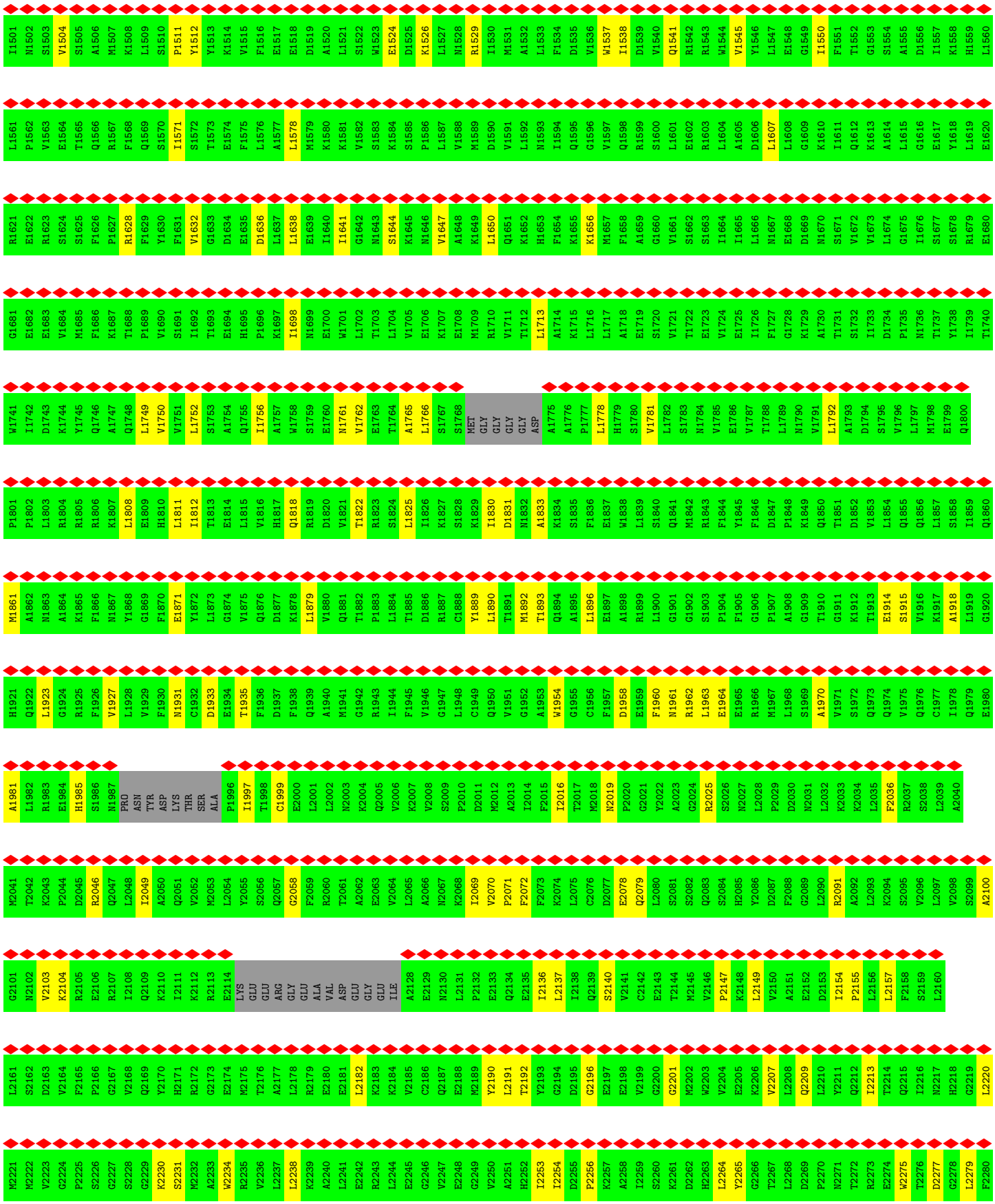
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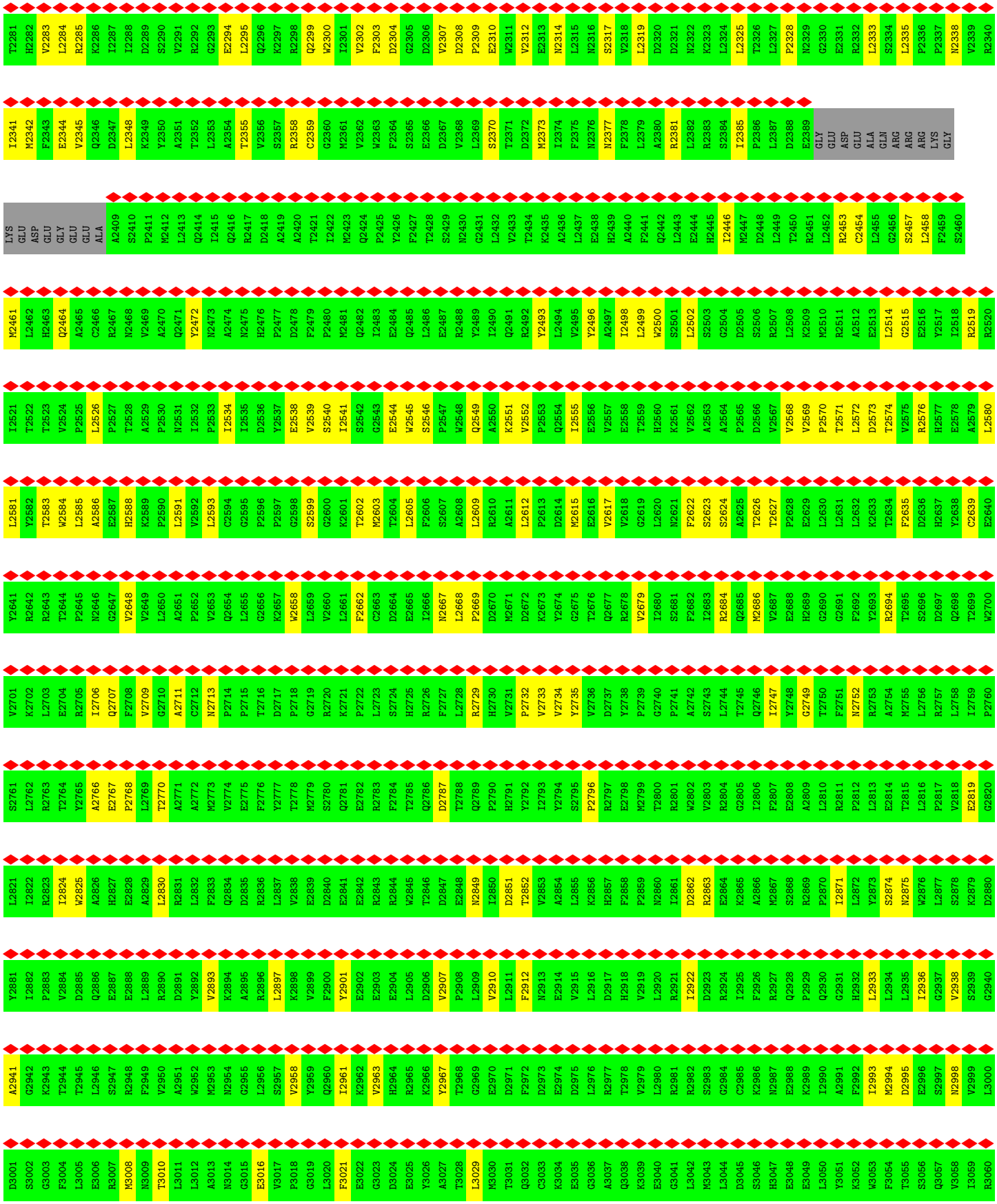
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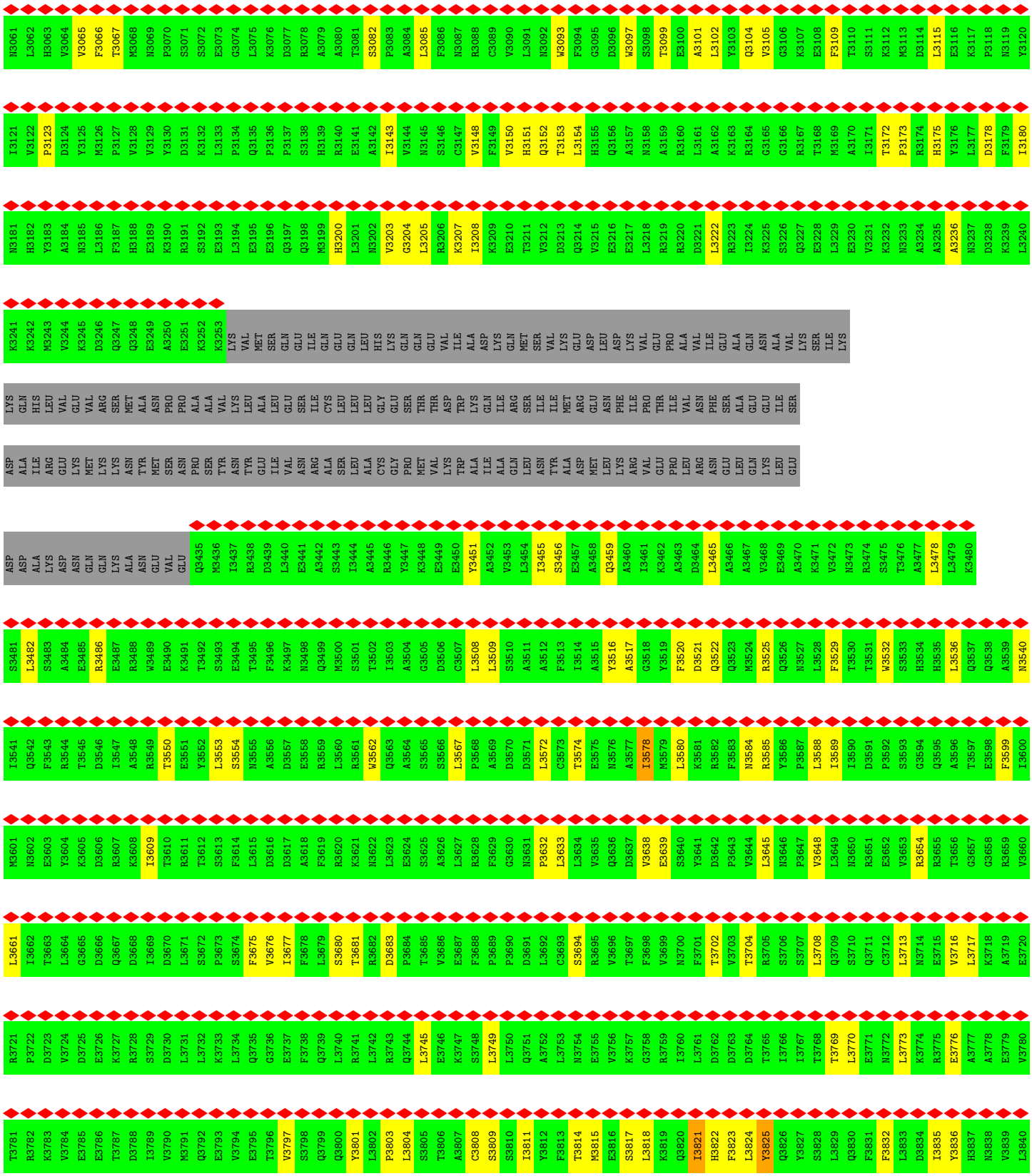
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K3241 K3242 M3243 V3244 K3245 D3246 Q3247 Q3248 E3249 A3250 E3251 K3252 K3253 LYS VAL MET SER GLN GLU ILE GLN GLU GLN LEU HIS LYS GLN GLU VAL ILE ALA ASP LYS GLN MET SER VAL LYS GLU ASP LEU ASP LYS VAL GLU PRO ALA VAL ILE GLU ALA GLN ASN ALA VAL LYS SER ILE LYS
LYS GLN HIS LEU VAL GLU VAL ARG SER MET ALA ASN PRO PRO ALA ALA VAL LYS LEU ALA LEU GLU SER ILE CYS LEU LEU LEU GLY GLU SER THR THR ASP TRP LYS GLN ILE ARG SER ILE ILE MET ARG GLU ASN PHE ILE PRO THR ILE VAL ASN PHE SER ALA GLU GLU ILE SER
ASP ALA ILE ARG GLU LYS MET LYS LYS ASN TYR MET SER ASN PRO SER TYR ASN TYR GLU ILE VAL ASN ARG ALA SER LEU ALA CYS GLY PRO MET VAL LYS TRP ALA ILE ALA GLN LEU ASN TYR ALA ASP MET LEU LYS ARG VAL GLU PRO LEU ARG ASN GLU LEU GLN LYS LEU GLU
ASP ASP ALA LYS ASP ASN GLN GLN LYS ALA ASN GLU VAL GLU Q3435 M3436 I3437 R3438 D3439 L3440 E3441 A3442 S3443 I3444 A3445 R3446 Y3447 K3448 E3449 E3450 Y3451 A3452 V3453 L3454 I3455 S3456 E3457 A3458 Q3459 A3460 I3461 K3462 A3463 D3464 L3465 A3466 A3467 V3468 E3469 A3470 K3471 V3472 N3473 R3474 S3475 T3476 A3477 L3478 L3479 K3480
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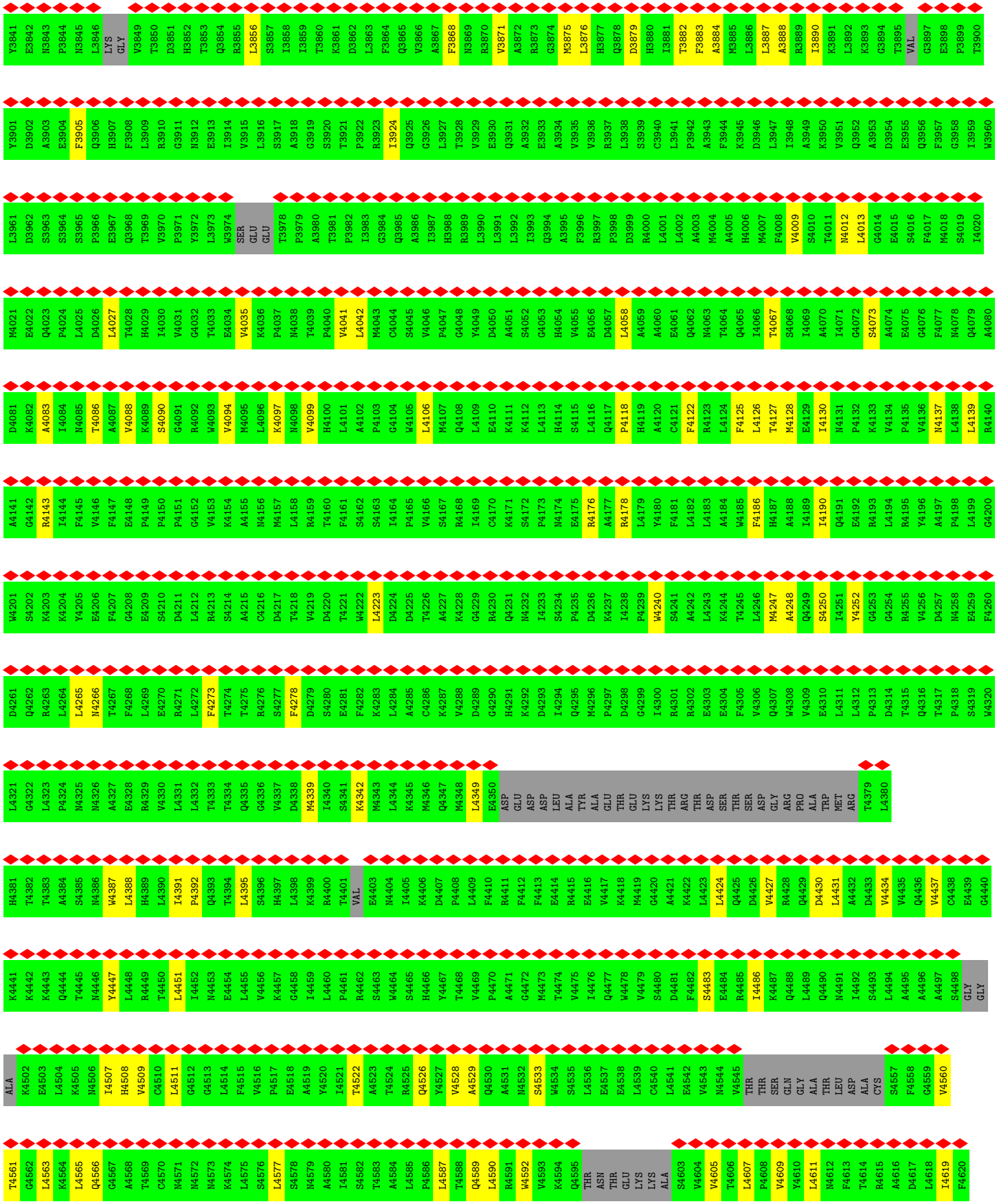
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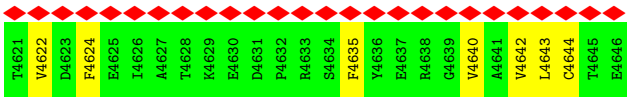
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Y4636
E4637
R4638
G4639
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V4642
L4643
C4644
T4645
E4646

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	233227	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 ($e^-/Å^2$)	1.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	106061	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.309	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	528.0, 528.0, 528.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.43	0/23474	0.71	4/31851 (0.0%)
1	B	0.43	0/23474	0.71	4/31851 (0.0%)
All	All	0.43	0/46948	0.71	8/63702 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3821	ILE	N-CA-C	5.74	126.51	111.00
1	B	3821	ILE	N-CA-C	5.74	126.51	111.00
1	A	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	4250	SER	N-CA-C	5.52	125.91	111.00
1	B	3578	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	3578	ILE	CB-CA-C	-5.10	101.40	111.60
1	A	2019	ASN	C-N-CD	5.02	138.94	128.40
1	B	2019	ASN	C-N-CD	5.00	138.91	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	23003	0	22805	587	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	23003	0	22805	582	0
2	A	81	0	36	13	0
2	B	81	0	36	13	0
3	A	31	0	12	4	0
3	B	31	0	12	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	46232	0	45706	1155	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 13.

All (1155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3638:VAL:HG12	1:A:3681:THR:CG2	1.29	1.60
1:B:3638:VAL:HG12	1:B:3681:THR:CG2	1.29	1.54
1:B:3749:LEU:HD13	1:B:3773:LEU:CD1	1.44	1.46
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG2	1.50	1.45
1:A:3749:LEU:HD13	1:A:3773:LEU:CD1	1.44	1.43
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG2	1.50	1.43
1:A:1931:ASN:ND2	1:A:2317:SER:HB3	1.28	1.42
1:B:1931:ASN:ND2	1:B:2317:SER:HB3	1.28	1.41
1:A:3815:MET:CE	1:A:3871:VAL:CG2	2.07	1.33
1:B:3815:MET:CE	1:B:3871:VAL:CG2	2.07	1.32
1:A:3815:MET:HE2	1:A:3871:VAL:CG2	1.61	1.29
1:A:3456:SER:CB	1:B:3459:GLN:HG3	1.64	1.27
1:A:2584:TRP:CZ3	1:A:2732:PRO:CG	2.17	1.25
1:A:3459:GLN:HG3	1:B:3456:SER:CB	1.65	1.25
1:A:3638:VAL:CG1	1:A:3681:THR:CG2	2.14	1.25
1:B:2584:TRP:CZ3	1:B:2732:PRO:CG	2.18	1.24
1:B:3638:VAL:CG1	1:B:3681:THR:CG2	2.14	1.24
1:A:3115:LEU:HD13	1:A:3143:ILE:CD1	1.67	1.24
1:B:3115:LEU:HD13	1:B:3143:ILE:CD1	1.67	1.24
1:A:3456:SER:OG	1:B:3459:GLN:HG3	1.34	1.22
1:A:4622:VAL:HG12	1:A:4624:PHE:CE2	1.75	1.21
1:A:3459:GLN:HG3	1:B:3456:SER:OG	1.38	1.19
1:B:4622:VAL:HG12	1:B:4624:PHE:CE2	1.76	1.19
1:A:2609:LEU:HD11	1:A:2615:MET:HB2	1.23	1.17
1:B:3815:MET:CE	1:B:3871:VAL:HG21	1.72	1.16
1:B:2325:LEU:HD23	1:B:2333:LEU:HD12	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3821:ILE:HD12	1:A:4342:LYS:CG	1.77	1.14
1:B:3815:MET:HE1	1:B:3871:VAL:CG2	1.70	1.14
1:A:3749:LEU:HD13	1:A:3773:LEU:HD11	1.26	1.13
1:A:3815:MET:CE	1:A:3871:VAL:HG21	1.72	1.13
1:B:3821:ILE:HD12	1:B:4342:LYS:CG	1.78	1.12
1:A:2549:GLN:NE2	1:A:2572:LEU:HD22	1.65	1.12
1:A:3456:SER:OG	1:B:3459:GLN:CG	1.96	1.12
1:A:4607:LEU:HD21	1:A:4635:PHE:HZ	1.08	1.11
1:A:4511:LEU:HD22	1:A:4644:CYS:SG	1.90	1.11
1:B:2549:GLN:NE2	1:B:2572:LEU:HD22	1.65	1.11
1:B:2196:GLY:HA2	1:B:2201:GLY:HA3	1.32	1.11
1:A:3821:ILE:HD12	1:A:4342:LYS:HG3	1.33	1.10
1:B:2457:SER:HB3	1:B:2584:TRP:CH2	1.86	1.10
1:B:2457:SER:CB	1:B:2584:TRP:HH2	1.63	1.10
1:A:2457:SER:HB3	1:A:2584:TRP:CH2	1.86	1.10
1:A:2457:SER:CB	1:A:2584:TRP:HH2	1.63	1.10
1:A:3115:LEU:HD13	1:A:3143:ILE:HD11	1.31	1.10
1:A:4607:LEU:HD21	1:A:4635:PHE:CZ	1.85	1.10
1:B:2609:LEU:HD11	1:B:2615:MET:HB2	1.23	1.10
1:B:3821:ILE:CD1	1:B:4342:LYS:HD2	1.81	1.10
1:A:3459:GLN:CG	1:B:3456:SER:OG	1.99	1.10
1:B:4511:LEU:HD22	1:B:4644:CYS:SG	1.90	1.10
1:B:4607:LEU:HD21	1:B:4635:PHE:CZ	1.85	1.10
1:B:3115:LEU:HD13	1:B:3143:ILE:HD11	1.31	1.09
1:A:3749:LEU:HD13	1:A:3773:LEU:HD13	1.33	1.09
1:B:1931:ASN:ND2	1:B:2317:SER:CB	2.14	1.09
1:B:4424:LEU:HD13	1:B:4486:ILE:CD1	1.83	1.09
1:A:3821:ILE:CD1	1:A:4342:LYS:HD2	1.81	1.09
1:A:1931:ASN:ND2	1:A:2317:SER:CB	2.14	1.09
1:A:2196:GLY:HA2	1:A:2201:GLY:HA3	1.32	1.09
1:A:3815:MET:HE1	1:A:3871:VAL:CG2	1.80	1.09
1:A:3815:MET:HE2	1:A:3871:VAL:HG21	1.13	1.08
1:A:4424:LEU:HD13	1:A:4486:ILE:CD1	1.83	1.08
1:A:4622:VAL:CG1	1:A:4624:PHE:CE2	2.34	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD11	1.26	1.08
1:B:4607:LEU:HD21	1:B:4635:PHE:HZ	1.08	1.08
1:B:4622:VAL:CG1	1:B:4624:PHE:CE2	2.34	1.08
1:B:3815:MET:HE2	1:B:3871:VAL:CG2	1.71	1.08
1:A:2325:LEU:HD23	1:A:2333:LEU:HD12	1.28	1.08
1:B:3821:ILE:HD12	1:B:4342:LYS:HG3	1.34	1.08
1:B:3749:LEU:HD13	1:B:3773:LEU:HD13	1.33	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3815:MET:HE1	1:B:3871:VAL:HG23	1.29	1.07
1:B:1766:LEU:HD23	1:B:1833:ALA:HA	1.36	1.07
1:B:2580:LEU:O	1:B:2584:TRP:HD1	1.36	1.07
1:B:3815:MET:HE2	1:B:3871:VAL:HG21	1.17	1.06
1:A:1879:LEU:HD12	1:A:1918:ALA:HB2	1.36	1.06
1:B:3638:VAL:CG1	1:B:3681:THR:HG23	1.79	1.06
1:A:3638:VAL:CG1	1:A:3681:THR:HG23	1.79	1.05
1:A:3815:MET:HE1	1:A:3871:VAL:HG23	1.37	1.05
1:A:1766:LEU:HD23	1:A:1833:ALA:HA	1.36	1.05
1:A:2580:LEU:O	1:A:2584:TRP:HD1	1.36	1.04
1:B:1879:LEU:HD12	1:B:1918:ALA:HB2	1.36	1.03
1:A:2609:LEU:HD11	1:A:2615:MET:CB	1.87	1.03
1:A:2549:GLN:HE21	1:A:2572:LEU:HD22	1.18	1.03
1:B:4605:VAL:CG1	1:B:4635:PHE:CE2	2.42	1.03
1:B:4424:LEU:HD13	1:B:4486:ILE:HD11	1.38	1.02
1:A:4605:VAL:CG1	1:A:4635:PHE:CE2	2.42	1.02
1:A:3749:LEU:CD1	1:A:3773:LEU:CD1	2.37	1.01
1:A:4424:LEU:HD13	1:A:4486:ILE:HD11	1.38	1.01
1:B:2609:LEU:HD11	1:B:2615:MET:CB	1.88	1.01
1:B:3749:LEU:CD1	1:B:3773:LEU:CD1	2.37	1.01
1:A:3099:THR:HG22	1:A:3152:GLN:NE2	1.75	1.01
1:B:2549:GLN:HE21	1:B:2572:LEU:HD22	1.18	1.01
1:B:3099:THR:HG22	1:B:3152:GLN:NE2	1.75	1.01
1:A:1778:LEU:CD1	1:A:1830:ILE:HD12	1.91	1.00
1:B:4605:VAL:HG11	1:B:4635:PHE:CE2	1.96	1.00
1:B:1778:LEU:CD1	1:B:1830:ILE:HD12	1.91	1.00
1:A:3638:VAL:CG1	1:A:3681:THR:HG21	1.91	0.99
1:A:4605:VAL:HG11	1:A:4635:PHE:CE2	1.96	0.99
1:A:2549:GLN:HG3	1:A:2572:LEU:HD13	1.44	0.98
1:B:1879:LEU:HD12	1:B:1918:ALA:CB	1.93	0.98
1:A:3638:VAL:HG12	1:A:3681:THR:HG21	1.45	0.98
1:B:2819:GLU:OE2	1:B:2862:ASP:CB	2.12	0.98
1:B:3638:VAL:CG1	1:B:3681:THR:HG21	1.91	0.97
1:B:2457:SER:CB	1:B:2584:TRP:CH2	2.44	0.97
1:B:3638:VAL:HG12	1:B:3681:THR:HG21	1.45	0.97
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG2	1.15	0.97
1:A:3749:LEU:CD1	1:A:3773:LEU:HD11	1.95	0.97
1:B:2358:ARG:NH2	2:B:4801:ADP:O1B	1.97	0.97
1:A:2819:GLU:OE2	1:A:2862:ASP:CB	2.12	0.97
1:A:3817:SER:OG	1:A:4349:LEU:HD12	1.65	0.97
1:B:2549:GLN:HG3	1:B:2572:LEU:HD13	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2358:ARG:NH2	2:A:4801:ADP:O1B	1.97	0.96
1:A:1879:LEU:HD12	1:A:1918:ALA:CB	1.93	0.96
1:A:2302:VAL:HG22	1:A:2342:MET:HB2	1.46	0.96
1:A:3459:GLN:HG3	1:B:3456:SER:HB3	1.46	0.96
1:B:3817:SER:OG	1:B:4349:LEU:CD1	2.14	0.96
1:B:3822:HIS:O	1:B:3823:PHE:CG	2.19	0.96
1:B:3749:LEU:CD1	1:B:3773:LEU:HD11	1.95	0.95
1:A:3172:THR:HG21	1:A:3694:SER:OG	1.66	0.95
1:A:3822:HIS:O	1:A:3823:PHE:CG	2.19	0.95
1:A:3817:SER:OG	1:A:4349:LEU:CD1	2.14	0.95
1:A:3821:ILE:HD12	1:A:4342:LYS:CD	1.97	0.95
1:A:2457:SER:CB	1:A:2584:TRP:CH2	2.44	0.95
1:B:1931:ASN:HD22	1:B:2317:SER:HB3	1.15	0.95
1:A:2609:LEU:CD1	1:A:2615:MET:HB2	1.97	0.95
1:A:2220:LEU:HD23	1:A:2342:MET:HG2	1.48	0.95
1:A:3456:SER:HB3	1:B:3459:GLN:HG3	1.49	0.95
1:A:3638:VAL:HG12	1:A:3681:THR:HG23	0.97	0.95
1:B:3817:SER:OG	1:B:4349:LEU:HD12	1.65	0.94
1:B:1981:ALA:HB2	1:B:1999:CYS:SG	2.07	0.94
1:B:3638:VAL:HG12	1:B:3681:THR:HG23	0.97	0.94
1:B:2302:VAL:HG22	1:B:2342:MET:HB2	1.46	0.94
1:B:3822:HIS:O	1:B:3823:PHE:CD2	2.21	0.94
1:A:4622:VAL:HG11	1:A:4624:PHE:CZ	2.03	0.94
1:B:3821:ILE:HD12	1:B:4342:LYS:CD	1.97	0.94
1:B:2609:LEU:CD1	1:B:2615:MET:HB2	1.97	0.94
1:B:1931:ASN:HD22	1:B:2317:SER:CB	1.76	0.94
1:B:3172:THR:HG21	1:B:3694:SER:OG	1.66	0.94
1:A:1981:ALA:HB2	1:A:1999:CYS:SG	2.07	0.93
1:A:3822:HIS:O	1:A:3823:PHE:CD2	2.21	0.93
1:B:4622:VAL:HG11	1:B:4624:PHE:CZ	2.03	0.93
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.48	0.93
1:A:3115:LEU:CD1	1:A:3143:ILE:HD11	1.99	0.92
1:A:1778:LEU:HD11	1:A:1830:ILE:HD12	1.52	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:HB3	1.15	0.92
1:A:1931:ASN:HD22	1:A:2317:SER:CB	1.77	0.92
1:A:4622:VAL:CG1	1:A:4624:PHE:CZ	2.53	0.92
1:B:3115:LEU:CD1	1:B:3143:ILE:HD11	1.99	0.91
1:B:4622:VAL:CG1	1:B:4624:PHE:CZ	2.53	0.91
1:B:2220:LEU:HD23	1:B:2342:MET:HG2	1.49	0.91
1:B:2464:GLN:HG2	1:B:2583:THR:HG23	1.51	0.91
1:B:2605:LEU:CD2	1:B:2662:PHE:CE1	2.54	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.49	0.91
1:B:1778:LEU:HD11	1:B:1830:ILE:HD12	1.52	0.91
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG2	1.15	0.90
1:A:3123:PRO:HB3	1:A:3540:ASN:ND2	1.85	0.90
1:A:2605:LEU:CD2	1:A:2662:PHE:CE1	2.54	0.90
1:B:3123:PRO:HB3	1:B:3540:ASN:ND2	1.85	0.90
1:B:2580:LEU:O	1:B:2584:TRP:CD1	2.24	0.90
1:A:2584:TRP:HZ3	1:A:2732:PRO:CG	1.70	0.89
1:A:2464:GLN:HG2	1:A:2583:THR:HG23	1.51	0.89
1:A:2580:LEU:O	1:A:2584:TRP:CD1	2.24	0.89
1:B:3115:LEU:CD1	1:B:3143:ILE:CD1	2.50	0.89
1:A:4186:PHE:HZ	1:A:4265:LEU:CD1	1.85	0.89
1:B:4186:PHE:HZ	1:B:4265:LEU:CD1	1.85	0.89
1:A:2457:SER:HB3	1:A:2584:TRP:HH2	1.29	0.89
1:A:1632:VAL:CG1	1:A:1636:ASP:HB2	2.03	0.88
1:A:4186:PHE:HZ	1:A:4265:LEU:HD11	1.39	0.88
1:B:2584:TRP:HZ3	1:B:2732:PRO:CG	1.70	0.88
1:B:1632:VAL:CG1	1:B:1636:ASP:HB2	2.03	0.88
1:B:2752:ASN:ND2	1:B:2770:THR:HG22	1.90	0.87
1:A:4067:THR:HB	1:A:4094:VAL:HG22	1.56	0.87
1:B:4186:PHE:HZ	1:B:4265:LEU:HD11	1.38	0.87
1:A:3115:LEU:HD13	1:A:3143:ILE:HD13	1.55	0.87
1:B:3115:LEU:HD13	1:B:3143:ILE:HD13	1.55	0.87
1:A:3638:VAL:HG12	1:A:3681:THR:HG22	1.57	0.86
1:A:3708:LEU:CD2	1:A:3809:SER:HA	2.05	0.86
1:B:2612:LEU:HD13	1:B:2615:MET:HE3	1.56	0.86
1:A:2612:LEU:HD13	1:A:2615:MET:HE3	1.56	0.85
1:B:4067:THR:HB	1:B:4094:VAL:HG22	1.56	0.85
1:A:4424:LEU:CD1	1:A:4486:ILE:HD13	2.07	0.85
1:B:3821:ILE:HD13	1:B:4342:LYS:HD2	1.59	0.85
1:B:3708:LEU:CD2	1:B:3809:SER:HA	2.05	0.85
1:B:2863:ARG:O	1:B:2863:ARG:HD3	1.76	0.85
1:B:3808:CYS:SG	1:B:3836:TYR:OH	2.35	0.85
1:A:2863:ARG:O	1:A:2863:ARG:HD3	1.76	0.85
1:B:4424:LEU:CD1	1:B:4486:ILE:HD13	2.07	0.85
1:A:2091:ARG:NH1	2:A:4801:ADP:O1A	2.10	0.84
1:A:2752:ASN:ND2	1:A:2770:THR:HG22	1.90	0.84
1:A:3115:LEU:CD1	1:A:3143:ILE:CD1	2.50	0.84
1:A:3821:ILE:HD13	1:A:4342:LYS:HD2	1.59	0.84
1:B:2091:ARG:NH1	2:B:4801:ADP:O1A	2.10	0.84
1:A:3821:ILE:CD1	1:A:4342:LYS:CD	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4605:VAL:HG11	1:A:4635:PHE:CZ	2.13	0.83
1:B:2091:ARG:NH1	2:B:4801:ADP:H5'2	1.94	0.83
1:B:4605:VAL:HG11	1:B:4635:PHE:CZ	2.13	0.83
1:A:3808:CYS:SG	1:A:3836:TYR:OH	2.35	0.83
1:A:2446:ILE:HD11	1:A:2735:TYR:CD1	2.14	0.82
1:A:3815:MET:HE2	1:A:3871:VAL:HG22	1.59	0.82
1:B:1879:LEU:CD1	1:B:1918:ALA:HB2	2.10	0.82
1:B:2446:ILE:HD11	1:B:2735:TYR:CD1	2.14	0.82
1:A:2851:ASP:OD2	1:A:2863:ARG:NH1	2.12	0.82
1:A:2091:ARG:NH1	2:A:4801:ADP:H5'2	1.94	0.81
1:B:3821:ILE:CD1	1:B:4342:LYS:CD	2.55	0.81
1:A:1879:LEU:CD1	1:A:1918:ALA:HB2	2.10	0.81
1:B:2851:ASP:OD2	1:B:2863:ARG:NH1	2.12	0.81
1:B:3638:VAL:HG12	1:B:3681:THR:HG22	1.57	0.81
1:A:3882:THR:HG22	1:A:4339:MET:HG3	1.64	0.80
1:B:3822:HIS:ND1	1:B:3824:LEU:HB3	1.97	0.80
1:B:4424:LEU:HD13	1:B:4486:ILE:HD13	1.61	0.80
1:B:2609:LEU:CD2	1:B:2617:VAL:HG23	2.12	0.80
1:A:1931:ASN:OD1	1:A:1958:ASP:HB2	1.82	0.80
1:B:2551:LYS:O	1:B:2551:LYS:HD3	1.82	0.80
1:B:3882:THR:HG22	1:B:4339:MET:HG3	1.64	0.80
1:B:3175:HIS:CD2	1:B:3585:ARG:NH2	2.50	0.80
1:B:2609:LEU:CD2	1:B:2617:VAL:CG2	2.60	0.79
1:A:1636:ASP:OD2	1:A:1656:LYS:NZ	2.14	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:HG23	2.12	0.79
1:B:1879:LEU:HD11	1:B:1914:GLU:O	1.83	0.79
1:A:3822:HIS:ND1	1:A:3824:LEU:HB3	1.97	0.79
1:A:2551:LYS:O	1:A:2551:LYS:HD3	1.82	0.79
1:B:1636:ASP:OD2	1:B:1656:LYS:NZ	2.14	0.79
1:B:2593:LEU:HD23	1:B:2734:VAL:CG2	2.13	0.79
1:A:2609:LEU:CD2	1:A:2617:VAL:CG2	2.60	0.79
1:B:1931:ASN:OD1	1:B:1958:ASP:HB2	1.82	0.78
1:A:3675:PHE:O	1:A:3676:VAL:HG13	1.83	0.78
1:B:3675:PHE:O	1:B:3676:VAL:HG13	1.83	0.78
1:A:1825:LEU:HD12	1:A:1830:ILE:HD11	1.64	0.78
1:A:2605:LEU:CD2	1:A:2662:PHE:CD1	2.66	0.78
1:A:1879:LEU:HD11	1:A:1914:GLU:O	1.83	0.78
1:A:3175:HIS:CD2	1:A:3585:ARG:NH2	2.50	0.78
1:A:2265:TYR:CE2	1:A:2314:ASN:ND2	2.52	0.78
1:A:2609:LEU:HD21	1:A:2617:VAL:HG23	1.66	0.78
1:B:2265:TYR:CE2	1:B:2314:ASN:ND2	2.52	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2605:LEU:CD2	1:B:2662:PHE:CD1	2.66	0.78
1:A:2593:LEU:HD23	1:A:2734:VAL:CG2	2.13	0.78
1:B:2549:GLN:HE21	1:B:2572:LEU:CD2	1.97	0.78
1:A:3008:MET:HE2	1:A:3066:PHE:CZ	2.19	0.77
1:B:3815:MET:CE	1:B:3871:VAL:HG22	2.14	0.77
1:B:1825:LEU:HD12	1:B:1830:ILE:HD11	1.64	0.77
1:B:2609:LEU:HD21	1:B:2617:VAL:HG23	1.66	0.77
1:B:2058:GLY:O	1:B:2104:LYS:HE3	1.85	0.77
1:B:3151:HIS:HD1	1:B:3516:TYR:HH	1.30	0.77
1:B:4622:VAL:HG11	1:B:4624:PHE:CE2	2.17	0.77
1:A:2581:LEU:HD21	1:A:2593:LEU:HD21	1.67	0.76
1:B:2581:LEU:HD21	1:B:2593:LEU:HD21	1.67	0.76
1:A:4622:VAL:HG11	1:A:4624:PHE:CE2	2.17	0.76
1:B:4605:VAL:HG13	1:B:4635:PHE:CE2	2.19	0.76
1:A:4605:VAL:HG13	1:A:4635:PHE:CE2	2.19	0.76
1:A:2584:TRP:CE3	1:A:2732:PRO:HG2	2.17	0.76
1:A:4035:VAL:HG22	1:A:4143:ARG:HG3	1.68	0.76
1:B:2609:LEU:CD1	1:B:2615:MET:CB	2.59	0.76
1:B:2549:GLN:CG	1:B:2572:LEU:HD13	2.16	0.76
1:A:2571:THR:HG1	1:A:2574:THR:HG1	1.29	0.75
1:A:3562:TRP:HB3	1:A:3567:LEU:HD23	1.69	0.75
1:A:4424:LEU:CD1	1:A:4486:ILE:CD1	2.61	0.75
1:A:2058:GLY:O	1:A:2104:LYS:HE3	1.85	0.75
1:A:4190:ILE:HD11	1:A:4252:TYR:HE1	1.52	0.75
1:B:2149:LEU:HD11	1:B:2157:LEU:HD22	1.68	0.75
1:B:4035:VAL:HG22	1:B:4143:ARG:HG3	1.68	0.75
1:A:2609:LEU:CD1	1:A:2615:MET:CB	2.59	0.75
1:A:3008:MET:CE	1:A:3066:PHE:CZ	2.69	0.75
1:A:1778:LEU:HD13	1:A:1830:ILE:HD12	1.68	0.75
1:B:3008:MET:CE	1:B:3066:PHE:CZ	2.69	0.75
1:B:4190:ILE:HD11	1:B:4252:TYR:HE1	1.52	0.75
1:A:1933:ASP:OD1	1:A:1962:ARG:NH2	2.20	0.75
1:A:2549:GLN:CG	1:A:2572:LEU:HD13	2.16	0.75
1:A:2149:LEU:HD11	1:A:2157:LEU:HD22	1.68	0.74
1:B:2584:TRP:CZ3	1:B:2732:PRO:HG3	2.20	0.74
1:B:2584:TRP:CE3	1:B:2732:PRO:HG2	2.17	0.74
1:B:1933:ASP:OD1	1:B:1962:ARG:NH2	2.20	0.74
1:B:1778:LEU:HD13	1:B:1830:ILE:HD12	1.68	0.74
1:B:2749:GLY:HA2	1:B:2770:THR:HG21	1.70	0.74
1:B:2605:LEU:HD23	1:B:2662:PHE:CE1	2.21	0.74
1:B:3562:TRP:HB3	1:B:3567:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2549:GLN:HE21	1:A:2572:LEU:CD2	1.97	0.74
1:A:2605:LEU:HD23	1:A:2662:PHE:CE1	2.21	0.74
1:A:3082:SER:OG	1:A:3085:LEU:HD12	1.87	0.74
1:B:4388:LEU:O	1:B:4392:PRO:HD3	1.88	0.74
1:A:3459:GLN:CG	1:B:3456:SER:CB	2.58	0.73
1:A:4388:LEU:O	1:A:4392:PRO:HD3	1.88	0.73
1:B:2457:SER:OG	1:B:2584:TRP:HH2	1.71	0.73
1:B:3082:SER:OG	1:B:3085:LEU:HD12	1.87	0.73
1:B:3154:LEU:HD22	1:B:3516:TYR:CD2	2.23	0.73
1:B:4424:LEU:CD1	1:B:4486:ILE:CD1	2.61	0.73
1:A:3151:HIS:HD1	1:A:3516:TYR:HH	1.30	0.72
1:A:2749:GLY:HA2	1:A:2770:THR:HG21	1.70	0.72
1:A:3154:LEU:HD22	1:A:3516:TYR:CD2	2.23	0.72
1:A:2078:GLU:OE1	1:A:4522:THR:HG21	1.90	0.72
1:A:2312:VAL:HG11	1:A:2355:THR:HG23	1.70	0.72
1:A:2605:LEU:HD22	1:A:2662:PHE:HE1	1.55	0.72
1:B:2078:GLU:OE1	1:B:4522:THR:HG21	1.90	0.72
1:A:2457:SER:OG	1:A:2584:TRP:HH2	1.71	0.72
1:B:2312:VAL:HG11	1:B:2355:THR:HG23	1.70	0.72
1:B:3550:THR:OG1	1:B:3574:THR:HG22	1.90	0.72
1:A:3638:VAL:HG13	1:A:3681:THR:HG21	1.71	0.72
1:B:2605:LEU:HD22	1:B:2662:PHE:HE1	1.55	0.71
1:A:3822:HIS:CE1	1:A:3824:LEU:HB3	2.25	0.71
1:B:3099:THR:HG22	1:B:3152:GLN:HE22	1.54	0.71
1:A:3550:THR:OG1	1:A:3574:THR:HG22	1.89	0.71
1:B:3099:THR:CG2	1:B:3152:GLN:NE2	2.52	0.71
1:A:3099:THR:CG2	1:A:3152:GLN:HE22	2.04	0.71
1:B:3638:VAL:HG13	1:B:3681:THR:HG21	1.71	0.70
1:B:3008:MET:HE2	1:B:3066:PHE:CZ	2.25	0.70
1:B:4607:LEU:CD2	1:B:4635:PHE:CZ	2.70	0.70
1:B:3822:HIS:CE1	1:B:3824:LEU:HB3	2.25	0.70
1:A:2584:TRP:CZ3	1:A:2732:PRO:HG3	2.20	0.70
1:B:2571:THR:HG1	1:B:2574:THR:HG1	1.22	0.70
1:A:3562:TRP:HB3	1:A:3567:LEU:CD2	2.22	0.70
1:A:2933:LEU:HD23	1:A:3065:VAL:HG13	1.73	0.70
1:A:3099:THR:CG2	1:A:3152:GLN:NE2	2.52	0.70
1:A:1762:VAL:O	1:A:1766:LEU:HD13	1.92	0.69
1:B:3099:THR:CG2	1:B:3152:GLN:HE22	2.04	0.69
1:B:1766:LEU:CD2	1:B:1833:ALA:HA	2.19	0.69
1:B:2912:PHE:HB2	1:B:3104:GLN:OE1	1.93	0.69
1:B:3815:MET:HE2	1:B:3871:VAL:HG22	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1766:LEU:CD2	1:A:1833:ALA:HA	2.19	0.69
1:A:3456:SER:OG	1:B:3459:GLN:CD	2.30	0.69
1:B:2457:SER:HB3	1:B:2584:TRP:CZ2	2.28	0.69
1:A:3456:SER:CB	1:B:3459:GLN:CG	2.58	0.69
1:A:4607:LEU:CD2	1:A:4635:PHE:CZ	2.70	0.69
1:B:3562:TRP:HB3	1:B:3567:LEU:CD2	2.22	0.69
1:A:1931:ASN:HD21	1:A:2317:SER:HB3	1.51	0.69
1:A:4190:ILE:HD11	1:A:4252:TYR:CE1	2.28	0.69
1:B:2933:LEU:HD23	1:B:3065:VAL:HG13	1.73	0.69
1:A:3099:THR:HG22	1:A:3152:GLN:HE22	1.54	0.69
1:B:1762:VAL:O	1:B:1766:LEU:HD13	1.92	0.69
1:A:2912:PHE:HB2	1:A:3104:GLN:OE1	1.93	0.69
1:B:3824:LEU:CD2	1:B:4130:ILE:HG12	2.23	0.69
1:B:1632:VAL:CG1	1:B:1636:ASP:CB	2.71	0.68
1:B:2995:ASP:OD1	1:B:3067:THR:HB	1.94	0.68
1:A:2626:THR:O	1:A:2627:THR:HG23	1.93	0.68
1:A:1632:VAL:CG1	1:A:1636:ASP:CB	2.71	0.68
1:A:2995:ASP:OD1	1:A:3067:THR:HB	1.94	0.68
1:B:2626:THR:O	1:B:2627:THR:HG23	1.93	0.68
1:A:2457:SER:HB3	1:A:2584:TRP:CZ2	2.28	0.68
1:A:2196:GLY:CA	1:A:2201:GLY:HA3	2.19	0.68
1:A:3550:THR:OG1	1:A:3574:THR:CG2	2.42	0.68
1:B:3478:LEU:HD13	1:B:3770:LEU:HD13	1.75	0.68
1:B:4247:MET:HE2	1:B:4252:TYR:CE2	2.28	0.68
1:A:3459:GLN:CD	1:B:3456:SER:OG	2.32	0.68
1:A:3824:LEU:CD2	1:A:4130:ILE:HG12	2.23	0.68
1:B:3522:GLN:OE1	1:B:3704:THR:HG21	1.94	0.68
1:A:4247:MET:CE	1:A:4252:TYR:HE2	2.07	0.68
1:B:2196:GLY:CA	1:B:2201:GLY:HA3	2.19	0.68
1:B:3550:THR:OG1	1:B:3574:THR:CG2	2.42	0.68
1:B:4190:ILE:HD11	1:B:4252:TYR:CE1	2.28	0.68
1:B:4247:MET:CE	1:B:4252:TYR:HE2	2.07	0.68
1:A:2580:LEU:HG	1:A:2584:TRP:HE1	1.59	0.67
1:A:3815:MET:CE	1:A:3871:VAL:HG22	2.14	0.67
1:A:2605:LEU:HD22	1:A:2662:PHE:CE1	2.27	0.67
1:A:3522:GLN:OE1	1:A:3704:THR:HG21	1.94	0.67
1:B:2549:GLN:NE2	1:B:2572:LEU:CD2	2.53	0.67
1:B:3175:HIS:HD2	1:B:3585:ARG:NH2	1.92	0.67
1:A:4186:PHE:CZ	1:A:4265:LEU:HD11	2.28	0.67
1:B:2555:ILE:HG21	1:B:2570:PRO:HD2	1.76	0.67
1:B:2580:LEU:HG	1:B:2584:TRP:HE1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2910:VAL:HG11	1:A:3105:VAL:HG23	1.77	0.67
1:A:2555:ILE:HG21	1:A:2570:PRO:HD2	1.76	0.67
1:A:2612:LEU:HD13	1:A:2615:MET:CE	2.25	0.67
1:A:3200:HIS:O	1:A:3204:GLY:N	2.28	0.67
1:B:1931:ASN:HD21	1:B:2317:SER:HB3	1.51	0.67
1:A:3675:PHE:O	1:A:3676:VAL:CG1	2.43	0.66
1:B:2910:VAL:HG11	1:B:3105:VAL:HG23	1.77	0.66
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.77	0.66
1:B:3200:HIS:O	1:B:3204:GLY:N	2.28	0.66
1:B:4186:PHE:CZ	1:B:4265:LEU:HD11	2.28	0.66
1:A:3924:ILE:O	1:A:3924:ILE:HG22	1.95	0.66
1:A:4247:MET:HE2	1:A:4252:TYR:CE2	2.30	0.66
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	1.77	0.66
1:A:2863:ARG:HD3	1:A:2863:ARG:C	2.16	0.66
1:A:3478:LEU:HD13	1:A:3770:LEU:HD13	1.76	0.66
1:B:1632:VAL:HG12	1:B:1636:ASP:HB2	1.77	0.66
1:B:3675:PHE:O	1:B:3676:VAL:CG1	2.43	0.66
1:A:3021:PHE:CD1	1:A:3029:LEU:HD12	2.31	0.65
1:B:3021:PHE:CD1	1:B:3029:LEU:HD12	2.31	0.65
1:A:2584:TRP:CH2	1:A:2732:PRO:CG	2.79	0.65
1:A:2593:LEU:HD23	1:A:2734:VAL:HG23	1.78	0.65
1:B:2863:ARG:HD3	1:B:2863:ARG:C	2.16	0.65
1:A:2787:ASP:OD1	1:A:2787:ASP:O	2.15	0.65
1:A:3175:HIS:HD2	1:A:3585:ARG:NH2	1.92	0.65
1:B:3021:PHE:CE1	1:B:3029:LEU:HD12	2.32	0.65
1:A:2609:LEU:HD22	1:A:2617:VAL:CG2	2.27	0.65
1:B:2091:ARG:NH1	2:B:4801:ADP:C5'	2.60	0.65
1:B:2593:LEU:HD23	1:B:2734:VAL:HG23	1.78	0.65
1:A:3021:PHE:CE1	1:A:3029:LEU:HD12	2.32	0.64
1:B:2612:LEU:HD13	1:B:2615:MET:CE	2.25	0.64
1:B:3924:ILE:HG22	1:B:3924:ILE:O	1.95	0.64
1:A:1632:VAL:HG12	1:A:1636:ASP:HB2	1.77	0.64
1:B:2584:TRP:HZ3	1:B:2732:PRO:HG3	1.60	0.64
1:B:4388:LEU:HD21	1:B:4434:VAL:HG13	1.79	0.64
1:B:4565:LEU:HD23	1:B:4642:VAL:HG22	1.79	0.64
1:B:2584:TRP:CH2	1:B:2732:PRO:CG	2.79	0.64
1:A:1778:LEU:HD11	1:A:1830:ILE:CD1	2.27	0.64
1:B:2602:THR:OG1	2:B:4804:ADP:O1A	2.16	0.64
1:A:2091:ARG:NH1	2:A:4801:ADP:C5'	2.60	0.64
1:B:2609:LEU:HD22	1:B:2617:VAL:CG2	2.27	0.64
1:B:2787:ASP:O	1:B:2787:ASP:OD1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3580:LEU:HD21	1:A:3589:ILE:HD11	1.80	0.64
1:A:1766:LEU:HD23	1:A:1833:ALA:CA	2.22	0.63
1:A:4560:VAL:O	1:A:4587:LEU:HD12	1.98	0.63
1:A:4388:LEU:HD21	1:A:4434:VAL:HG13	1.79	0.63
1:B:3817:SER:HG	1:B:4349:LEU:HD12	1.62	0.63
1:A:2602:THR:OG1	2:A:4804:ADP:O1A	2.16	0.63
1:A:2667:ASN:ND2	1:A:2713:ASN:O	2.32	0.63
1:B:4560:VAL:O	1:B:4587:LEU:HD12	1.98	0.63
1:B:2667:ASN:ND2	1:B:2713:ASN:O	2.32	0.63
1:B:3580:LEU:HD21	1:B:3589:ILE:HD11	1.81	0.63
1:A:4565:LEU:HD23	1:A:4642:VAL:HG22	1.79	0.63
1:B:3708:LEU:HD23	1:B:3809:SER:CA	2.26	0.63
1:B:4190:ILE:CD1	1:B:4252:TYR:CE1	2.82	0.62
1:A:3811:ILE:HD12	1:A:3887:LEU:HD22	1.81	0.62
1:B:2612:LEU:CD1	1:B:2615:MET:HE3	2.29	0.62
1:B:3824:LEU:HD22	1:B:4130:ILE:HG12	1.79	0.62
1:B:3482:LEU:O	1:B:3486:ARG:N	2.32	0.62
1:A:3824:LEU:HD22	1:A:4130:ILE:HG12	1.80	0.62
1:B:2605:LEU:HD22	1:B:2662:PHE:CE1	2.27	0.62
1:B:3008:MET:HE1	1:B:3066:PHE:CZ	2.35	0.62
1:A:1879:LEU:HD12	1:A:1918:ALA:HB3	1.82	0.62
1:A:4508:HIS:CE1	1:A:4587:LEU:HD21	2.35	0.62
1:B:3811:ILE:CD1	1:B:3887:LEU:HD22	2.30	0.62
1:A:2568:VAL:HG22	1:A:2603:MET:CE	2.30	0.61
1:B:2568:VAL:HG22	1:B:2603:MET:CE	2.30	0.61
1:A:2549:GLN:NE2	1:A:2572:LEU:CD2	2.53	0.61
1:B:2103:VAL:HG13	1:B:2136:ILE:HG23	1.82	0.61
1:B:2593:LEU:CD1	1:B:2605:LEU:HB2	2.30	0.61
1:A:1931:ASN:ND2	1:A:2317:SER:CA	2.63	0.61
1:A:4190:ILE:CD1	1:A:4252:TYR:CE1	2.82	0.61
1:B:3811:ILE:HD12	1:B:3887:LEU:HD22	1.81	0.61
1:A:2072:PHE:HZ	1:A:2157:LEU:HD11	1.64	0.61
1:B:2100:ALA:HA	1:B:2140:SER:OG	2.01	0.61
1:A:1927:VAL:HG12	1:A:1954:TRP:HB2	1.83	0.61
1:A:2103:VAL:HG13	1:A:2136:ILE:HG23	1.82	0.61
1:A:3482:LEU:O	1:A:3486:ARG:N	2.32	0.61
1:B:3824:LEU:HD22	1:B:4130:ILE:HG23	1.82	0.60
1:B:4508:HIS:CE1	1:B:4587:LEU:HD21	2.35	0.60
1:A:2593:LEU:CD1	1:A:2605:LEU:HB2	2.30	0.60
1:A:2612:LEU:CD1	1:A:2615:MET:HE3	2.29	0.60
1:B:1879:LEU:HD12	1:B:1918:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3459:GLN:CG	1:B:3456:SER:HB3	2.28	0.60
1:B:1931:ASN:ND2	1:B:2317:SER:CA	2.63	0.60
1:A:2549:GLN:CD	1:A:2572:LEU:HD22	2.22	0.60
1:A:2571:THR:CG2	1:A:2747:ILE:HG12	2.32	0.60
1:B:1766:LEU:HD23	1:B:1833:ALA:CA	2.22	0.60
1:B:2571:THR:CG2	1:B:2747:ILE:HG12	2.32	0.60
1:A:2936:ILE:HG21	1:A:3093:TRP:CZ3	2.36	0.60
1:A:3708:LEU:HD23	1:A:3809:SER:CA	2.26	0.60
1:A:3824:LEU:HD22	1:A:4130:ILE:HG23	1.82	0.60
1:B:2072:PHE:HZ	1:B:2157:LEU:HD11	1.64	0.60
1:B:2936:ILE:HG21	1:B:3093:TRP:CZ3	2.36	0.60
1:A:3639:GLU:OE2	1:A:4137:ASN:ND2	2.22	0.60
1:A:4561:THR:CG2	1:A:4587:LEU:HD13	2.32	0.60
1:B:2540:SER:OG	1:B:2544:GLU:O	2.16	0.60
1:A:2551:LYS:HD3	1:A:2551:LYS:C	2.22	0.60
1:A:3811:ILE:CD1	1:A:3887:LEU:HD22	2.30	0.60
1:B:4561:THR:CG2	1:B:4587:LEU:HD13	2.32	0.60
1:A:2100:ALA:HA	1:A:2140:SER:OG	2.01	0.60
1:A:2605:LEU:HD21	1:A:2662:PHE:CD1	2.37	0.60
1:B:2549:GLN:CD	1:B:2572:LEU:HD22	2.22	0.60
1:B:2830:LEU:HD12	1:B:2871:ILE:HG21	1.84	0.60
1:B:4622:VAL:HG12	1:B:4624:PHE:CZ	2.28	0.59
1:B:1927:VAL:HG12	1:B:1954:TRP:HB2	1.83	0.59
1:B:4507:ILE:HG13	1:B:4509:VAL:HG23	1.83	0.59
1:A:4507:ILE:HG13	1:A:4509:VAL:HG23	1.83	0.59
1:B:2472:TYR:HB2	1:B:2541:ILE:HD11	1.84	0.59
1:B:3822:HIS:CE1	1:B:3824:LEU:CB	2.86	0.59
1:B:2551:LYS:HD3	1:B:2551:LYS:C	2.22	0.59
1:B:3099:THR:HG22	1:B:3152:GLN:HE21	1.65	0.59
1:A:3099:THR:HG22	1:A:3152:GLN:HE21	1.65	0.59
1:A:3822:HIS:CE1	1:A:3824:LEU:CB	2.86	0.59
1:B:4186:PHE:CZ	1:B:4265:LEU:CD1	2.77	0.59
1:B:1778:LEU:HD11	1:B:1830:ILE:CD1	2.27	0.59
1:B:1830:ILE:HG22	1:B:1831:ASP:N	2.18	0.59
1:B:2584:TRP:CZ3	1:B:2732:PRO:CB	2.86	0.59
1:B:3150:VAL:HG22	1:B:3532:TRP:CD1	2.38	0.59
1:B:4247:MET:CE	1:B:4252:TYR:CE2	2.86	0.59
1:B:3822:HIS:HB3	1:B:3825:TYR:CZ	2.38	0.59
1:A:3150:VAL:HG22	1:A:3532:TRP:CD1	2.38	0.58
1:B:2549:GLN:HG3	1:B:2572:LEU:CD1	2.29	0.58
1:A:2830:LEU:HD12	1:A:2871:ILE:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3683:ASP:HB2	1:A:4137:ASN:OD1	2.03	0.58
1:A:2294:GLU:OE1	1:A:2299:GLN:NE2	2.37	0.58
1:A:4247:MET:CE	1:A:4252:TYR:CE2	2.86	0.58
1:B:3639:GLU:OE2	1:B:4137:ASN:ND2	2.22	0.58
1:A:2472:TYR:HB2	1:A:2541:ILE:HD11	1.84	0.58
1:A:4027:LEU:HD23	1:A:4058:LEU:HD13	1.86	0.58
1:B:2588:HIS:HA	1:B:2707:GLN:NE2	2.18	0.58
1:A:2588:HIS:HA	1:A:2707:GLN:NE2	2.18	0.58
1:B:2279:LEU:O	1:B:2283:VAL:HG23	2.04	0.58
1:A:3822:HIS:HB3	1:A:3825:TYR:CZ	2.38	0.58
1:B:2294:GLU:OE1	1:B:2299:GLN:NE2	2.37	0.58
1:B:4027:LEU:HD23	1:B:4058:LEU:HD13	1.86	0.58
1:A:1896:LEU:HD21	1:A:1954:TRP:CZ2	2.39	0.58
1:A:2963:VAL:HG23	1:A:2967:TYR:CD2	2.39	0.58
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.36	0.58
1:B:2605:LEU:HD21	1:B:2662:PHE:CD1	2.37	0.58
1:B:4388:LEU:CD2	1:B:4434:VAL:HG13	2.33	0.58
1:A:1830:ILE:HG22	1:A:1831:ASP:N	2.18	0.58
1:A:2295:LEU:C	1:A:2338:ASN:HD21	2.07	0.58
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.36	0.58
1:B:1935:THR:HG22	1:B:2328:PRO:HG2	1.86	0.58
1:B:2295:LEU:C	1:B:2338:ASN:HD21	2.07	0.58
1:B:2912:PHE:CE2	1:B:3101:ALA:HB1	2.39	0.58
1:A:2912:PHE:CE2	1:A:3101:ALA:HB1	2.39	0.57
1:A:4388:LEU:CD2	1:A:4434:VAL:HG13	2.33	0.57
1:A:4424:LEU:HD11	1:A:4486:ILE:HD13	1.86	0.57
1:B:2963:VAL:HG23	1:B:2967:TYR:CD2	2.39	0.57
1:A:2295:LEU:HA	1:A:2338:ASN:HD22	1.70	0.57
1:A:4605:VAL:HG13	1:A:4635:PHE:CD2	2.39	0.57
1:A:2279:LEU:O	1:A:2283:VAL:HG23	2.04	0.57
1:B:1889:TYR:O	1:B:1893:THR:HG23	2.05	0.57
1:B:3683:ASP:HB2	1:B:4137:ASN:OD1	2.04	0.57
1:B:4605:VAL:HG13	1:B:4635:PHE:CD2	2.39	0.57
1:A:1571:ILE:HD13	1:A:1607:LEU:HD22	1.87	0.57
1:B:1896:LEU:HD21	1:B:1954:TRP:CZ2	2.39	0.57
1:B:2568:VAL:HG22	1:B:2603:MET:HE2	1.87	0.57
1:B:2571:THR:HG21	1:B:2747:ILE:HG12	1.87	0.57
1:B:3203:VAL:C	1:B:3204:GLY:N	2.58	0.57
1:B:4086:THR:O	1:B:4090:SER:N	2.37	0.57
1:B:4186:PHE:HE2	1:B:4252:TYR:CD2	2.23	0.57
1:A:4247:MET:HE3	1:A:4252:TYR:HE2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4508:HIS:CE1	1:A:4587:LEU:CD2	2.88	0.57
1:B:1571:ILE:HD13	1:B:1607:LEU:HD22	1.87	0.57
1:A:1935:THR:HG22	1:A:2328:PRO:HG2	1.86	0.57
1:A:3082:SER:OG	1:A:3085:LEU:CD1	2.53	0.57
1:B:4508:HIS:CE1	1:B:4587:LEU:CD2	2.88	0.57
1:A:4186:PHE:HE2	1:A:4252:TYR:CD2	2.23	0.56
1:B:1778:LEU:CD1	1:B:1830:ILE:CD1	2.75	0.56
1:A:3451:TYR:CE1	1:A:3455:ILE:HD11	2.40	0.56
1:A:4067:THR:HG21	1:A:4083:ALA:HB1	1.87	0.56
1:B:2499:LEU:HD12	1:B:2514:LEU:HD23	1.87	0.56
1:A:1892:MET:O	1:A:1896:LEU:HD13	2.05	0.56
1:A:2499:LEU:HD12	1:A:2514:LEU:HD23	1.87	0.56
1:A:2571:THR:OG1	1:A:2574:THR:OG1	2.06	0.56
1:A:2584:TRP:CZ3	1:A:2732:PRO:CB	2.86	0.56
1:A:2626:THR:O	1:A:2627:THR:CG2	2.53	0.56
1:A:3203:VAL:C	1:A:3204:GLY:N	2.58	0.56
1:B:2295:LEU:HA	1:B:2338:ASN:HD22	1.70	0.56
1:B:3451:TYR:CE1	1:B:3455:ILE:HD11	2.40	0.56
1:A:3818:LEU:O	1:A:3821:ILE:HG22	2.06	0.56
1:A:4507:ILE:CD1	1:A:4509:VAL:CG2	2.84	0.56
1:A:1778:LEU:CD1	1:A:1830:ILE:CD1	2.75	0.56
1:A:1889:TYR:O	1:A:1893:THR:HG23	2.05	0.56
1:A:2591:LEU:HG	1:A:2709:VAL:HG12	1.88	0.56
1:A:3456:SER:HB3	1:B:3459:GLN:CG	2.30	0.56
1:B:4067:THR:HG21	1:B:4083:ALA:HB1	1.87	0.56
1:B:4560:VAL:HG12	1:B:4563:LEU:HD11	1.88	0.56
1:A:1644:SER:HA	1:A:1650:LEU:HD11	1.88	0.56
1:A:3822:HIS:HB3	1:A:3825:TYR:CE1	2.41	0.56
1:A:4186:PHE:CZ	1:A:4265:LEU:CD1	2.77	0.56
1:B:1644:SER:HA	1:B:1650:LEU:HD11	1.88	0.56
1:B:1879:LEU:HD11	1:B:1914:GLU:C	2.27	0.56
1:B:4507:ILE:CD1	1:B:4509:VAL:CG2	2.84	0.56
1:B:2626:THR:O	1:B:2627:THR:CG2	2.53	0.56
1:A:2571:THR:HG21	1:A:2747:ILE:HG12	1.87	0.55
1:B:2461:MET:HE3	1:B:2584:TRP:CZ2	2.41	0.55
1:B:2994:MET:CE	1:B:3008:MET:SD	2.94	0.55
1:B:4561:THR:HG22	1:B:4587:LEU:HD13	1.88	0.55
1:A:1879:LEU:HD11	1:A:1914:GLU:C	2.27	0.55
1:A:2091:ARG:CZ	2:A:4801:ADP:H5'2	2.36	0.55
1:B:2609:LEU:HD11	1:B:2615:MET:HB3	1.83	0.55
1:A:2994:MET:CE	1:A:3008:MET:SD	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2591:LEU:HG	1:B:2709:VAL:HG12	1.88	0.55
1:A:1830:ILE:CG2	1:A:1831:ASP:N	2.69	0.55
1:A:4561:THR:HG22	1:A:4587:LEU:HD13	1.88	0.55
1:B:2464:GLN:HG2	1:B:2583:THR:CG2	2.32	0.55
1:A:2091:ARG:HH11	2:A:4801:ADP:H5'2	1.71	0.55
1:A:2897:LEU:HD23	1:A:2901:TYR:OH	2.07	0.55
1:B:1892:MET:O	1:B:1896:LEU:HD13	2.05	0.55
1:A:1765:ALA:CB	1:A:1778:LEU:HD23	2.37	0.55
1:B:2897:LEU:HD23	1:B:2901:TYR:OH	2.07	0.55
1:B:1830:ILE:CG2	1:B:1831:ASP:N	2.69	0.55
1:B:3082:SER:OG	1:B:3085:LEU:CD1	2.53	0.55
1:B:4395:LEU:HD21	1:B:4483:SER:HA	1.88	0.55
1:A:2609:LEU:HD11	1:A:2615:MET:HB3	1.83	0.55
1:A:4560:VAL:HG12	1:A:4563:LEU:HD11	1.88	0.55
1:B:3822:HIS:HB3	1:B:3825:TYR:CE1	2.41	0.55
1:B:4424:LEU:HD11	1:B:4486:ILE:HD13	1.86	0.55
1:A:3008:MET:HE1	1:A:3066:PHE:CZ	2.41	0.55
1:A:3236:ALA:HB1	1:A:3451:TYR:HE1	1.72	0.55
1:A:4186:PHE:HZ	1:A:4265:LEU:HD12	1.71	0.54
1:B:2091:ARG:CZ	2:B:4801:ADP:H5'2	2.36	0.54
1:A:4395:LEU:HD21	1:A:4483:SER:HA	1.88	0.54
1:B:4560:VAL:HG12	1:B:4563:LEU:CD1	2.38	0.54
1:B:1765:ALA:CB	1:B:1778:LEU:HD23	2.37	0.54
1:B:3818:LEU:O	1:B:3821:ILE:HG22	2.06	0.54
1:A:2457:SER:CA	1:A:2584:TRP:CH2	2.91	0.54
1:A:2893:VAL:O	1:A:2897:LEU:HD13	2.07	0.54
1:A:4560:VAL:HG12	1:A:4563:LEU:CD1	2.38	0.54
1:A:4067:THR:HG21	1:A:4083:ALA:CB	2.37	0.54
1:B:2893:VAL:O	1:B:2897:LEU:HD13	2.07	0.54
1:A:2192:THR:OG1	1:A:2373:MET:HG3	2.07	0.54
1:A:2312:VAL:HG11	1:A:2355:THR:CG2	2.38	0.54
1:A:2464:GLN:OE1	1:A:2586:ALA:HB3	2.08	0.54
1:A:2552:VAL:HG23	1:A:2552:VAL:O	2.08	0.54
1:B:2464:GLN:OE1	1:B:2586:ALA:HB3	2.08	0.54
1:B:3150:VAL:O	1:B:3153:THR:OG1	2.25	0.54
1:B:4511:LEU:HD22	1:B:4644:CYS:HG	1.66	0.54
1:A:2190:TYR:O	1:A:2377:ASN:CG	2.46	0.54
1:B:3745:LEU:HD11	1:B:3773:LEU:HA	1.89	0.54
1:A:2295:LEU:HA	1:A:2338:ASN:ND2	2.23	0.54
1:A:4086:THR:O	1:A:4090:SER:N	2.37	0.54
1:B:2190:TYR:O	1:B:2377:ASN:CG	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2767:GLU:N	1:B:2768:PRO:HD2	2.23	0.54
1:B:2819:GLU:CD	1:B:2862:ASP:CB	2.77	0.54
1:A:3745:LEU:HD11	1:A:3773:LEU:HA	1.89	0.54
1:B:1765:ALA:HB3	1:B:1778:LEU:HD23	1.89	0.53
1:B:2295:LEU:HA	1:B:2338:ASN:ND2	2.23	0.53
1:B:3222:LEU:HD12	1:B:3465:LEU:HD23	1.90	0.53
1:B:3803:PRO:C	1:B:3804:LEU:N	2.62	0.53
1:B:3822:HIS:C	1:B:3823:PHE:CD2	2.81	0.53
1:B:4067:THR:HG21	1:B:4083:ALA:CB	2.37	0.53
1:A:2767:GLU:N	1:A:2768:PRO:HD2	2.23	0.53
1:A:3803:PRO:C	1:A:3804:LEU:N	2.62	0.53
1:B:4247:MET:HE3	1:B:4252:TYR:HE2	1.72	0.53
1:A:2300:TRP:CD2	1:A:2342:MET:HE3	2.43	0.53
1:A:3150:VAL:O	1:A:3153:THR:OG1	2.25	0.53
1:A:1765:ALA:HB3	1:A:1778:LEU:HD23	1.89	0.53
1:A:2265:TYR:CD2	1:A:2314:ASN:ND2	2.76	0.53
1:A:2549:GLN:HG3	1:A:2572:LEU:CD1	2.29	0.53
1:A:3822:HIS:C	1:A:3823:PHE:CD2	2.81	0.53
1:B:1879:LEU:CD1	1:B:1914:GLU:O	2.55	0.53
1:B:2552:VAL:HG23	1:B:2552:VAL:O	2.08	0.53
1:B:4622:VAL:HG11	1:B:4624:PHE:HZ	1.69	0.53
1:A:2461:MET:HE3	1:A:2584:TRP:CZ2	2.44	0.53
1:B:2091:ARG:HH11	2:B:4801:ADP:H5'2	1.71	0.53
1:A:2182:LEU:HD11	1:A:2207:VAL:HG11	1.91	0.53
1:A:3175:HIS:CD2	1:A:3585:ARG:CZ	2.92	0.53
1:B:2192:THR:OG1	1:B:2373:MET:HG3	2.07	0.53
1:B:3205:LEU:O	1:B:3208:ILE:HG22	2.09	0.53
1:A:2464:GLN:HG2	1:A:2583:THR:CG2	2.32	0.53
1:B:2457:SER:CA	1:B:2584:TRP:CH2	2.91	0.53
1:A:2238:LEU:HD13	1:A:2300:TRP:CE3	2.44	0.53
1:A:2584:TRP:HZ3	1:A:2732:PRO:HG3	1.60	0.53
1:A:3811:ILE:CD1	1:A:3887:LEU:CD2	2.87	0.53
1:B:2046:ARG:HA	1:B:2049:ILE:HG22	1.90	0.53
1:B:2238:LEU:HD13	1:B:2300:TRP:CE3	2.44	0.53
1:B:3236:ALA:HB1	1:B:3451:TYR:HE1	1.72	0.53
1:B:4607:LEU:CD2	1:B:4635:PHE:CE2	2.92	0.53
1:A:1762:VAL:O	1:A:1766:LEU:CD1	2.58	0.52
1:A:3205:LEU:O	1:A:3208:ILE:HG22	2.09	0.52
1:B:3236:ALA:HB1	1:B:3451:TYR:CE1	2.44	0.52
1:B:3749:LEU:HD13	1:B:3773:LEU:HD12	1.74	0.52
1:B:2265:TYR:CD2	1:B:2314:ASN:ND2	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2302:VAL:HG22	1:B:2342:MET:CB	2.31	0.52
1:B:3175:HIS:CD2	1:B:3585:ARG:CZ	2.92	0.52
1:B:3882:THR:OG1	1:B:4342:LYS:NZ	2.35	0.52
1:A:1825:LEU:HD12	1:A:1830:ILE:CD1	2.38	0.52
1:B:2345:VAL:HG11	1:B:2348:LEU:HD21	1.91	0.52
1:B:3010:THR:HG22	1:B:3016:GLU:O	2.10	0.52
1:A:1970:ALA:CB	1:A:4073:SER:HB2	2.40	0.52
1:A:2046:ARG:HA	1:A:2049:ILE:HG22	1.90	0.52
1:A:2584:TRP:CH2	1:A:2732:PRO:HB3	2.45	0.52
1:A:2819:GLU:CD	1:A:2862:ASP:CB	2.76	0.52
1:A:3236:ALA:HB1	1:A:3451:TYR:CE1	2.44	0.52
1:B:2312:VAL:HG11	1:B:2355:THR:CG2	2.38	0.52
1:A:4607:LEU:CD2	1:A:4635:PHE:CE2	2.92	0.52
1:B:3824:LEU:HD21	1:B:4130:ILE:HG12	1.92	0.52
1:A:2091:ARG:CZ	2:A:4801:ADP:H4'	2.40	0.52
1:A:2345:VAL:HG11	1:A:2348:LEU:HD21	1.91	0.52
1:A:2994:MET:HE1	1:A:3008:MET:SD	2.49	0.52
1:A:3222:LEU:HD12	1:A:3465:LEU:HD23	1.90	0.52
1:B:2182:LEU:HD11	1:B:2207:VAL:HG11	1.91	0.52
1:B:2307:VAL:HG13	1:B:2312:VAL:HG21	1.92	0.52
1:A:2302:VAL:HG22	1:A:2342:MET:CB	2.31	0.52
1:A:3102:LEU:O	1:A:3105:VAL:HG12	2.10	0.52
1:A:3817:SER:HG	1:A:4349:LEU:HD12	1.72	0.52
1:B:2091:ARG:CZ	2:B:4801:ADP:H4'	2.40	0.52
1:B:2300:TRP:CD2	1:B:2342:MET:HE3	2.46	0.51
1:A:2230:LYS:NZ	3:A:4802:ATP:O3G	2.43	0.51
1:A:2549:GLN:CG	1:A:2572:LEU:HD22	2.40	0.51
1:A:2648:VAL:HG11	1:A:2694:ARG:NH2	2.26	0.51
1:A:3882:THR:OG1	1:A:4342:LYS:NZ	2.35	0.51
1:B:3811:ILE:CD1	1:B:3887:LEU:CD2	2.87	0.51
1:A:4589:GLN:C	1:A:4590:LEU:HD12	2.31	0.51
1:B:2078:GLU:OE1	1:B:4522:THR:CG2	2.58	0.51
1:A:1490:TRP:CG	1:A:1538:ILE:HD12	2.45	0.51
1:A:2588:HIS:HA	1:A:2707:GLN:HE22	1.76	0.51
1:A:2849:ASN:O	1:A:2852:THR:HG22	2.11	0.51
1:A:3021:PHE:CG	1:A:3029:LEU:CD1	2.93	0.51
1:B:1970:ALA:CB	1:B:4073:SER:HB2	2.40	0.51
1:B:4589:GLN:C	1:B:4590:LEU:HD12	2.31	0.51
1:A:4186:PHE:HE2	1:A:4252:TYR:CG	2.28	0.51
1:A:4622:VAL:HG11	1:A:4624:PHE:HZ	1.70	0.51
1:B:2584:TRP:CH2	1:B:2732:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2584:TRP:CH2	1:B:2732:PRO:CB	2.93	0.51
1:B:4042:LEU:CD2	1:B:4139:LEU:HD23	2.41	0.51
1:A:3888:ALA:HB1	1:A:4012:ASN:HD22	1.75	0.51
1:A:4609:VAL:HG23	1:A:4622:VAL:HG23	1.93	0.51
1:A:1750:VAL:HG12	1:A:1811:LEU:HD13	1.93	0.51
1:B:1750:VAL:HG12	1:B:1811:LEU:HD13	1.93	0.51
1:B:2605:LEU:HD21	1:B:2662:PHE:HD1	1.75	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:CD1	2.93	0.51
1:B:4186:PHE:HE2	1:B:4252:TYR:CG	2.28	0.51
1:B:2149:LEU:HD11	1:B:2157:LEU:CD2	2.40	0.51
1:B:2230:LYS:NZ	3:B:4802:ATP:O3G	2.43	0.51
1:A:2307:VAL:HG13	1:A:2312:VAL:HG21	1.92	0.51
1:A:2584:TRP:CH2	1:A:2732:PRO:CB	2.93	0.51
1:B:4609:VAL:HG23	1:B:4622:VAL:HG23	1.93	0.51
1:A:2568:VAL:HG22	1:A:2603:MET:HE3	1.91	0.51
1:B:1490:TRP:CG	1:B:1538:ILE:HD12	2.45	0.51
1:B:1762:VAL:O	1:B:1766:LEU:CD1	2.57	0.51
1:B:2588:HIS:HA	1:B:2707:GLN:HE22	1.76	0.51
1:B:2648:VAL:HG11	1:B:2694:ARG:NH2	2.26	0.51
1:B:3021:PHE:CG	1:B:3029:LEU:HD13	2.46	0.51
1:B:3102:LEU:O	1:B:3105:VAL:HG12	2.10	0.51
1:B:4507:ILE:HD12	1:B:4509:VAL:HG22	1.93	0.51
1:B:4560:VAL:CG1	1:B:4563:LEU:HD11	2.41	0.51
1:B:4622:VAL:CG1	1:B:4624:PHE:HE2	2.15	0.51
1:A:2593:LEU:HD11	1:A:2605:LEU:HB2	1.93	0.50
1:A:4607:LEU:HD21	1:A:4635:PHE:CE2	2.41	0.50
1:B:1752:LEU:CD2	1:B:1756:ILE:HD11	2.41	0.50
1:B:2549:GLN:CG	1:B:2572:LEU:HD22	2.41	0.50
1:A:1752:LEU:CD2	1:A:1756:ILE:HD11	2.41	0.50
1:A:2593:LEU:CD2	1:A:2734:VAL:CG2	2.89	0.50
1:A:4622:VAL:HG12	1:A:4624:PHE:CZ	2.28	0.50
1:B:3888:ALA:HB1	1:B:4012:ASN:HD22	1.75	0.50
1:B:4186:PHE:HZ	1:B:4265:LEU:HD12	1.71	0.50
1:A:3010:THR:HG22	1:A:3016:GLU:O	2.10	0.50
1:A:3021:PHE:CG	1:A:3029:LEU:HD13	2.46	0.50
1:A:3097:TRP:CE3	1:A:3173:PRO:HB3	2.47	0.50
1:A:1879:LEU:CD1	1:A:1914:GLU:O	2.55	0.50
1:B:2849:ASN:O	1:B:2852:THR:HG22	2.11	0.50
1:A:3521:ASP:OD1	1:A:3702:THR:HG21	2.11	0.50
1:A:4560:VAL:CG1	1:A:4563:LEU:HD11	2.41	0.50
1:A:2072:PHE:CZ	1:A:2157:LEU:HD11	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2635:PHE:CZ	1:A:2686:MET:HE1	2.46	0.50
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.93	0.50
1:A:3824:LEU:HD21	1:A:4130:ILE:HG12	1.92	0.50
1:A:1537:TRP:CH2	1:A:1578:LEU:HD21	2.47	0.50
1:A:4042:LEU:CD2	1:A:4139:LEU:HD23	2.41	0.50
1:B:1537:TRP:CH2	1:B:1578:LEU:HD21	2.47	0.50
1:B:2961:ILE:HD11	1:B:2998:ASN:HB3	1.93	0.49
1:A:3821:ILE:HG23	1:A:3822:HIS:N	2.28	0.49
1:B:3097:TRP:CE3	1:B:3173:PRO:HB3	2.47	0.49
1:B:2635:PHE:CZ	1:B:2686:MET:HE1	2.48	0.49
1:B:4447:TYR:CE2	1:B:4451:LEU:HD11	2.47	0.49
1:A:2078:GLU:OE1	1:A:4522:THR:CG2	2.58	0.49
1:B:3478:LEU:CD1	1:B:3770:LEU:HD13	2.43	0.49
1:B:3521:ASP:OD1	1:B:3702:THR:HG21	2.11	0.49
1:A:1792:LEU:HD13	1:A:1812:ILE:HG13	1.95	0.49
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.94	0.49
1:A:4507:ILE:HD12	1:A:4509:VAL:HG22	1.93	0.49
1:B:3822:HIS:C	1:B:3823:PHE:CG	2.86	0.49
1:A:3208:ILE:HD12	1:A:3482:LEU:HB3	1.95	0.49
1:A:3680:SER:O	1:A:3681:THR:HG23	2.12	0.49
1:A:3708:LEU:HD21	1:A:3809:SER:HA	1.93	0.49
1:B:1792:LEU:HD13	1:B:1812:ILE:HG13	1.95	0.49
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.94	0.49
1:B:2493:TYR:HA	1:B:2539:VAL:HG11	1.95	0.49
1:B:3821:ILE:HG23	1:B:3822:HIS:N	2.28	0.49
1:A:2457:SER:HA	1:A:2584:TRP:CH2	2.47	0.49
1:A:4434:VAL:HA	1:A:4437:VAL:HG22	1.95	0.49
1:B:2072:PHE:CZ	1:B:2157:LEU:HD11	2.45	0.49
1:B:2457:SER:HA	1:B:2584:TRP:CH2	2.47	0.49
1:B:2593:LEU:HD11	1:B:2605:LEU:HB2	1.93	0.49
1:B:2994:MET:HE2	1:B:3008:MET:SD	2.53	0.49
1:A:3509:LEU:HB3	1:A:3529:PHE:CE1	2.48	0.49
1:A:3639:GLU:CD	1:A:4137:ASN:HD21	2.11	0.49
1:A:3716:VAL:HG21	1:A:3804:LEU:HD23	1.95	0.49
1:B:3208:ILE:HD12	1:B:3482:LEU:HB3	1.95	0.49
1:A:2662:PHE:CZ	1:A:2711:ALA:HB2	2.48	0.48
1:B:1825:LEU:HD12	1:B:1830:ILE:CD1	2.38	0.48
1:B:3639:GLU:CD	1:B:4137:ASN:HD21	2.11	0.48
1:A:2585:LEU:HB2	1:A:2612:LEU:HD11	1.95	0.48
1:B:3509:LEU:HB3	1:B:3529:PHE:CE1	2.48	0.48
1:B:3680:SER:O	1:B:3681:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4635:PHE:CZ	1:B:4640:VAL:HB	2.48	0.48
1:A:2605:LEU:HD21	1:A:2662:PHE:HD1	1.75	0.48
1:A:4635:PHE:CZ	1:A:4640:VAL:HB	2.48	0.48
1:B:2662:PHE:CZ	1:B:2711:ALA:HB2	2.48	0.48
1:B:4434:VAL:HA	1:B:4437:VAL:HG22	1.95	0.48
1:A:3745:LEU:HD22	1:A:3776:GLU:CB	2.44	0.48
1:B:4248:ALA:HB1	1:B:4266:ASN:OD1	2.14	0.48
1:A:2230:LYS:N	3:A:4802:ATP:O1B	2.46	0.48
1:A:3638:VAL:H	1:A:3681:THR:HG22	1.79	0.48
1:B:4609:VAL:CG2	1:B:4622:VAL:CG2	2.92	0.48
1:A:4447:TYR:CE2	1:A:4451:LEU:HD11	2.47	0.48
1:B:2626:THR:HG22	1:B:2679:VAL:HG21	1.96	0.48
1:A:2602:THR:HG22	1:A:2662:PHE:CZ	2.49	0.48
1:B:2591:LEU:C	1:B:2591:LEU:HD12	2.34	0.48
1:A:4622:VAL:CG1	1:A:4624:PHE:HE2	2.15	0.48
1:B:3745:LEU:HD22	1:B:3776:GLU:CB	2.44	0.48
1:A:2493:TYR:HA	1:A:2539:VAL:HG11	1.95	0.48
1:A:3021:PHE:CD1	1:A:3029:LEU:CD1	2.97	0.48
1:B:2668:LEU:N	1:B:2669:PRO:CD	2.77	0.48
1:B:3811:ILE:HD12	1:B:3887:LEU:CD2	2.44	0.48
1:B:4041:VAL:HG11	1:B:4125:PHE:CE2	2.49	0.48
1:B:4186:PHE:CZ	1:B:4265:LEU:HD12	2.48	0.48
1:A:2069:ILE:HD12	1:A:2137:LEU:HD21	1.96	0.47
1:A:3822:HIS:C	1:A:3823:PHE:CG	2.86	0.47
1:A:4041:VAL:HG11	1:A:4125:PHE:CE2	2.49	0.47
1:B:2585:LEU:HB2	1:B:2612:LEU:HD11	1.95	0.47
1:B:2599:SER:N	2:B:4804:ADP:O2A	2.43	0.47
1:B:3021:PHE:CD1	1:B:3029:LEU:CD1	2.97	0.47
1:B:3638:VAL:H	1:B:3681:THR:HG22	1.79	0.47
1:A:2591:LEU:C	1:A:2591:LEU:HD12	2.34	0.47
1:A:4609:VAL:CG2	1:A:4622:VAL:CG2	2.92	0.47
1:B:2602:THR:HG22	1:B:2662:PHE:CZ	2.49	0.47
1:B:3509:LEU:HD21	1:B:3536:LEU:HD12	1.96	0.47
1:A:2149:LEU:HD11	1:A:2157:LEU:CD2	2.40	0.47
1:B:1778:LEU:HD13	1:B:1830:ILE:CD1	2.40	0.47
1:A:2231:SER:OG	1:A:2344:GLU:OE2	2.32	0.47
1:A:2729:ARG:NH1	3:A:4802:ATP:O1G	2.40	0.47
1:A:4387:TRP:CZ3	1:A:4391:ILE:HD13	2.49	0.47
1:B:2230:LYS:N	3:B:4802:ATP:O1B	2.46	0.47
1:B:2729:ARG:NH1	3:B:4802:ATP:O1G	2.40	0.47
1:B:3824:LEU:HD22	1:B:4130:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4042:LEU:HD12	1:B:4126:LEU:HB2	1.95	0.47
1:A:2191:LEU:HD22	3:A:4802:ATP:C5	2.50	0.47
1:A:2568:VAL:CG2	1:A:2603:MET:HE3	2.44	0.47
1:A:4508:HIS:ND1	1:A:4587:LEU:CD2	2.77	0.47
1:B:1766:LEU:HD12	1:B:1778:LEU:HD21	1.96	0.47
1:B:2231:SER:OG	1:B:2344:GLU:OE2	2.32	0.47
1:B:4508:HIS:ND1	1:B:4587:LEU:CD2	2.77	0.47
1:A:4248:ALA:HB1	1:A:4266:ASN:OD1	2.14	0.47
1:B:2069:ILE:HD12	1:B:2137:LEU:HD21	1.96	0.47
1:A:2154:ILE:N	1:A:2155:PRO:CD	2.78	0.47
1:A:3554:SER:HB2	1:A:3578:ILE:HD12	1.96	0.47
1:A:4042:LEU:HD12	1:A:4126:LEU:HB2	1.95	0.47
1:A:4566:GLN:HE21	1:A:4643:LEU:HD11	1.80	0.47
1:B:2154:ILE:N	1:B:2155:PRO:CD	2.78	0.47
1:B:2191:LEU:HD22	3:B:4802:ATP:C5	2.50	0.47
1:B:3478:LEU:HD22	1:B:3770:LEU:HD13	1.96	0.47
1:B:3716:VAL:HG21	1:B:3804:LEU:HD23	1.95	0.47
1:B:4387:TRP:CZ3	1:B:4391:ILE:HD13	2.49	0.47
1:A:1541:GLN:O	1:A:1545:VAL:HG23	2.15	0.47
1:A:2626:THR:HG22	1:A:2679:VAL:HG21	1.96	0.47
1:A:3478:LEU:HD22	1:A:3770:LEU:HD13	1.96	0.47
1:B:3554:SER:HB2	1:B:3578:ILE:HD12	1.96	0.47
1:A:1766:LEU:HD12	1:A:1778:LEU:HD21	1.96	0.47
1:A:2568:VAL:HG22	1:A:2603:MET:HE2	1.95	0.47
1:A:4427:VAL:O	1:A:4431:LEU:HG	2.15	0.47
1:B:3522:GLN:HB2	1:B:3704:THR:HG22	1.97	0.47
1:B:3888:ALA:HA	1:B:4013:LEU:HD21	1.97	0.47
1:A:2668:LEU:N	1:A:2669:PRO:CD	2.77	0.47
1:A:3478:LEU:CD1	1:A:3770:LEU:HD22	2.45	0.47
1:A:3645:LEU:HD23	1:A:3648:VAL:HB	1.97	0.47
1:B:2461:MET:CE	1:B:2584:TRP:CZ2	2.98	0.47
1:B:2922:ILE:HD12	1:B:2933:LEU:HD21	1.96	0.47
1:A:3888:ALA:HA	1:A:4013:LEU:HD21	1.97	0.46
1:B:1504:VAL:HG11	1:B:1524:GLU:HB2	1.97	0.46
1:B:2103:VAL:HG13	1:B:2136:ILE:CG2	2.46	0.46
1:A:2308:ASP:OD2	1:A:2310:GLU:HB3	2.15	0.46
1:A:2461:MET:CE	1:A:2584:TRP:CZ2	2.98	0.46
1:B:2752:ASN:HD22	1:B:2770:THR:HG22	1.76	0.46
1:A:3008:MET:HE2	1:A:3066:PHE:HZ	1.75	0.46
1:A:3811:ILE:HD12	1:A:3887:LEU:CD2	2.44	0.46
1:A:4507:ILE:HD12	1:A:4509:VAL:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2958:VAL:HG13	1:B:2993:ILE:HG12	1.98	0.46
1:B:4427:VAL:O	1:B:4431:LEU:HG	2.15	0.46
1:A:2058:GLY:O	1:A:2104:LYS:CE	2.61	0.46
1:A:3509:LEU:HD21	1:A:3536:LEU:HD12	1.96	0.46
1:A:2922:ILE:HD12	1:A:2933:LEU:HD21	1.96	0.46
1:A:3478:LEU:CD1	1:A:3770:LEU:HD13	2.43	0.46
1:A:3824:LEU:HD22	1:A:4130:ILE:CG2	2.45	0.46
1:B:3645:LEU:HD23	1:B:3648:VAL:HB	1.97	0.46
1:A:4387:TRP:CH2	1:A:4391:ILE:HG21	2.51	0.46
1:B:2191:LEU:HD23	1:B:2377:ASN:ND2	2.30	0.46
1:B:4566:GLN:HE21	1:B:4643:LEU:HD11	1.80	0.46
1:A:2103:VAL:HG13	1:A:2136:ILE:CG2	2.46	0.46
1:B:3478:LEU:CD1	1:B:3770:LEU:HD22	2.45	0.46
1:B:3817:SER:OG	1:B:4349:LEU:HD13	2.10	0.46
1:A:1504:VAL:HG11	1:A:1524:GLU:HB2	1.97	0.46
1:B:1541:GLN:O	1:B:1545:VAL:HG23	2.15	0.46
1:B:3203:VAL:O	1:B:3207:LYS:N	2.47	0.46
1:B:1792:LEU:HD22	1:B:1808:LEU:HD22	1.97	0.46
1:B:4607:LEU:HD12	1:B:4624:PHE:CE2	2.51	0.46
1:A:3522:GLN:HB2	1:A:3704:THR:HG22	1.97	0.46
1:A:3683:ASP:CB	1:A:4137:ASN:OD1	2.64	0.46
1:B:3683:ASP:CB	1:B:4137:ASN:OD1	2.64	0.46
1:A:2304:ASP:OD1	1:A:2684:ARG:NH2	2.47	0.45
1:A:2958:VAL:HG13	1:A:2993:ILE:HG12	1.98	0.45
1:A:3745:LEU:HD22	1:A:3776:GLU:HB2	1.98	0.45
1:A:4042:LEU:HD11	1:A:4128:MET:HE3	1.98	0.45
1:B:2058:GLY:O	1:B:2104:LYS:CE	2.61	0.45
1:B:2308:ASP:OD2	1:B:2310:GLU:HB3	2.16	0.45
1:B:3745:LEU:HD11	1:B:3773:LEU:HD22	1.98	0.45
1:A:1778:LEU:HD13	1:A:1830:ILE:CD1	2.40	0.45
1:A:2191:LEU:HD23	1:A:2377:ASN:ND2	2.30	0.45
1:A:4186:PHE:CZ	1:A:4265:LEU:HD12	2.48	0.45
1:A:3814:THR:OG1	1:A:3890:ILE:HD11	2.16	0.45
1:A:3817:SER:OG	1:A:4349:LEU:HD13	2.10	0.45
1:B:4387:TRP:CH2	1:B:4391:ILE:HG21	2.51	0.45
1:B:4507:ILE:HD12	1:B:4509:VAL:CG2	2.46	0.45
1:B:3717:LEU:HD11	1:B:3797:VAL:HG11	1.99	0.45
1:A:2254:ILE:HG12	1:A:2279:LEU:HD21	1.98	0.45
1:B:1931:ASN:HD22	1:B:2317:SER:CA	2.26	0.45
1:A:1931:ASN:HD22	1:A:2317:SER:N	2.15	0.45
1:A:2213:ILE:CG2	1:A:2220:LEU:HD13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4607:LEU:HD12	1:A:4624:PHE:CE2	2.51	0.45
1:B:2079:GLN:OE1	1:B:4526:GLN:NE2	2.47	0.45
1:A:2461:MET:HE3	1:A:2584:TRP:HZ2	1.80	0.45
1:A:2709:VAL:HG23	1:A:2709:VAL:O	2.17	0.45
1:A:3745:LEU:HD11	1:A:3773:LEU:HD22	1.98	0.45
1:B:1985:HIS:CD2	1:B:1997:ILE:HD12	2.52	0.45
1:B:2213:ILE:CG2	1:B:2220:LEU:HD13	2.47	0.45
1:B:2254:ILE:HG12	1:B:2279:LEU:HD21	1.98	0.45
1:B:2994:MET:HE1	1:B:3008:MET:SD	2.57	0.45
1:B:3871:VAL:HG11	1:B:3883:PHE:CE2	2.52	0.45
1:B:4042:LEU:HD11	1:B:4128:MET:CE	2.47	0.45
1:A:1792:LEU:HD22	1:A:1808:LEU:HD22	1.97	0.45
1:A:3871:VAL:HG11	1:A:3883:PHE:CE2	2.52	0.45
1:B:3814:THR:OG1	1:B:3890:ILE:HD11	2.16	0.45
1:B:4178:ARG:HG2	1:B:4278:PHE:CE1	2.52	0.45
1:A:3680:SER:O	1:A:3681:THR:CG2	2.65	0.45
1:A:3801:TYR:CD1	1:A:3856:LEU:HD22	2.52	0.45
1:B:4240:TRP:CZ3	1:B:4273:PHE:O	2.70	0.45
1:A:3203:VAL:O	1:A:3207:LYS:N	2.47	0.45
1:A:3822:HIS:NE2	1:A:3876:LEU:CD1	2.79	0.45
1:A:4097:LYS:HA	1:A:4127:THR:HG22	1.98	0.45
1:B:2593:LEU:CD2	1:B:2734:VAL:CG2	2.89	0.45
1:B:3822:HIS:NE2	1:B:3876:LEU:CD1	2.79	0.45
1:B:4088:VAL:HG22	1:B:4122:PHE:CE2	2.52	0.45
1:B:4097:LYS:HA	1:B:4127:THR:HG22	1.98	0.45
1:A:4178:ARG:HG2	1:A:4278:PHE:CE1	2.52	0.44
1:B:2568:VAL:HG22	1:B:2603:MET:HE3	1.99	0.44
1:B:2569:VAL:O	1:B:2569:VAL:HG13	2.17	0.44
1:B:3102:LEU:HB3	1:B:3148:VAL:HG22	1.99	0.44
1:B:3683:ASP:CG	1:B:4137:ASN:OD1	2.56	0.44
1:A:2458:LEU:HD13	1:A:2498:ILE:HG22	1.99	0.44
1:B:2515:GLY:HA2	1:B:2534:ILE:HD12	1.99	0.44
1:A:2358:ARG:HH22	2:A:4801:ADP:PB	2.40	0.44
1:A:2453:ARG:HD2	1:A:2733:VAL:HG12	2.00	0.44
1:A:2515:GLY:HA2	1:A:2534:ILE:HD12	1.99	0.44
1:A:3567:LEU:HB2	1:A:3599:PHE:CD1	2.52	0.44
1:A:4042:LEU:HD11	1:A:4128:MET:CE	2.47	0.44
1:B:2622:PHE:CE2	1:B:2679:VAL:HG11	2.52	0.44
1:A:2766:ALA:O	1:A:2770:THR:HG23	2.18	0.44
1:A:4088:VAL:HG22	1:A:4122:PHE:CE2	2.52	0.44
1:A:4508:HIS:ND1	1:A:4587:LEU:HD21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1931:ASN:ND2	1:B:2317:SER:N	2.65	0.44
1:B:3745:LEU:HD22	1:B:3776:GLU:HB2	1.98	0.44
1:A:1931:ASN:HD22	1:A:2317:SER:CA	2.27	0.44
1:A:1985:HIS:CD2	1:A:1997:ILE:HD12	2.52	0.44
1:A:3822:HIS:O	1:A:3822:HIS:CG	2.71	0.44
1:B:2304:ASP:OD1	1:B:2684:ARG:NH2	2.47	0.44
1:B:2358:ARG:NH2	2:B:4801:ADP:PB	2.89	0.44
1:B:3567:LEU:HB2	1:B:3599:PHE:CD1	2.52	0.44
1:A:2358:ARG:NH2	2:A:4801:ADP:PB	2.89	0.44
1:A:2874:SER:OG	1:A:2875:ASN:N	2.51	0.44
1:A:3717:LEU:HD11	1:A:3797:VAL:HG11	1.99	0.44
1:B:3572:LEU:HD23	1:B:3572:LEU:C	2.38	0.44
1:A:2605:LEU:HD23	1:A:2662:PHE:CD1	2.44	0.44
1:A:2622:PHE:CE2	1:A:2679:VAL:HG11	2.52	0.44
1:A:3102:LEU:HB3	1:A:3148:VAL:HG22	1.99	0.44
1:B:1931:ASN:HD22	1:B:2317:SER:N	2.15	0.44
1:B:2358:ARG:HH22	2:B:4801:ADP:PB	2.40	0.44
1:B:2453:ARG:HD2	1:B:2733:VAL:HG12	2.00	0.44
1:B:2461:MET:HE3	1:B:2584:TRP:HZ2	1.79	0.44
1:B:2874:SER:OG	1:B:2875:ASN:N	2.51	0.44
1:B:3680:SER:O	1:B:3681:THR:CG2	2.65	0.44
1:B:4609:VAL:CG2	1:B:4622:VAL:HG23	2.48	0.44
1:B:1879:LEU:HD21	1:B:1914:GLU:CG	2.47	0.44
1:B:2551:LYS:C	1:B:2551:LYS:CD	2.86	0.44
1:B:2569:VAL:HG11	1:B:2747:ILE:HG23	1.99	0.44
1:B:4508:HIS:ND1	1:B:4587:LEU:HD21	2.33	0.44
1:A:2079:GLN:OE1	1:A:4526:GLN:NE2	2.47	0.44
1:A:2568:VAL:CG2	1:A:2603:MET:CE	2.95	0.44
1:A:3572:LEU:C	1:A:3572:LEU:HD23	2.38	0.44
1:A:3609:ILE:HG12	1:A:3632:PRO:HG2	1.99	0.44
1:A:4240:TRP:CZ3	1:A:4273:PHE:O	2.70	0.44
1:B:3708:LEU:HD21	1:B:3809:SER:HA	1.93	0.44
1:B:3801:TYR:CD1	1:B:3856:LEU:HD22	2.52	0.44
1:A:2284:LEU:HB3	1:A:2333:LEU:HD13	2.00	0.43
1:A:3822:HIS:CB	1:A:3825:TYR:CZ	3.01	0.43
1:B:1550:ILE:HD13	1:B:1638:LEU:HD22	2.00	0.43
1:B:3609:ILE:HG12	1:B:3632:PRO:HG2	1.99	0.43
1:B:3822:HIS:O	1:B:3822:HIS:CG	2.71	0.43
1:A:1879:LEU:HD21	1:A:1914:GLU:CG	2.47	0.43
1:A:2335:LEU:HD11	1:A:2341:ILE:HD11	2.00	0.43
1:A:2871:ILE:HG23	1:A:2871:ILE:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2335:LEU:HD11	1:B:2341:ILE:HD11	2.00	0.43
1:B:2709:VAL:HG23	1:B:2709:VAL:O	2.17	0.43
1:B:2910:VAL:CG1	1:B:3105:VAL:HG23	2.47	0.43
1:B:3832:PHE:O	1:B:3835:ILE:HB	2.18	0.43
1:A:2519:ARG:HA	1:A:2526:LEU:CD1	2.49	0.43
1:B:2568:VAL:CG2	1:B:2603:MET:CE	2.95	0.43
1:B:3822:HIS:CB	1:B:3825:TYR:CZ	3.01	0.43
1:A:1931:ASN:ND2	1:A:2317:SER:N	2.65	0.43
1:A:3832:PHE:O	1:A:3835:ILE:HB	2.18	0.43
1:B:2220:LEU:CD2	1:B:2342:MET:HE2	2.49	0.43
1:B:2571:THR:OG1	1:B:2574:THR:OG1	2.06	0.43
1:B:3574:THR:O	1:B:3578:ILE:HG12	2.19	0.43
1:A:2569:VAL:HG11	1:A:2747:ILE:HG23	1.99	0.43
1:A:2635:PHE:CE1	1:A:2706:ILE:HD13	2.54	0.43
1:A:3825:TYR:CE2	1:A:3875:MET:SD	3.12	0.43
1:B:1818:GLN:O	1:B:1822:THR:HG23	2.19	0.43
1:A:1818:GLN:O	1:A:1822:THR:HG23	2.19	0.43
1:A:1923:LEU:HD12	1:A:1954:TRP:CZ2	2.53	0.43
1:A:2302:VAL:HG12	1:A:2303:PHE:N	2.33	0.43
1:A:2910:VAL:CG1	1:A:3105:VAL:HG23	2.47	0.43
1:B:2295:LEU:C	1:B:2338:ASN:ND2	2.72	0.43
1:B:2302:VAL:HG12	1:B:2303:PHE:N	2.33	0.43
1:B:2766:ALA:O	1:B:2770:THR:HG23	2.18	0.43
1:A:1713:LEU:HD22	1:A:1749:LEU:HD21	2.00	0.43
1:B:1526:LYS:O	1:B:1529:ARG:HG2	2.19	0.43
1:B:1632:VAL:HG13	1:B:1636:ASP:HB2	1.95	0.43
1:B:2284:LEU:HB3	1:B:2333:LEU:HD13	2.00	0.43
1:B:3654:ARG:HB2	1:B:3661:LEU:HB2	2.01	0.43
1:A:1970:ALA:HB2	1:A:4073:SER:HB2	2.00	0.43
1:A:4609:VAL:CG2	1:A:4622:VAL:HG23	2.48	0.43
1:B:1970:ALA:HB2	1:B:4073:SER:HB2	2.00	0.43
1:B:4430:ASP:O	1:B:4434:VAL:HG12	2.19	0.43
1:A:2308:ASP:HB2	1:A:2309:PRO:HD2	2.00	0.43
1:A:2569:VAL:O	1:A:2569:VAL:HG13	2.17	0.43
1:A:3574:THR:O	1:A:3578:ILE:HG12	2.19	0.43
1:A:3683:ASP:CG	1:A:4137:ASN:OD1	2.56	0.43
1:A:4430:ASP:O	1:A:4434:VAL:HG12	2.19	0.43
1:B:1923:LEU:HD12	1:B:1954:TRP:CZ2	2.53	0.43
1:B:2458:LEU:HD13	1:B:2498:ILE:HG22	1.99	0.43
1:B:2519:ARG:HA	1:B:2526:LEU:CD1	2.49	0.43
1:B:2635:PHE:CE1	1:B:2706:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3769:THR:O	1:B:3773:LEU:HG	2.19	0.43
1:B:3825:TYR:CE2	1:B:3875:MET:SD	3.12	0.43
1:A:1632:VAL:HG11	1:A:1636:ASP:CB	2.48	0.43
1:A:2551:LYS:C	1:A:2551:LYS:CD	2.86	0.43
1:A:2213:ILE:HG21	1:A:2220:LEU:HD13	2.01	0.42
1:A:2256:PRO:HB3	1:A:2264:LEU:HD22	2.00	0.42
1:A:4088:VAL:HG13	1:A:4118:PRO:CB	2.49	0.42
1:B:1713:LEU:HD22	1:B:1749:LEU:HD21	2.00	0.42
1:B:2070:VAL:HB	1:B:2071:PRO:HD3	2.01	0.42
1:B:2213:ILE:HG21	1:B:2220:LEU:HD13	2.01	0.42
1:A:2234:TRP:HH2	1:A:2253:ILE:HD11	1.84	0.42
1:B:2319:LEU:HD13	1:B:2359:CYS:SG	2.59	0.42
1:B:2571:THR:HG22	1:B:2747:ILE:HG12	2.00	0.42
1:B:2871:ILE:HG23	1:B:2871:ILE:O	2.18	0.42
1:B:4088:VAL:HG13	1:B:4118:PRO:CB	2.49	0.42
1:A:1526:LYS:O	1:A:1529:ARG:HG2	2.19	0.42
1:A:2496:TYR:CZ	1:A:2500:TRP:CD1	3.08	0.42
1:A:3109:PHE:CD2	1:A:3180:ILE:HG21	2.54	0.42
1:B:2275:TRP:NE1	1:B:2277:ASP:OD1	2.53	0.42
1:B:3550:THR:OG1	1:B:3574:THR:HG21	2.19	0.42
1:A:2588:HIS:HB3	1:A:2658:TRP:CZ3	2.54	0.42
1:B:1961:ASN:ND2	1:B:2025:ARG:CB	2.82	0.42
1:B:2234:TRP:HH2	1:B:2253:ILE:HD11	1.84	0.42
1:B:2526:LEU:HA	1:B:2545:TRP:CZ3	2.54	0.42
1:B:2907:VAL:O	1:B:2907:VAL:HG23	2.20	0.42
1:B:4577:LEU:HD21	1:B:4635:PHE:HD1	1.84	0.42
1:A:1452:VAL:HG13	1:A:1512:TYR:CE1	2.55	0.42
1:A:2275:TRP:NE1	1:A:2277:ASP:OD1	2.53	0.42
1:A:3609:ILE:HG12	1:A:3632:PRO:HB2	2.01	0.42
1:B:2308:ASP:HB2	1:B:2309:PRO:HD2	2.00	0.42
1:B:3879:ASP:O	1:B:3882:THR:OG1	2.30	0.42
1:B:4529:ALA:O	1:B:4533:SER:N	2.52	0.42
1:A:1550:ILE:HD13	1:A:1638:LEU:HD22	2.00	0.42
1:A:2381:ARG:HG2	1:A:2385:ILE:HD11	2.02	0.42
1:B:1452:VAL:HG13	1:B:1512:TYR:CE1	2.55	0.42
1:B:2824:ILE:HG13	1:B:2825:TRP:N	2.34	0.42
1:B:4609:VAL:CG2	1:B:4622:VAL:HG21	2.50	0.42
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	2.01	0.42
1:A:2549:GLN:HG2	1:A:2572:LEU:HB2	2.02	0.42
1:A:2824:ILE:HG13	1:A:2825:TRP:N	2.34	0.42
1:A:3769:THR:O	1:A:3773:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1632:VAL:HG11	1:B:1636:ASP:CB	2.48	0.42
1:B:2605:LEU:HD23	1:B:2662:PHE:CD1	2.44	0.42
1:A:2147:PRO:HG3	1:A:2209:GLN:HB3	2.02	0.42
1:A:3178:ASP:OD1	1:A:3584:ASN:HB3	2.20	0.42
1:B:1861:MET:HE2	1:B:1890:LEU:HA	2.02	0.42
1:B:2256:PRO:HB3	1:B:2264:LEU:HD22	2.01	0.42
1:B:3178:ASP:OD1	1:B:3584:ASN:HB3	2.20	0.42
1:B:3588:LEU:HD23	1:B:3589:ILE:N	2.35	0.42
1:B:3609:ILE:HG12	1:B:3632:PRO:HB2	2.01	0.42
1:A:4609:VAL:CG2	1:A:4622:VAL:HG21	2.50	0.42
1:B:2285:ARG:NH1	1:B:2333:LEU:HD21	2.35	0.42
1:B:3508:LEU:HD23	1:B:3536:LEU:HD21	2.02	0.42
1:A:1961:ASN:ND2	1:A:2025:ARG:CB	2.82	0.42
1:A:2091:ARG:NH1	2:A:4801:ADP:PA	2.93	0.42
1:A:2571:THR:HG22	1:A:2747:ILE:HG12	2.00	0.42
1:A:2938:VAL:O	1:A:2941:ALA:HB2	2.20	0.42
1:A:3508:LEU:HD23	1:A:3536:LEU:HD21	2.02	0.42
1:A:3654:ARG:HB2	1:A:3661:LEU:HB2	2.01	0.42
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	2.01	0.42
1:B:2091:ARG:NH1	2:B:4801:ADP:PA	2.93	0.42
1:B:2220:LEU:HD23	1:B:2342:MET:HE2	2.02	0.42
1:B:2938:VAL:O	1:B:2941:ALA:HB2	2.20	0.42
1:B:3109:PHE:CD2	1:B:3180:ILE:HG21	2.54	0.42
1:B:3175:HIS:CD2	1:B:3585:ARG:HH22	2.36	0.42
1:B:1628:ARG:NH2	1:B:1871:GLU:OE2	2.53	0.41
1:B:2549:GLN:HG2	1:B:2572:LEU:HB2	2.02	0.41
1:A:1931:ASN:HD21	1:A:2317:SER:CB	2.21	0.41
1:A:2070:VAL:HB	1:A:2071:PRO:HD3	2.01	0.41
1:A:2623:SER:OG	1:A:2624:SER:N	2.53	0.41
1:A:2907:VAL:HG23	1:A:2907:VAL:O	2.20	0.41
1:B:1761:ASN:HB3	1:B:1781:VAL:HG22	2.02	0.41
1:B:3713:LEU:O	1:B:3717:LEU:HG	2.20	0.41
1:A:2319:LEU:HD13	1:A:2359:CYS:SG	2.59	0.41
1:B:2381:ARG:HG2	1:B:2385:ILE:HD11	2.02	0.41
1:B:2496:TYR:CZ	1:B:2500:TRP:CD1	3.08	0.41
1:A:1641:ILE:HA	1:A:1698:ILE:CD1	2.50	0.41
1:B:1960:PHE:CE1	1:B:1963:LEU:CD2	3.03	0.41
1:B:2588:HIS:HB3	1:B:2658:TRP:CZ3	2.54	0.41
1:B:4387:TRP:CZ3	1:B:4391:ILE:HG21	2.56	0.41
1:A:1632:VAL:HG11	1:A:1636:ASP:HB3	2.02	0.41
1:A:1960:PHE:CE1	1:A:1963:LEU:CD2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2454:CYS:HB3	1:A:2502:LEU:HD23	2.03	0.41
1:A:3550:THR:OG1	1:A:3574:THR:HG21	2.19	0.41
1:A:4387:TRP:CZ3	1:A:4391:ILE:HG21	2.56	0.41
1:A:4577:LEU:HD21	1:A:4635:PHE:HD1	1.84	0.41
1:B:2623:SER:OG	1:B:2624:SER:N	2.53	0.41
1:A:1628:ARG:NH2	1:A:1871:GLU:OE2	2.53	0.41
1:A:2526:LEU:HA	1:A:2545:TRP:CZ3	2.54	0.41
1:A:2538:GLU:N	1:A:2546:SER:O	2.53	0.41
1:A:4529:ALA:O	1:A:4533:SER:N	2.52	0.41
1:B:2091:ARG:HH11	2:B:4801:ADP:PA	2.43	0.41
1:B:2147:PRO:HG3	1:B:2209:GLN:HB3	2.02	0.41
1:B:4176:ARG:HD3	1:B:4223:LEU:HD22	2.03	0.41
1:A:3924:ILE:O	1:A:3924:ILE:CG2	2.67	0.41
1:A:4528:VAL:HG21	1:A:4592:TRP:CD1	2.56	0.41
1:A:2091:ARG:HH11	2:A:4801:ADP:PA	2.43	0.41
1:A:2295:LEU:C	1:A:2338:ASN:ND2	2.72	0.41
1:A:2369:LEU:O	1:A:2451:ARG:NH1	2.43	0.41
1:A:3745:LEU:CD1	1:A:3773:LEU:HD22	2.51	0.41
1:B:3633:LEU:O	1:B:3677:ILE:HA	2.21	0.41
1:B:4528:VAL:HG21	1:B:4592:TRP:CD1	2.56	0.41
1:B:4561:THR:HG23	1:B:4587:LEU:HD13	2.03	0.41
1:A:1761:ASN:HB3	1:A:1781:VAL:HG22	2.02	0.41
1:A:2635:PHE:O	1:A:2639:CYS:N	2.50	0.41
1:A:3151:HIS:CE1	1:A:3516:TYR:HH	2.36	0.41
1:A:3562:TRP:HB3	1:A:3567:LEU:HD22	2.01	0.41
1:A:3588:LEU:HD23	1:A:3589:ILE:N	2.35	0.41
1:A:3633:LEU:O	1:A:3677:ILE:HA	2.21	0.41
1:B:3638:VAL:N	1:B:3681:THR:HG22	2.36	0.41
1:A:1931:ASN:OD1	1:A:1958:ASP:CB	2.62	0.41
1:A:2540:SER:OG	1:A:2544:GLU:O	2.16	0.41
1:A:3871:VAL:HG11	1:A:3883:PHE:CD2	2.56	0.41
1:B:1641:ILE:HA	1:B:1698:ILE:CD1	2.50	0.41
1:B:2568:VAL:CG2	1:B:2603:MET:HE3	2.51	0.41
1:A:1632:VAL:HG13	1:A:1636:ASP:HB2	1.95	0.40
1:A:2285:ARG:NH1	1:A:2333:LEU:HD21	2.35	0.40
1:A:2599:SER:N	2:A:4804:ADP:O2A	2.43	0.40
1:A:2752:ASN:HD22	1:A:2770:THR:HG22	1.76	0.40
1:A:3648:VAL:HA	1:A:3662:ILE:HD11	2.03	0.40
1:B:3871:VAL:HG11	1:B:3883:PHE:CD2	2.56	0.40
1:A:2370:SER:O	1:A:2373:MET:HB3	2.21	0.40
1:A:3154:LEU:HD11	1:A:3520:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4042:LEU:HD21	1:A:4139:LEU:HD23	2.03	0.40
1:B:1879:LEU:HD13	1:B:1915:SER:HA	2.03	0.40
1:B:2454:CYS:HB3	1:B:2502:LEU:HD23	2.03	0.40
1:B:2538:GLU:N	1:B:2546:SER:O	2.53	0.40
1:A:1978:ILE:HG23	1:A:2012:MET:HE1	2.02	0.40
1:A:2091:ARG:NH2	1:A:2320:ASP:OD1	2.53	0.40
1:A:2639:CYS:SG	1:A:2652:PRO:HA	2.62	0.40
1:A:4009:VAL:HG13	1:A:4013:LEU:HD12	2.03	0.40
1:A:4176:ARG:HD3	1:A:4223:LEU:HD22	2.03	0.40
1:B:3154:LEU:HD11	1:B:3520:PHE:CE2	2.56	0.40
1:B:3553:LEU:HD13	1:B:3578:ILE:HG21	2.04	0.40
1:B:3868:PHE:CE1	1:B:3884:ALA:HB2	2.56	0.40
1:B:4009:VAL:HG13	1:B:4013:LEU:HD12	2.03	0.40
1:A:2994:MET:HE2	1:A:3008:MET:SD	2.61	0.40
1:A:3868:PHE:CE1	1:A:3884:ALA:HB2	2.56	0.40
1:A:4565:LEU:CD2	1:A:4642:VAL:HG22	2.50	0.40
1:B:1632:VAL:HG11	1:B:1636:ASP:HB3	2.02	0.40
1:B:2370:SER:O	1:B:2373:MET:HB3	2.21	0.40
1:B:2635:PHE:O	1:B:2639:CYS:N	2.50	0.40
1:A:2182:LEU:O	1:A:2185:VAL:HG22	2.22	0.40
1:A:4468:THR:HG21	1:A:4611:LEU:HD23	2.04	0.40
1:B:2016:ILE:HD12	1:B:2036:PHE:CD2	2.56	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	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	51	83
1	B	2888/4646 (62%)	2714 (94%)	171 (6%)	3 (0%)	51	83
All	All	5776/9292 (62%)	5428 (94%)	342 (6%)	6 (0%)	54	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1647	VAL
1	B	1647	VAL
1	A	1964	GLU
1	B	1964	GLU
1	A	1511	PRO
1	B	1511	PRO

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	2472/4125 (60%)	2469 (100%)	3 (0%)	93 97
1	B	2472/4125 (60%)	2469 (100%)	3 (0%)	93 97
All	All	4944/8250 (60%)	4938 (100%)	6 (0%)	93 97

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

Mol	Chain	Res	Type
1	A	2796	PRO
1	A	3825	TYR
1	A	3905	PHE
1	B	2796	PRO
1	B	3825	TYR
1	B	3905	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1612	GLN
1	A	1748	GLN
1	A	1784	ASN
1	A	1790	ASN
1	A	1856	GLN

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Mol	Chain	Res	Type
1	A	1863	ASN
1	A	1881	GLN
1	A	1894	GLN
1	A	1921	HIS
1	A	1931	ASN
1	A	1976	GLN
1	A	1979	GLN
1	A	1985	HIS
1	A	2079	GLN
1	A	2134	GLN
1	A	2139	GLN
1	A	2338	ASN
1	A	2549	GLN
1	A	2752	ASN
1	A	2913	ASN
1	A	2998	ASN
1	A	3014	ASN
1	A	3047	HIS
1	A	3152	GLN
1	A	3175	HIS
1	A	3182	HIS
1	A	3538	GLN
1	A	3540	ASN
1	A	3584	ASN
1	A	3646	ASN
1	A	3880	HIS
1	A	4012	ASN
1	A	4131	ASN
1	A	4393	GLN
1	A	4488	GLN
1	A	4490	GLN
1	A	4526	GLN
1	A	4566	GLN
1	B	1612	GLN
1	B	1748	GLN
1	B	1784	ASN
1	B	1790	ASN
1	B	1856	GLN
1	B	1863	ASN
1	B	1881	GLN
1	B	1894	GLN
1	B	1921	HIS

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Mol	Chain	Res	Type
1	B	1931	ASN
1	B	1976	GLN
1	B	1979	GLN
1	B	1985	HIS
1	B	2079	GLN
1	B	2134	GLN
1	B	2139	GLN
1	B	2338	ASN
1	B	2549	GLN
1	B	2752	ASN
1	B	2913	ASN
1	B	2998	ASN
1	B	3014	ASN
1	B	3047	HIS
1	B	3152	GLN
1	B	3175	HIS
1	B	3182	HIS
1	B	3538	GLN
1	B	3540	ASN
1	B	3584	ASN
1	B	3646	ASN
1	B	3880	HIS
1	B	4012	ASN
1	B	4131	ASN
1	B	4393	GLN
1	B	4488	GLN
1	B	4490	GLN
1	B	4526	GLN
1	B	4566	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	4805	-	24,29,29	0.86	0	29,45,45	1.58	7 (24%)
2	ADP	B	4805	-	24,29,29	0.86	0	29,45,45	1.58	7 (24%)
2	ADP	B	4801	-	24,29,29	1.09	2 (8%)	29,45,45	1.61	5 (17%)
3	ATP	B	4802	4	26,33,33	0.96	1 (3%)	31,52,52	1.77	7 (22%)
3	ATP	A	4802	4	26,33,33	0.97	1 (3%)	31,52,52	1.77	7 (22%)
2	ADP	B	4804	-	24,29,29	0.94	1 (4%)	29,45,45	1.69	5 (17%)
2	ADP	A	4801	-	24,29,29	1.10	2 (8%)	29,45,45	1.61	5 (17%)
2	ADP	A	4804	-	24,29,29	0.94	1 (4%)	29,45,45	1.69	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	4805	-	-	2/12/32/32	0/3/3/3
2	ADP	B	4805	-	-	2/12/32/32	0/3/3/3
2	ADP	B	4801	-	-	3/12/32/32	0/3/3/3
3	ATP	B	4802	4	-	1/18/38/38	0/3/3/3
3	ATP	A	4802	4	-	1/18/38/38	0/3/3/3
2	ADP	B	4804	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4801	-	-	3/12/32/32	0/3/3/3
2	ADP	A	4804	-	-	3/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4801	ADP	C5-C4	2.58	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4801	ADP	C5-C4	2.57	1.47	1.40
2	A	4801	ADP	C2-N3	2.51	1.36	1.32
3	A	4802	ATP	C5-C4	2.47	1.47	1.40
2	B	4801	ADP	C2-N3	2.45	1.36	1.32
3	B	4802	ATP	C5-C4	2.44	1.47	1.40
2	A	4804	ADP	C5-C4	2.13	1.46	1.40
2	B	4804	ADP	C5-C4	2.13	1.46	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4802	ATP	PA-O3A-PB	-5.44	114.16	132.83
3	B	4802	ATP	PA-O3A-PB	-5.44	114.16	132.83
2	A	4804	ADP	PA-O3A-PB	-4.51	117.35	132.83
2	B	4804	ADP	PA-O3A-PB	-4.51	117.35	132.83
2	B	4801	ADP	PA-O3A-PB	-4.15	118.57	132.83
2	A	4801	ADP	PA-O3A-PB	-4.15	118.59	132.83
3	A	4802	ATP	N3-C2-N1	-4.07	122.31	128.68
3	B	4802	ATP	N3-C2-N1	-4.07	122.31	128.68
2	A	4801	ADP	C3'-C2'-C1'	3.72	106.57	100.98
2	A	4805	ADP	N3-C2-N1	-3.71	122.88	128.68
2	B	4805	ADP	N3-C2-N1	-3.71	122.88	128.68
2	B	4801	ADP	C3'-C2'-C1'	3.70	106.56	100.98
2	B	4801	ADP	N3-C2-N1	-3.49	123.22	128.68
2	A	4801	ADP	N3-C2-N1	-3.48	123.24	128.68
2	A	4804	ADP	N3-C2-N1	-3.44	123.30	128.68
2	B	4804	ADP	N3-C2-N1	-3.42	123.33	128.68
2	B	4805	ADP	PA-O3A-PB	-3.41	121.11	132.83
2	A	4805	ADP	PA-O3A-PB	-3.41	121.12	132.83
3	B	4802	ATP	PB-O3B-PG	-3.30	121.49	132.83
3	A	4802	ATP	PB-O3B-PG	-3.29	121.52	132.83
2	A	4805	ADP	O4'-C1'-C2'	-3.14	102.33	106.93
2	B	4805	ADP	O4'-C1'-C2'	-3.14	102.33	106.93
3	A	4802	ATP	C1'-N9-C4	-2.89	121.57	126.64
3	B	4802	ATP	C1'-N9-C4	-2.88	121.57	126.64
2	A	4804	ADP	C3'-C2'-C1'	2.85	105.27	100.98
2	B	4804	ADP	C3'-C2'-C1'	2.85	105.27	100.98
2	B	4804	ADP	C1'-N9-C4	-2.85	121.64	126.64
2	A	4804	ADP	C1'-N9-C4	-2.83	121.67	126.64
2	A	4801	ADP	C4-C5-N7	-2.66	106.62	109.40
3	A	4802	ATP	C4-C5-N7	-2.63	106.66	109.40
2	B	4801	ADP	C4-C5-N7	-2.62	106.66	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	4802	ATP	C4-C5-N7	-2.61	106.67	109.40
2	A	4805	ADP	C4-C5-N7	-2.60	106.69	109.40
2	B	4805	ADP	C4-C5-N7	-2.57	106.72	109.40
3	A	4802	ATP	C2-N1-C6	2.31	122.70	118.75
3	B	4802	ATP	C2-N1-C6	2.31	122.70	118.75
2	A	4804	ADP	C4-C5-N7	-2.24	107.06	109.40
2	B	4804	ADP	C4-C5-N7	-2.24	107.06	109.40
3	B	4802	ATP	C3'-C2'-C1'	2.23	104.33	100.98
3	A	4802	ATP	C3'-C2'-C1'	2.20	104.30	100.98
2	A	4805	ADP	O3B-PB-O2B	2.14	115.80	107.64
2	B	4805	ADP	O3B-PB-O2B	2.14	115.80	107.64
2	A	4805	ADP	N6-C6-N1	2.02	122.76	118.57
2	B	4805	ADP	N6-C6-N1	2.02	122.76	118.57
2	B	4805	ADP	O2A-PA-O1A	2.01	122.18	112.24
2	A	4805	ADP	O2A-PA-O1A	2.01	122.16	112.24
2	A	4801	ADP	N6-C6-N1	2.00	122.73	118.57
2	B	4801	ADP	N6-C6-N1	2.00	122.73	118.57

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4804	ADP	PA-O3A-PB-O2B
2	A	4804	ADP	C5'-O5'-PA-O1A
2	A	4805	ADP	C5'-O5'-PA-O2A
2	A	4805	ADP	C5'-O5'-PA-O3A
2	B	4804	ADP	PA-O3A-PB-O2B
2	B	4804	ADP	C5'-O5'-PA-O1A
2	B	4805	ADP	C5'-O5'-PA-O2A
2	B	4805	ADP	C5'-O5'-PA-O3A
2	A	4801	ADP	O4'-C4'-C5'-O5'
2	B	4801	ADP	O4'-C4'-C5'-O5'
2	A	4801	ADP	C3'-C4'-C5'-O5'
2	B	4801	ADP	C3'-C4'-C5'-O5'
2	A	4804	ADP	C5'-O5'-PA-O3A
2	B	4804	ADP	C5'-O5'-PA-O3A
2	A	4801	ADP	C4'-C5'-O5'-PA
2	B	4801	ADP	C4'-C5'-O5'-PA
3	A	4802	ATP	PG-O3B-PB-O2B
3	B	4802	ATP	PG-O3B-PB-O2B

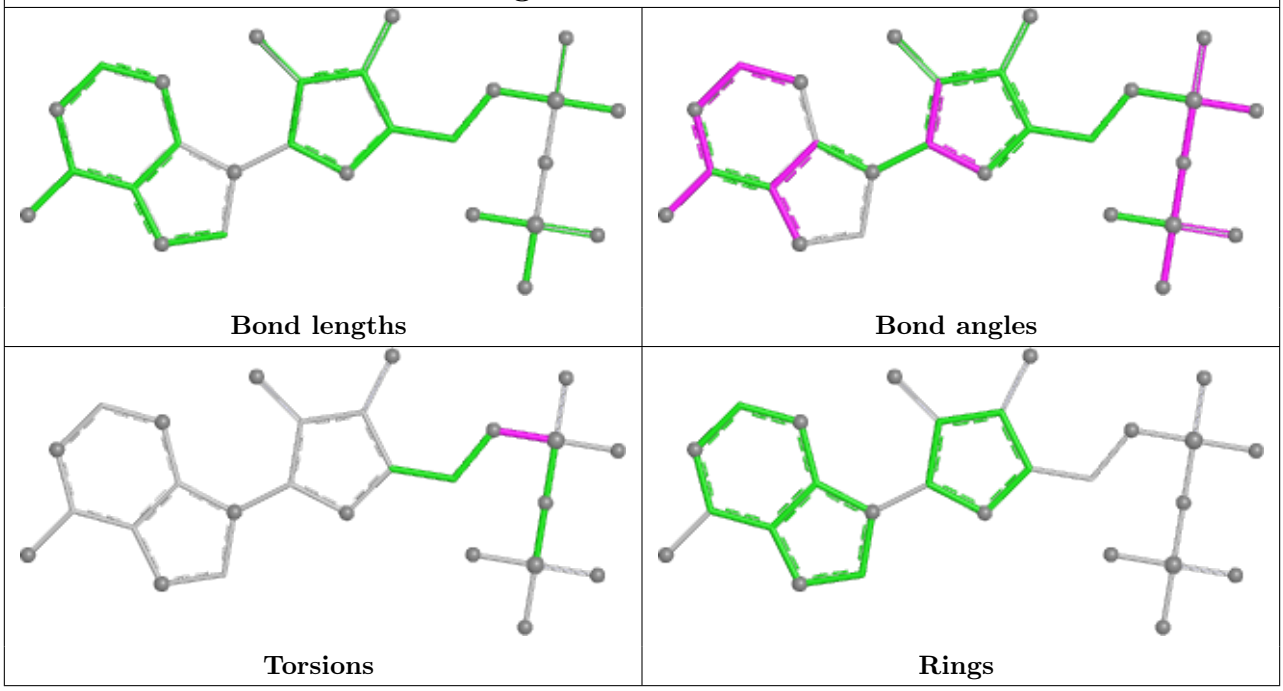
There are no ring outliers.

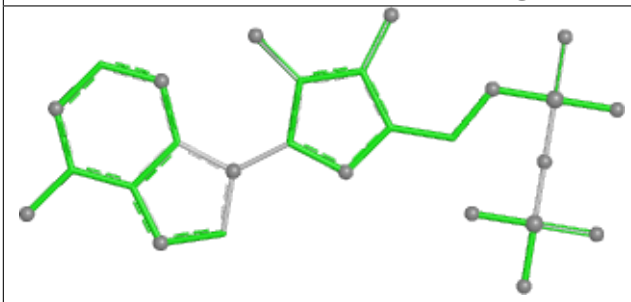
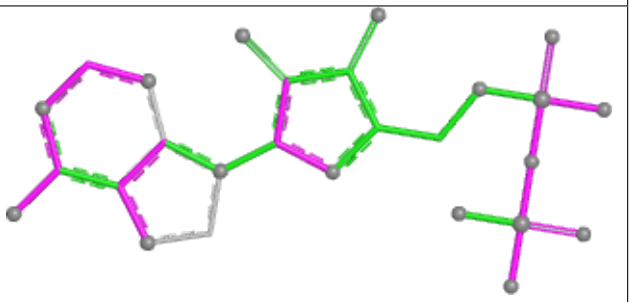
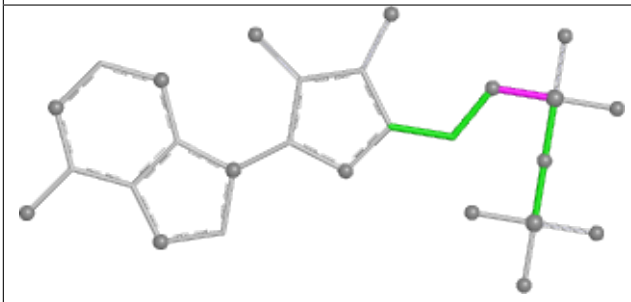
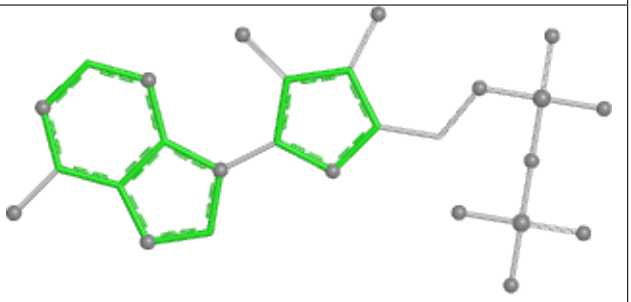
6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4801	ADP	11	0
3	B	4802	ATP	4	0
3	A	4802	ATP	4	0
2	B	4804	ADP	2	0
2	A	4801	ADP	11	0
2	A	4804	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 4805



Ligand ADP B 4805	
 Bond lengths	 Bond angles
 Torsions	 Rings

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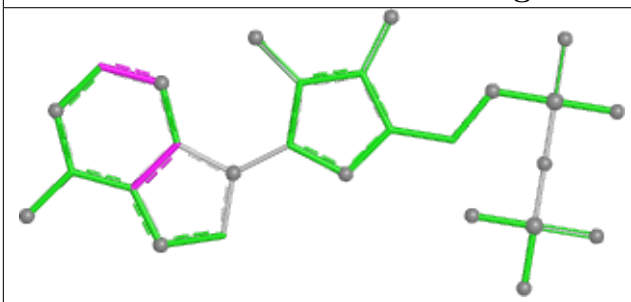
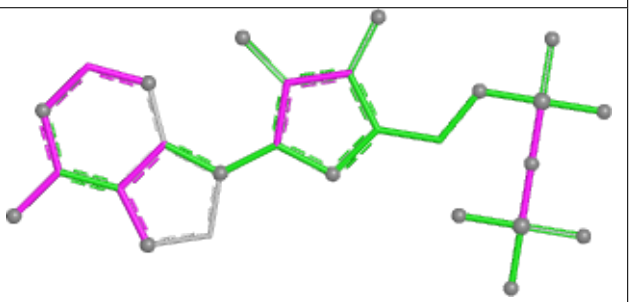
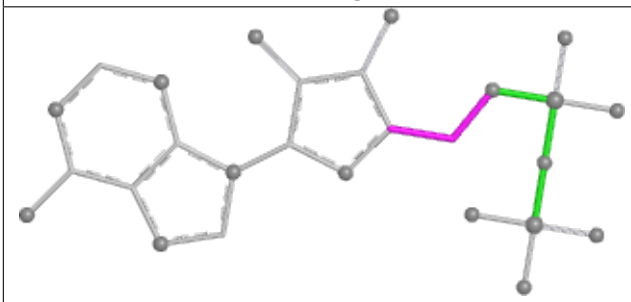
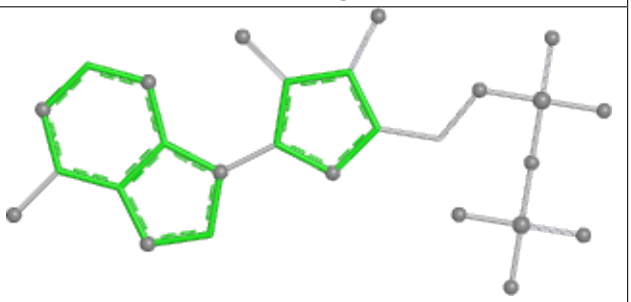
 Bond lengths	 Bond angles
 Torsions	 Rings

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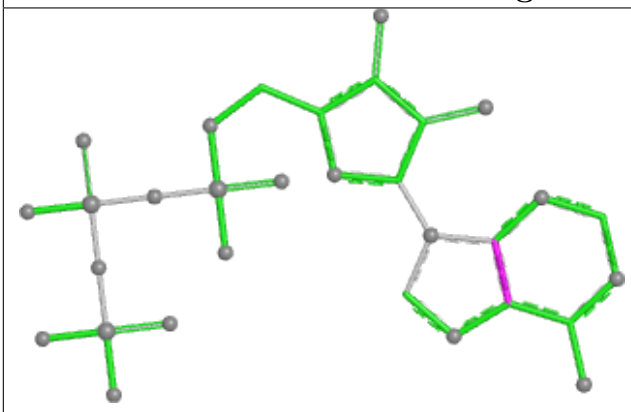
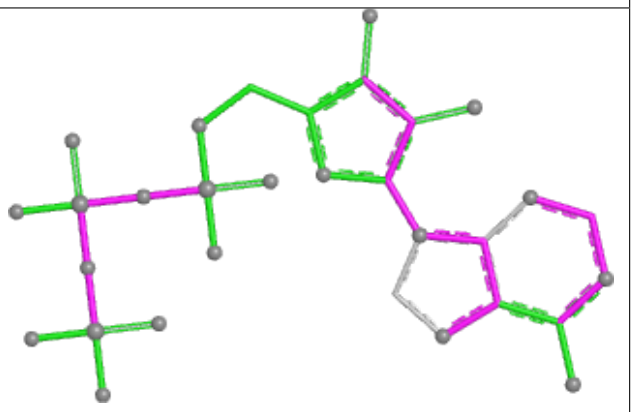
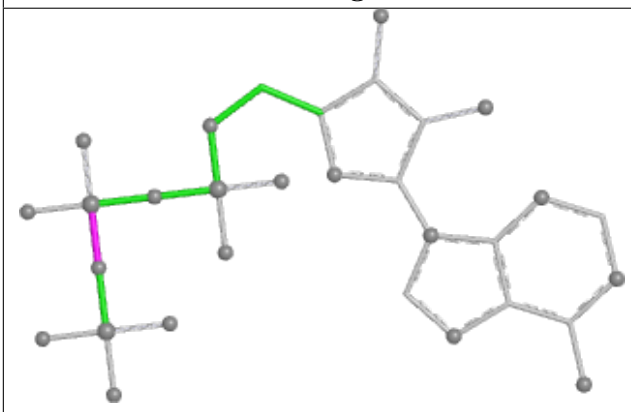


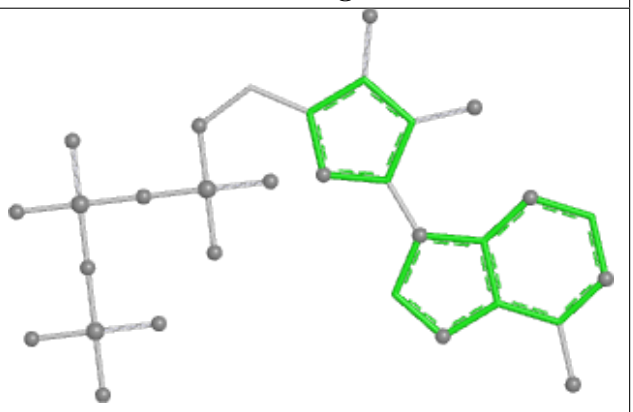
Bond lengths



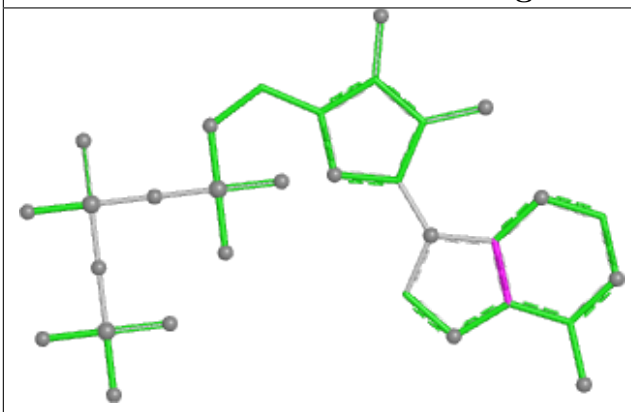
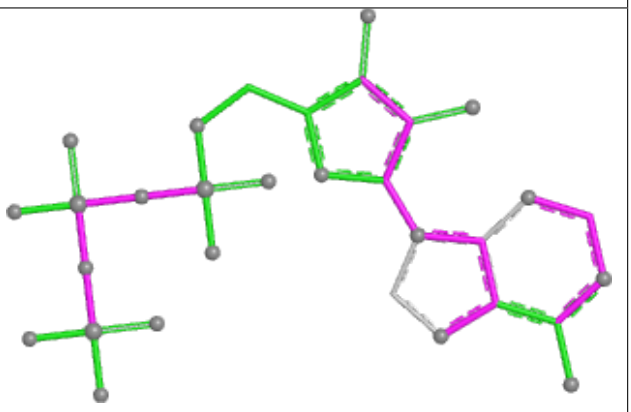
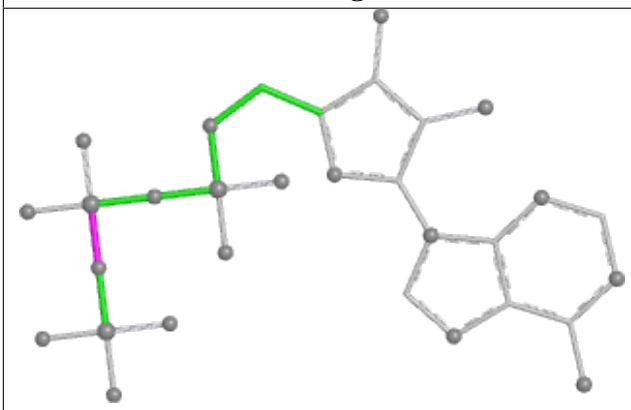
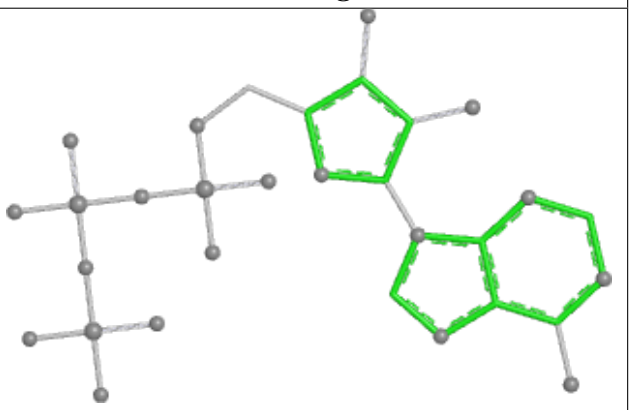
Bond angles

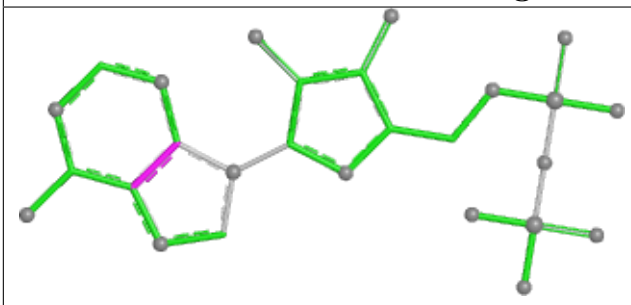
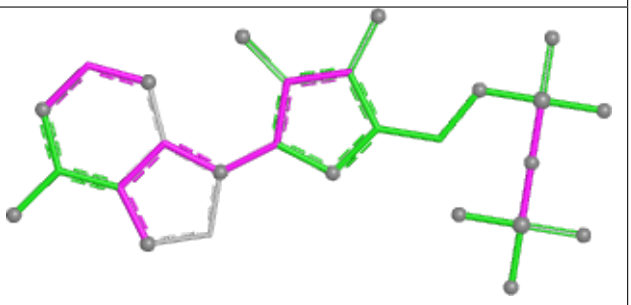
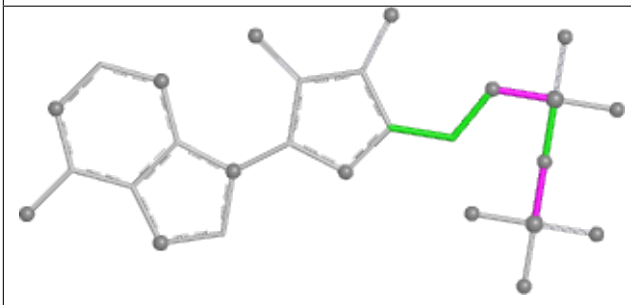
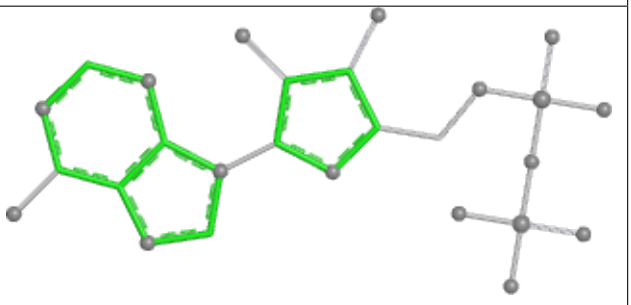


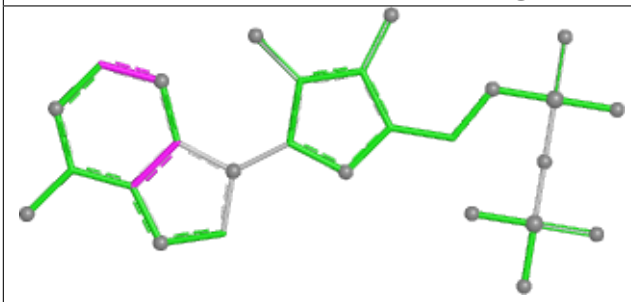
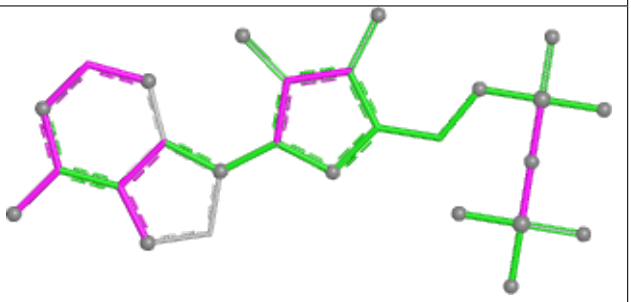
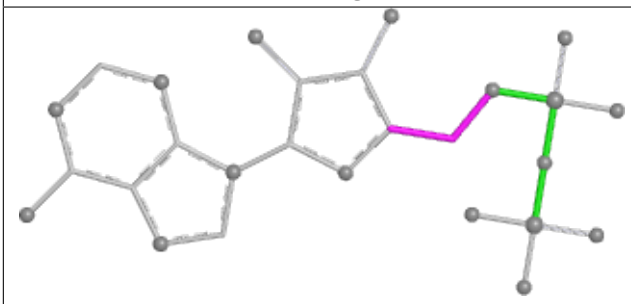
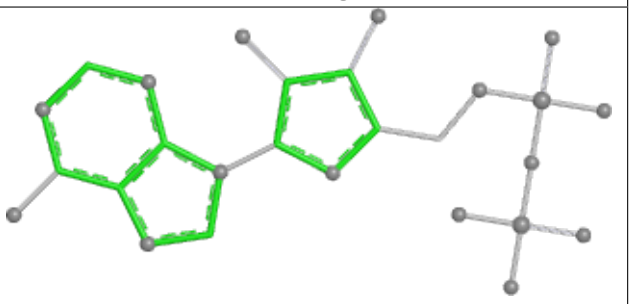
Torsions

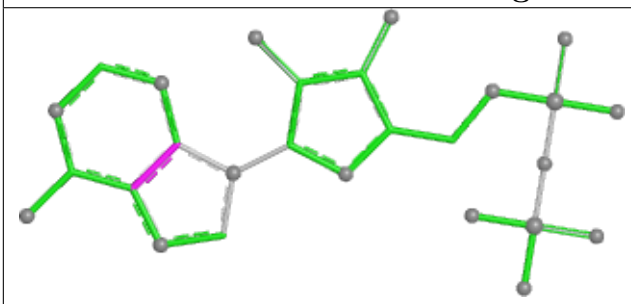
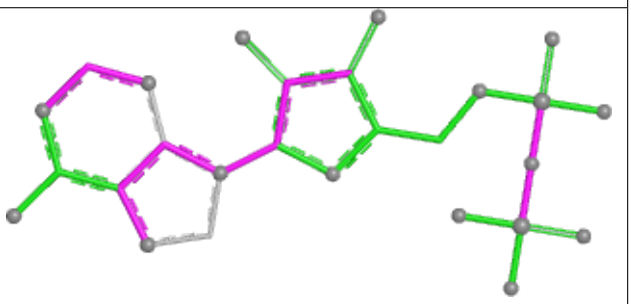
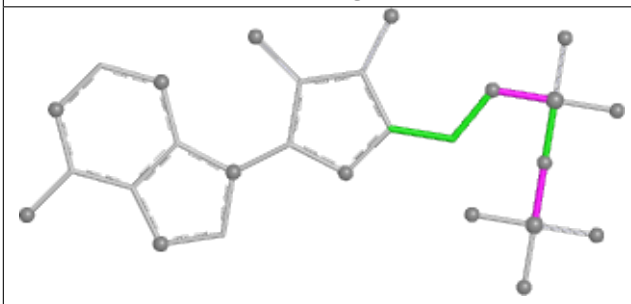
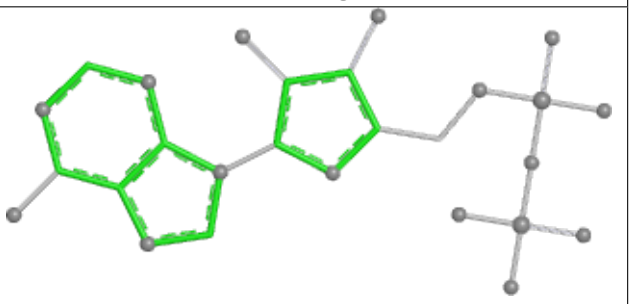


Rings

Ligand ATP A 4802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 4804	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 4801	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 4804	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3803:PRO	C	3804:LEU	N	2.62
1	B	3803:PRO	C	3804:LEU	N	2.62
1	A	3203:VAL	C	3204:GLY	N	2.58
1	B	3203:VAL	C	3204:GLY	N	2.58

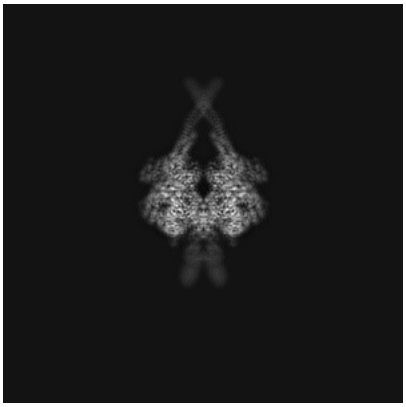
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3698. These allow visual inspection of the internal detail of the map and identification of artifacts.

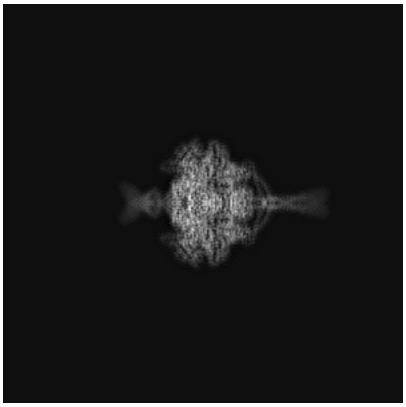
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

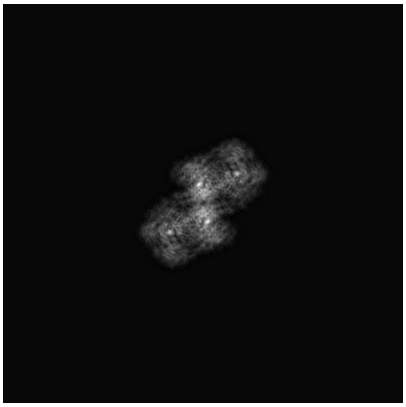
6.1.1 Primary map



X



Y

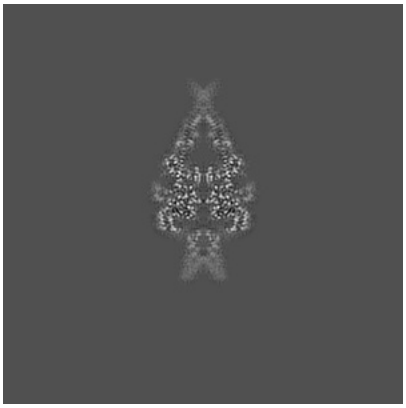


Z

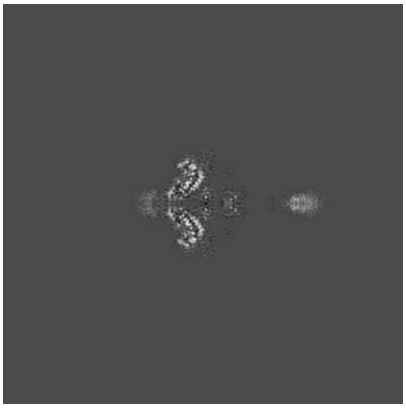
The images above show the map projected in three orthogonal directions.

6.2 Central slices

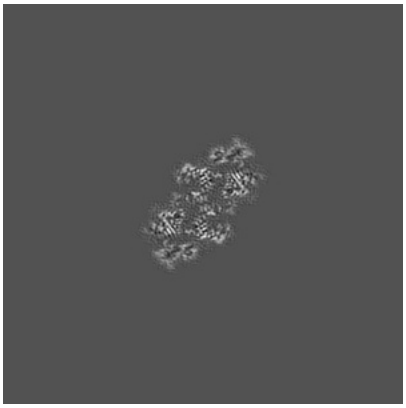
6.2.1 Primary map



X Index: 200



Y Index: 200

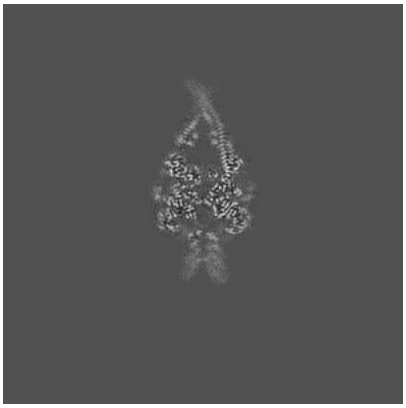


Z Index: 200

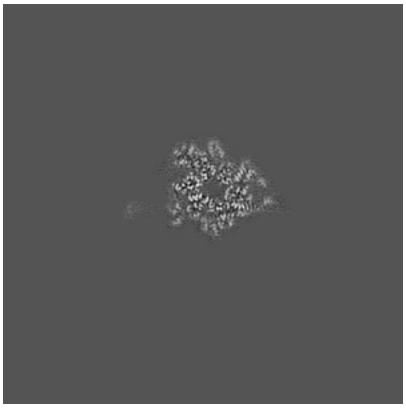
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

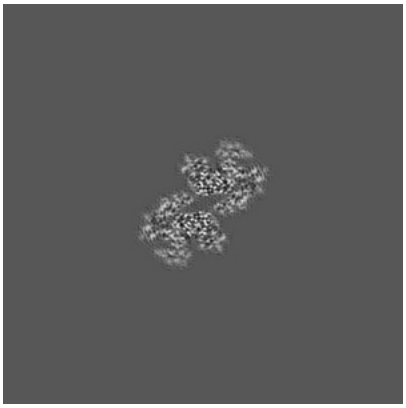
6.3.1 Primary map



X Index: 198



Y Index: 223



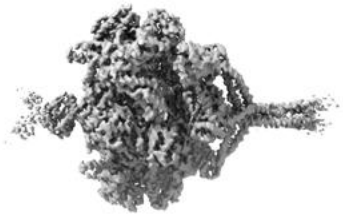
Z Index: 189

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

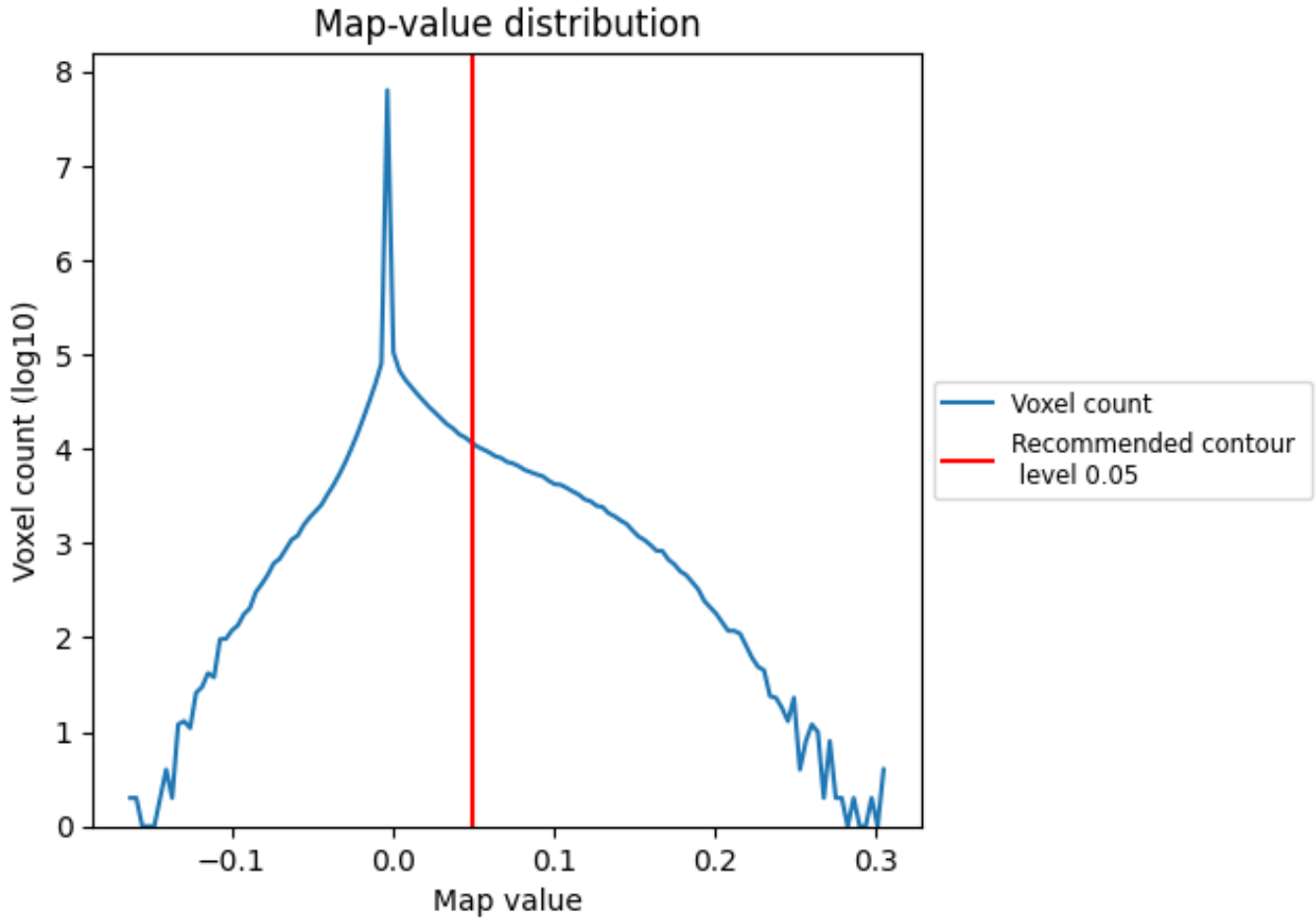
6.5 Mask visualisation (i)

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

7 Map analysis

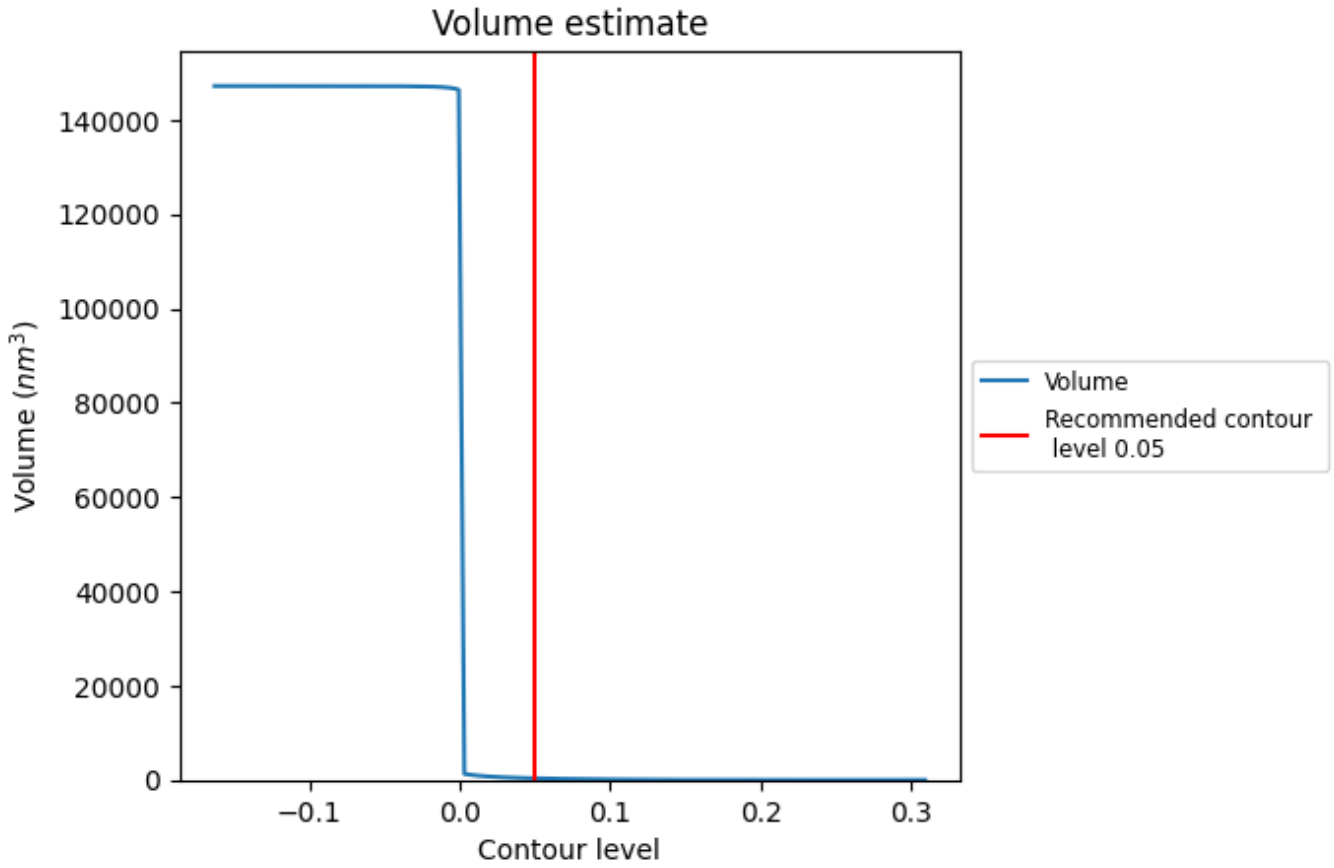
This section contains the results of statistical analysis of the map.

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.

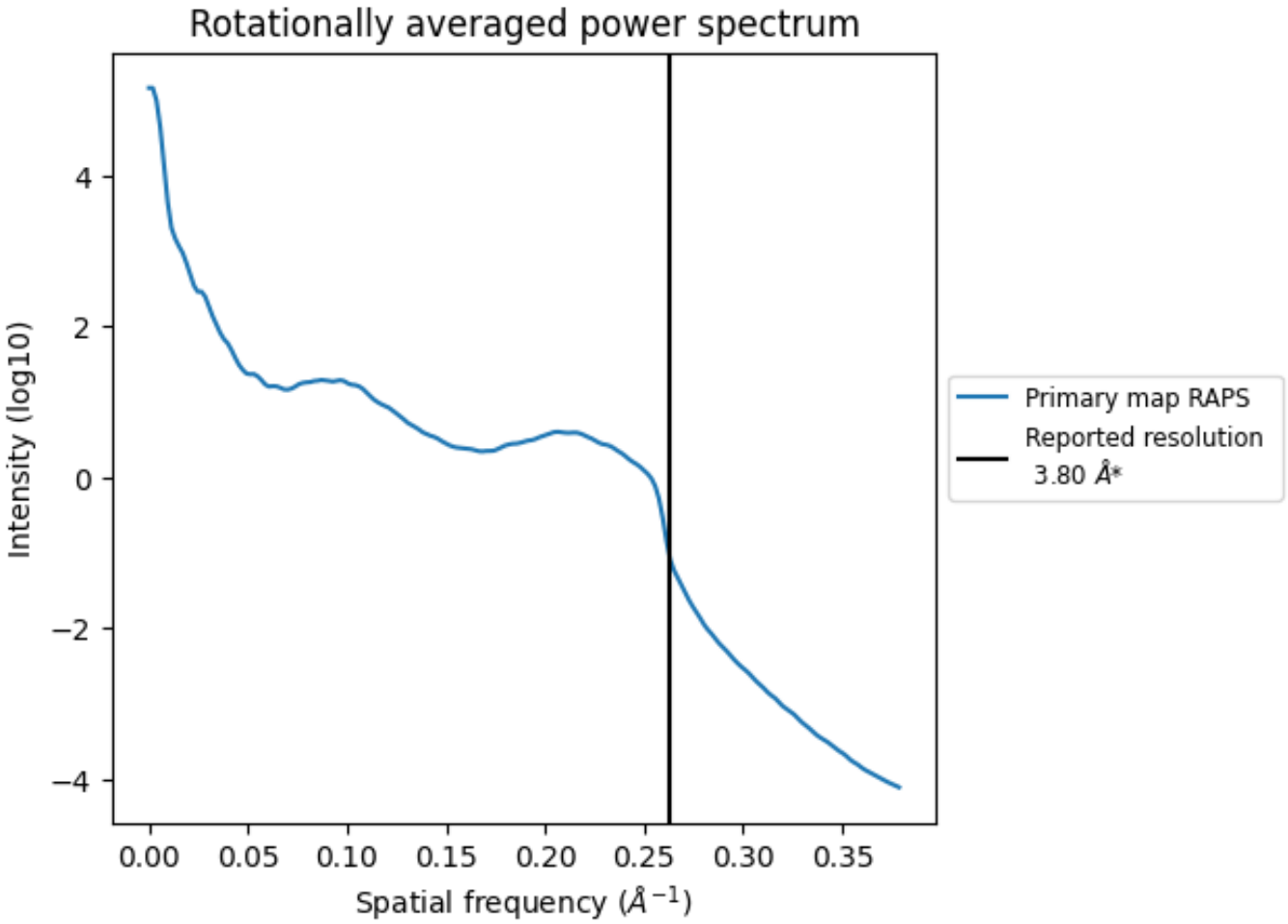
7.2 Volume estimate



The volume at the recommended contour level is 344 nm^3; this corresponds to an approximate mass of 311 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)

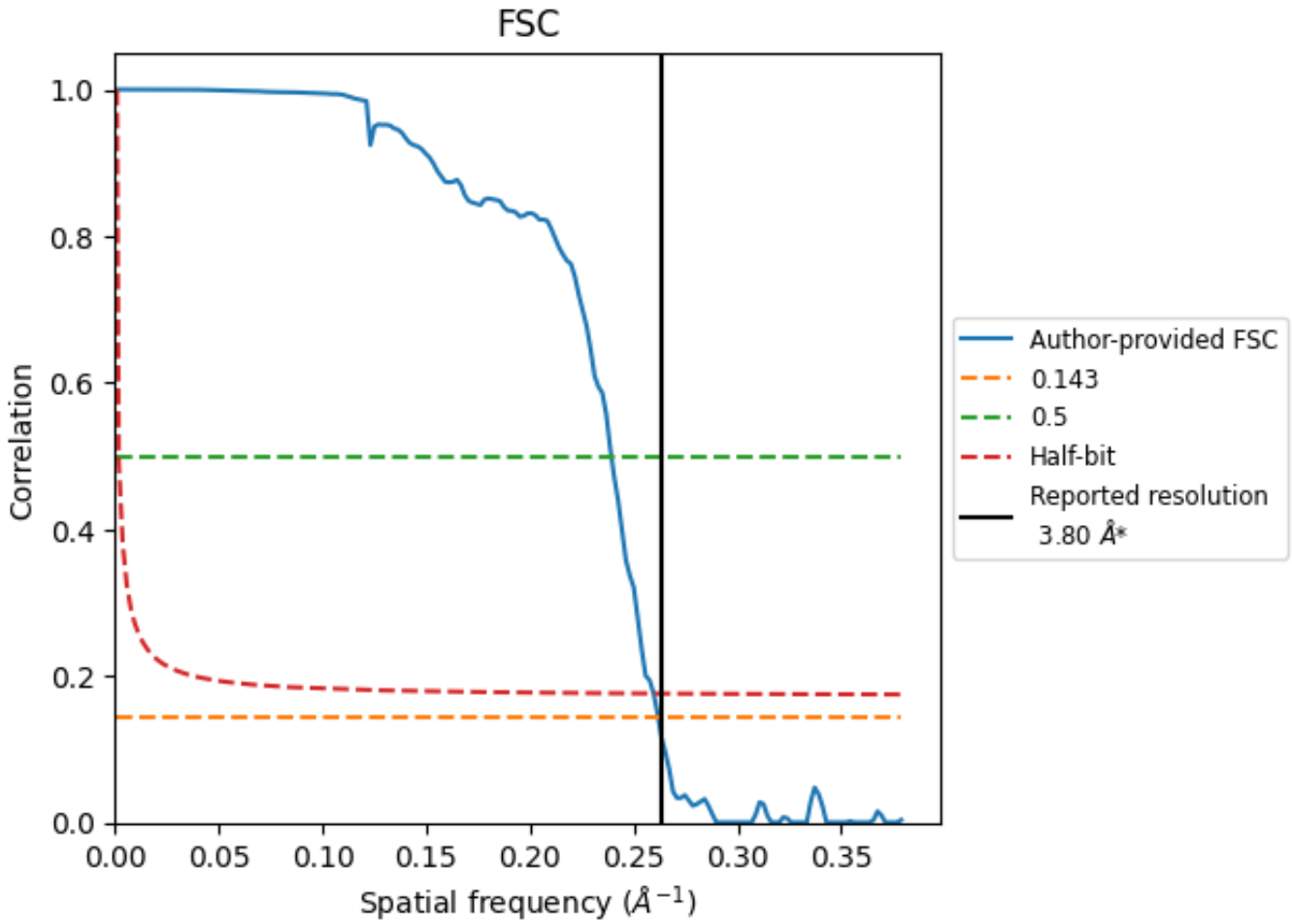


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

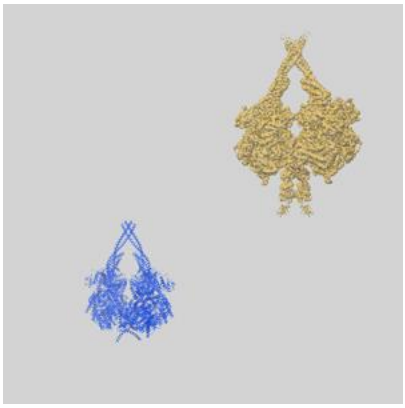
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.82	4.18	3.85
Unmasked-calculated*	-	-	-

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

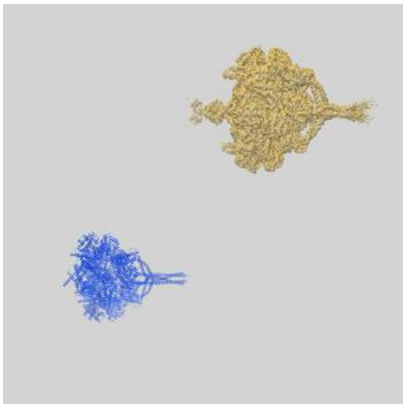
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3698 and PDB model 5NUG. Per-residue inclusion information can be found in section 3 on page 5.

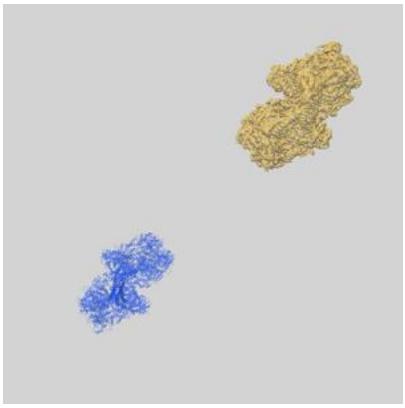
9.1 Map-model overlay



X



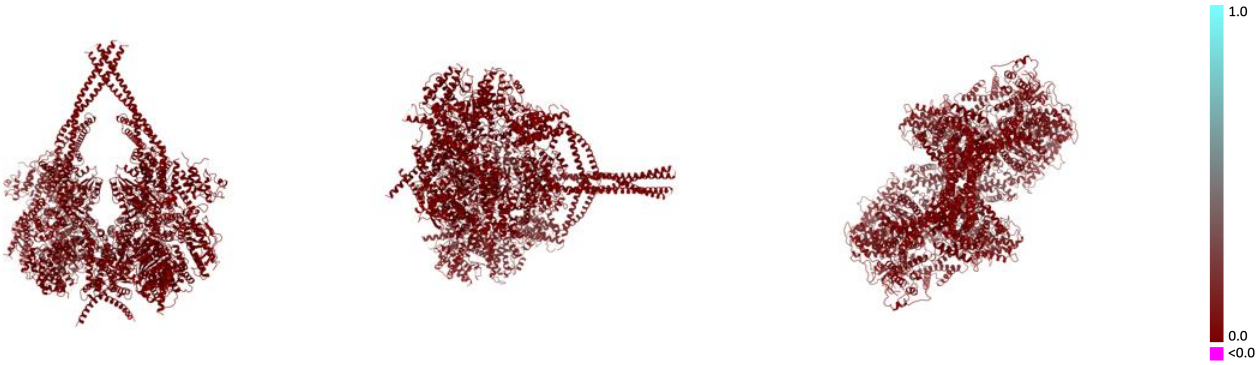
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

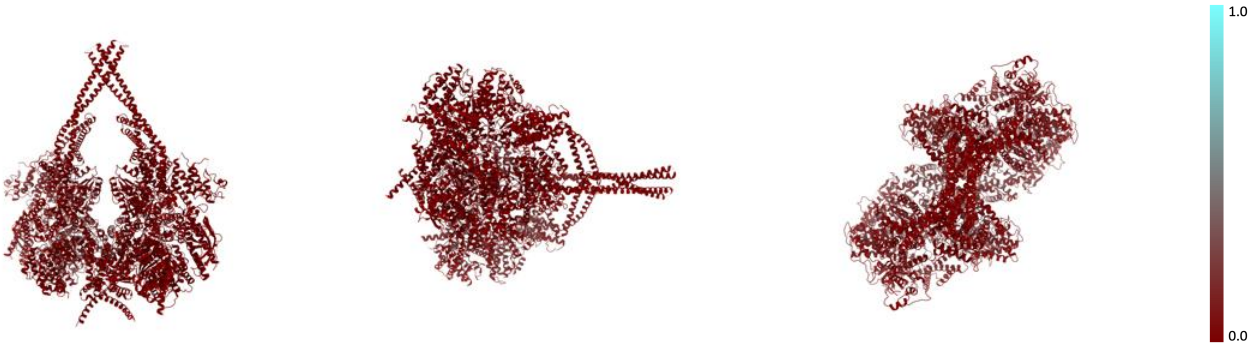
9.2 Q-score mapped to coordinate model (i)



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.

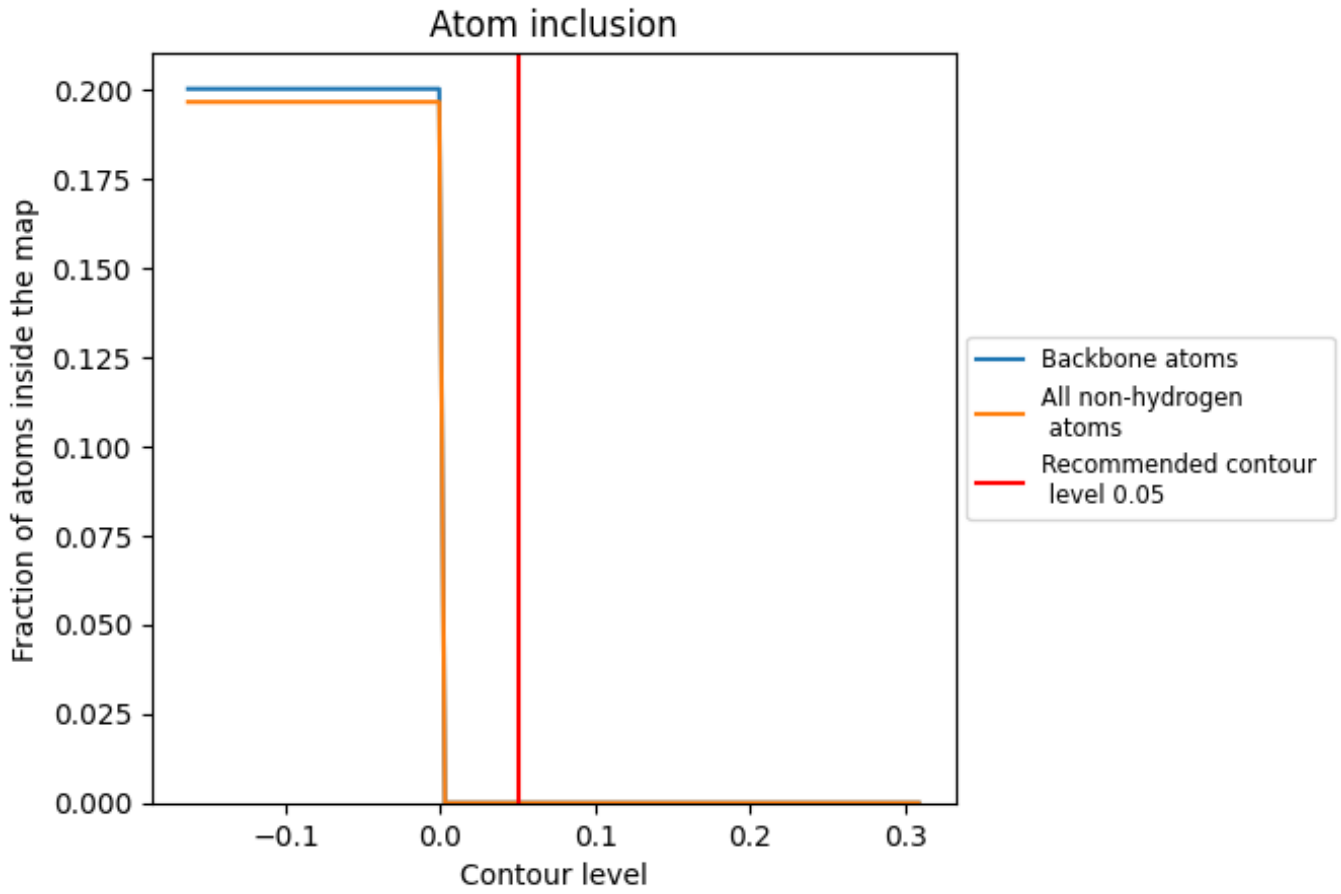
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.0000	0.0000
A	0.0000	0.0000
B	0.0000	0.0000