Full wwPDB EM Validation Report ⓘ

Jun 3, 2023 – 02:20 pm BST

PDB ID	:	8BH3
EMDB ID	:	EMD-16044
Title	:	DNA-PK Ku80 mediated dimer bound to PAXX
Authors	:	Hardwick, S.W.; Chaplin, A.K.
Deposited on	:	2022-10-28
Resolution	:	4.55 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:

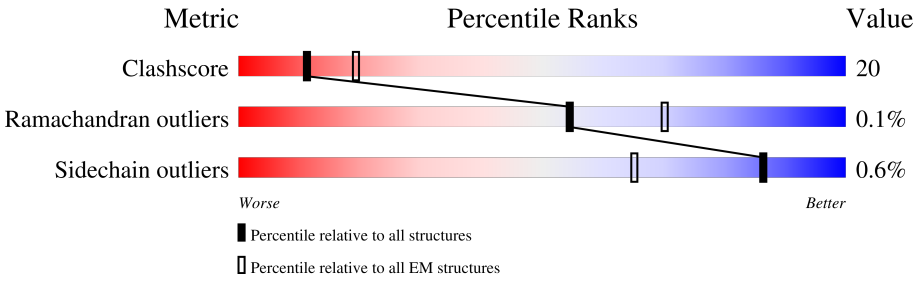
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

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

The reported resolution of this entry is 4.55 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	4128	48% 38% 14%
1	S	4128	48% 37% 14%
2	B	609	44% 40% 17%
2	T	609	46% 36% 18%
3	C	732	54% 37% 9%
3	L	732	53% 36% 11%
4	D	204	46% 59% 13% 28%
4	M	204	48% 65% 15% 20%

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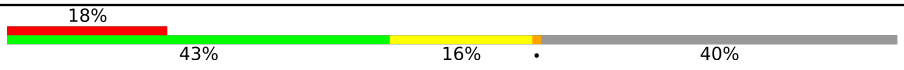
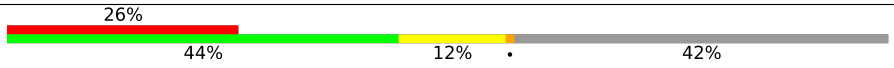
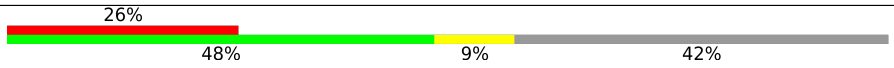
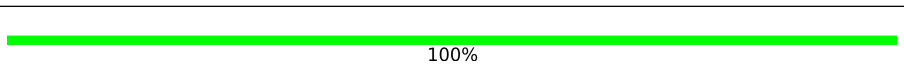
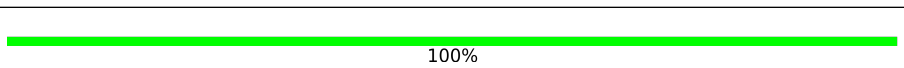
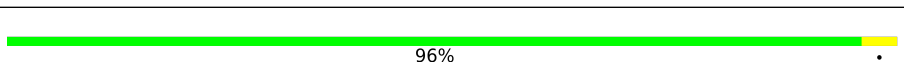
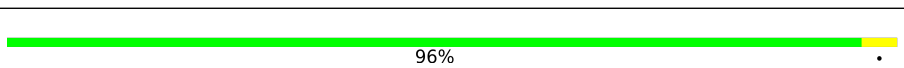
Mol	Chain	Length	Quality of chain
5	G	336	
5	H	336	
5	P	336	
5	Q	336	
6	I	911	
6	R	911	
7	j	25	
8	i	27	
9	d	26	
10	e	28	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 89245 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 DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3550	Total	C	N	O	S	0	0
			27927	17939	4728	5074	186		
1	S	3540	Total	C	N	O	S	0	0
			27999	18001	4725	5087	186		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	507	Total	C	N	O	S	0	0
			4038	2587	686	747	18		
2	T	502	Total	C	N	O	S	0	0
			4014	2569	680	747	18		

- Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	668	Total	C	N	O	S	0	0
			5292	3382	884	1000	26		
3	L	652	Total	C	N	O	S	0	0
			5174	3304	871	973	26		

- Molecule 4 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	147	Total	C	N	O	S	0	0
			1075	689	183	197	6		
4	M	164	Total	C	N	O	S	0	0
			1195	754	207	228	6		

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
5	H	194	Total	C	N	O	S	0	0
			1589	1009	271	302	7		
5	P	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
5	Q	194	Total	C	N	O	S	0	0
			1589	1009	271	302	7		

- Molecule 6 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	246	Total	C	N	O	S	0	0
			1977	1256	336	372	13		
6	R	246	Total	C	N	O	S	0	0
			1958	1240	332	373	13		

- Molecule 7 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	j	25	Total	C	N	O	P	0	0
			509	244	86	154	25		

- Molecule 8 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	27	Total	C	N	O	P	0	0
			552	265	102	158	27		

- Molecule 9 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	d	26	Total	C	N	O	P	0	0
			528	253	89	160	26		

- Molecule 10 is a DNA chain called DNA (28-MER).

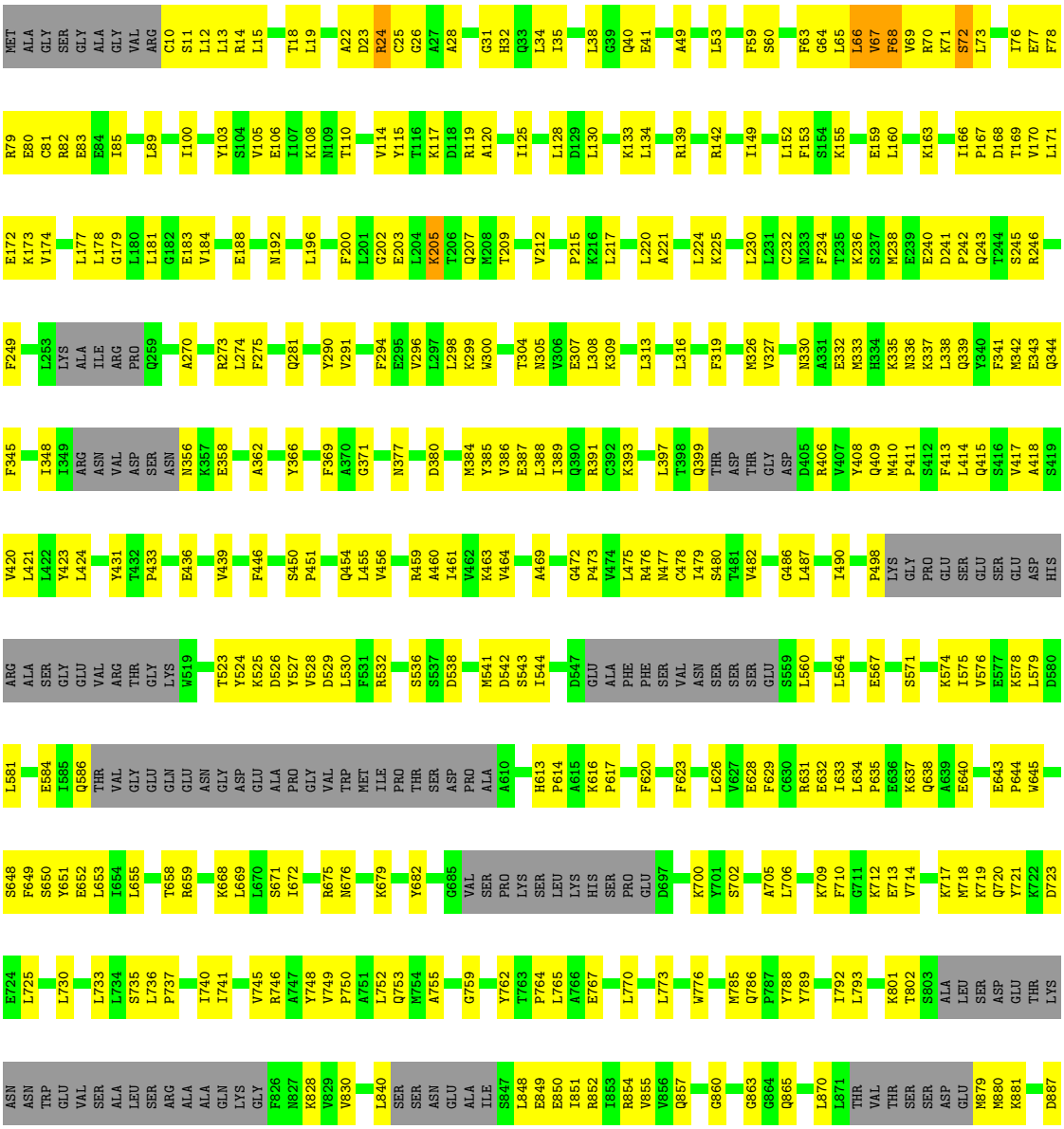
Mol	Chain	Residues	Atoms					AltConf	Trace
10	e	28	Total	C	N	O	P	0	0
			573	275	107	163	28		

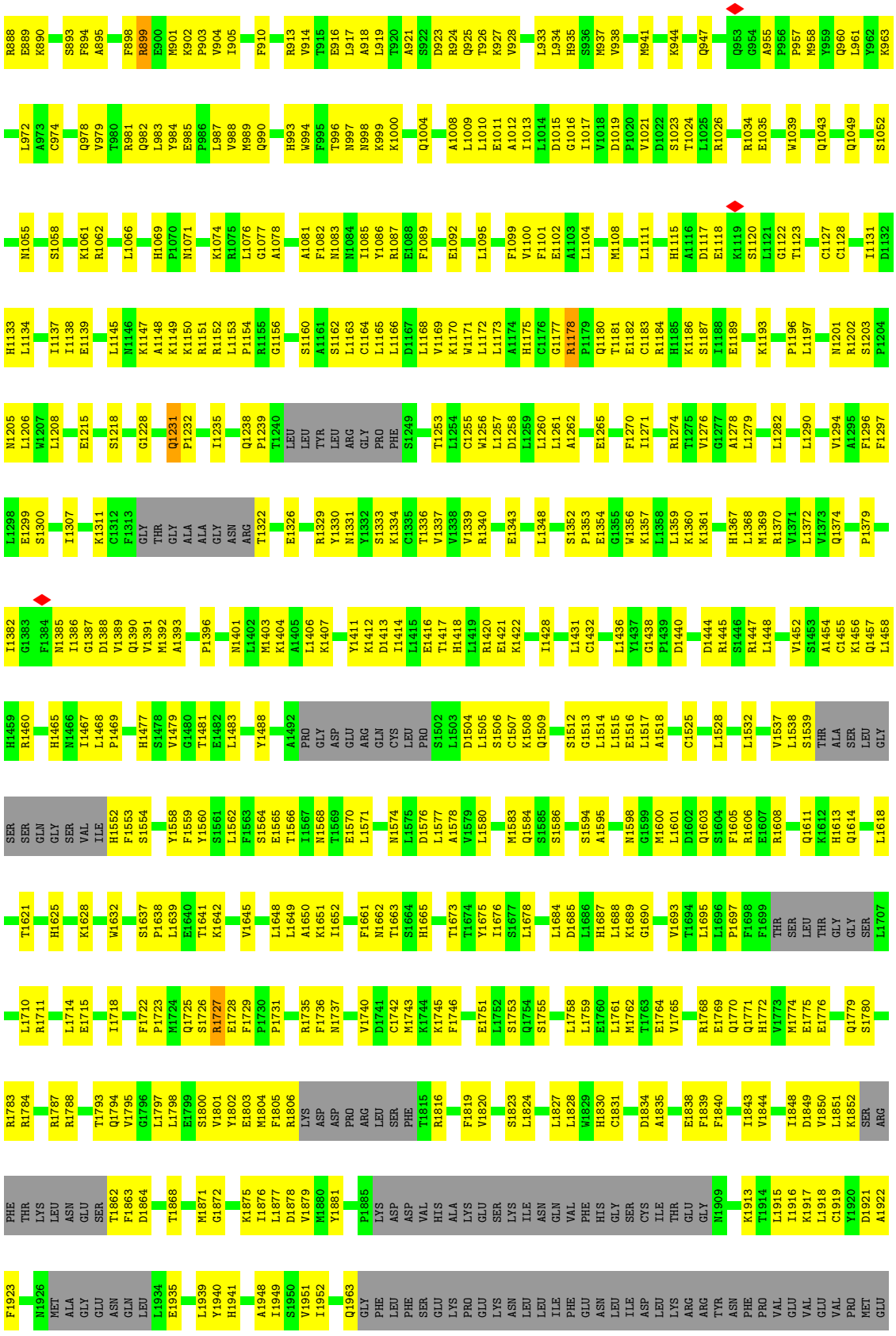
3 Residue-property plots (i)

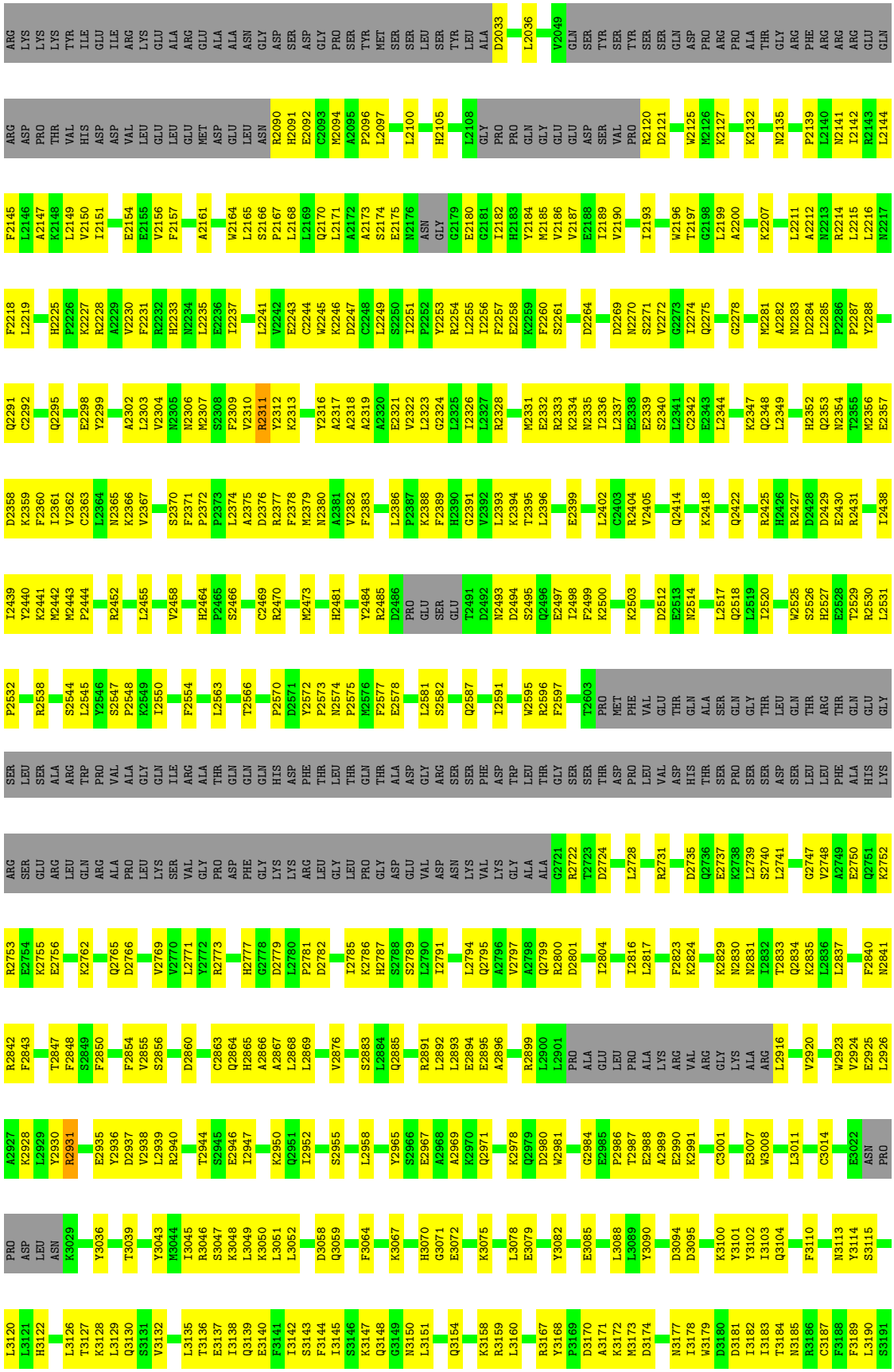
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

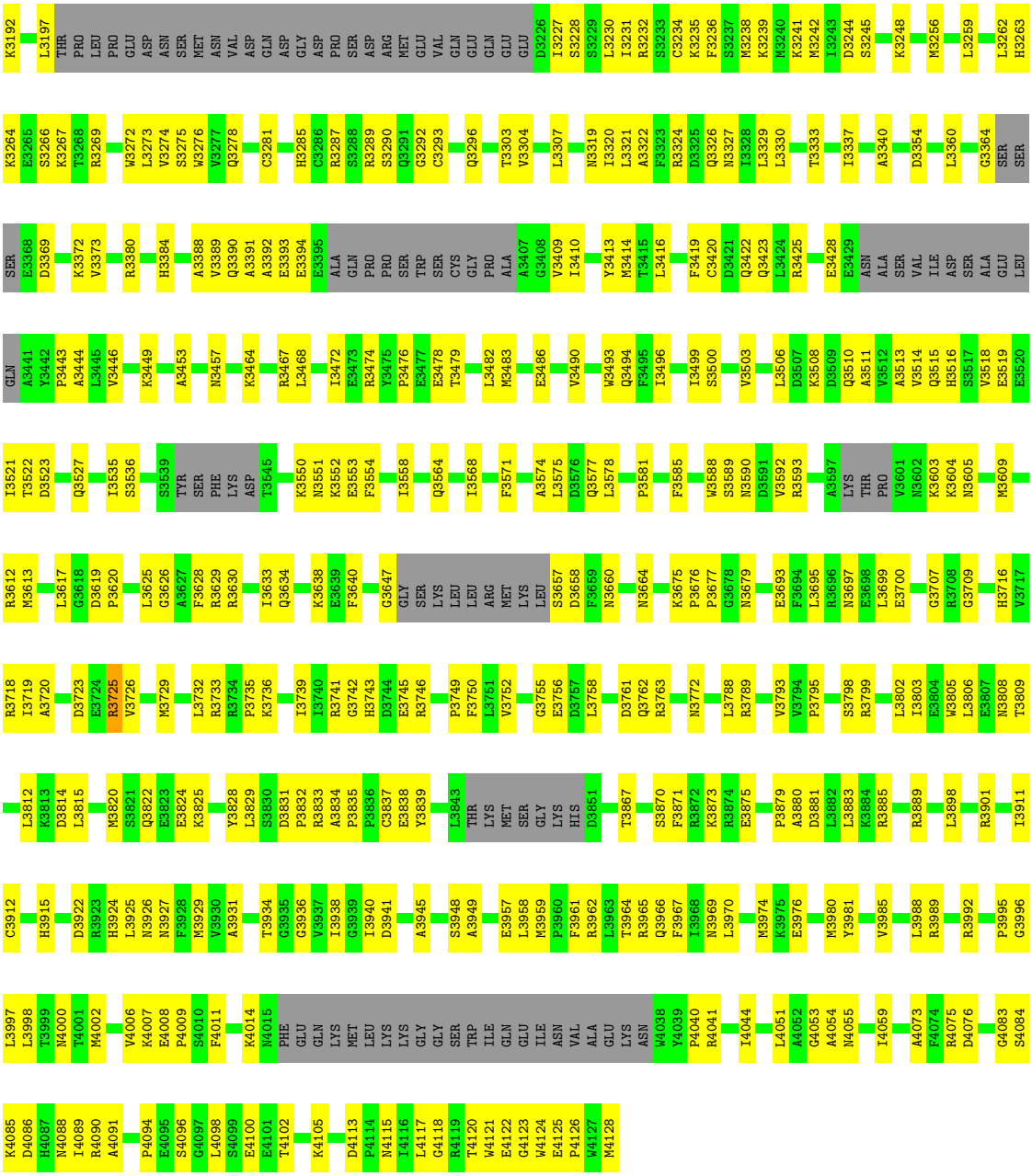
- Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain A:



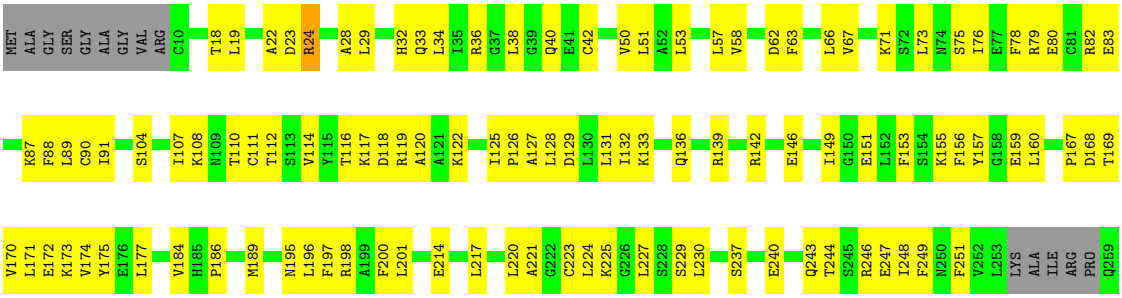


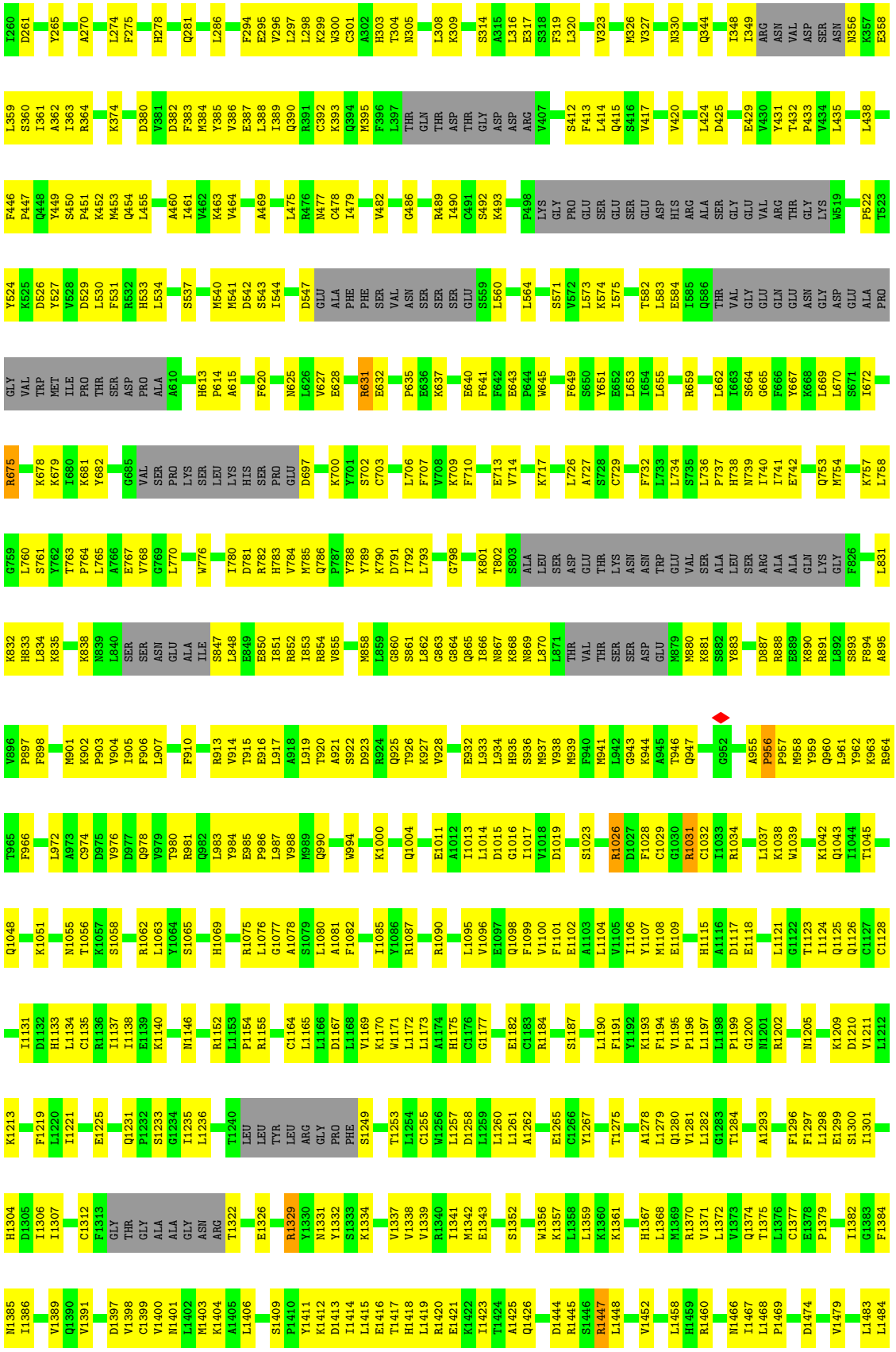


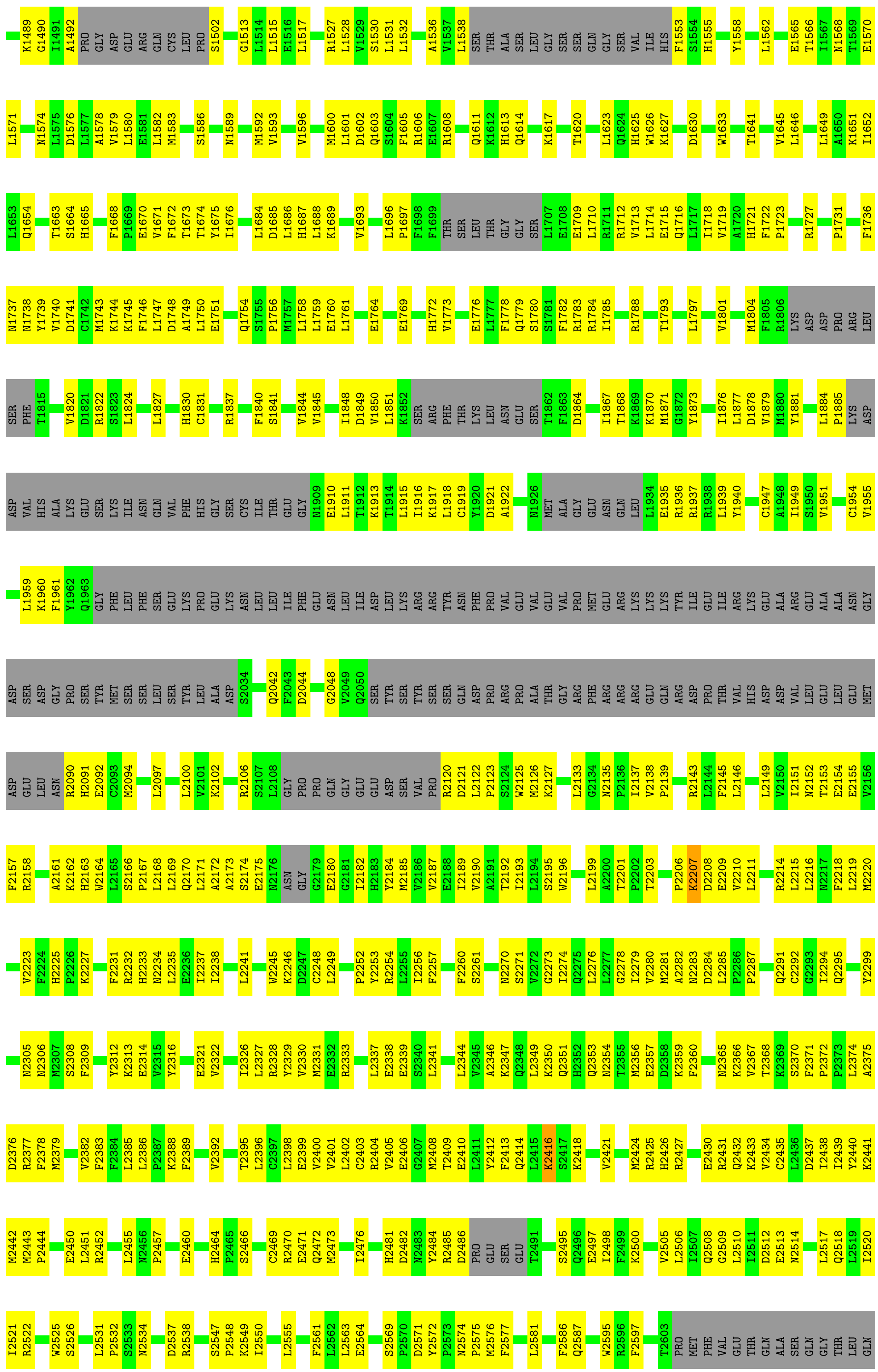


• Molecule 1: DNA-dependent protein kinase catalytic subunit

Chain S:



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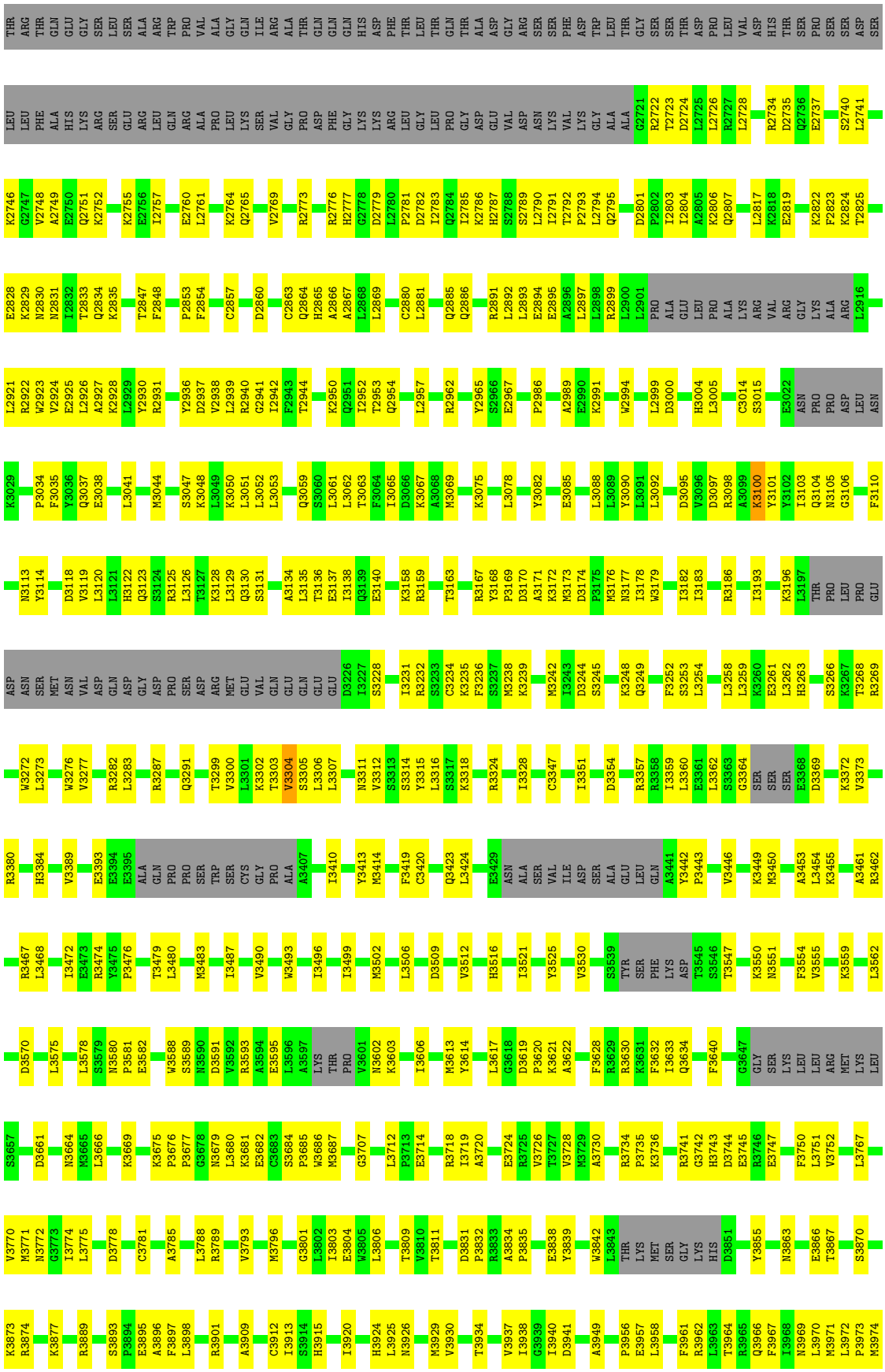
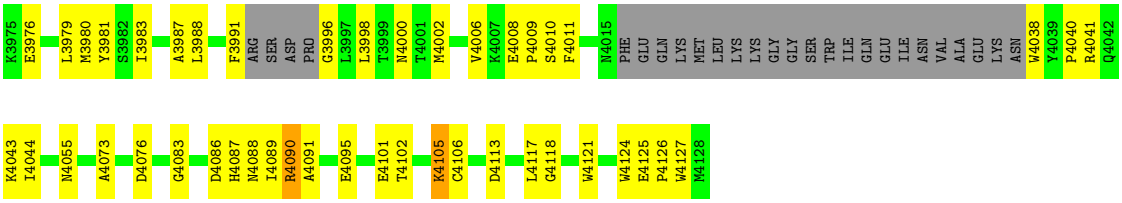
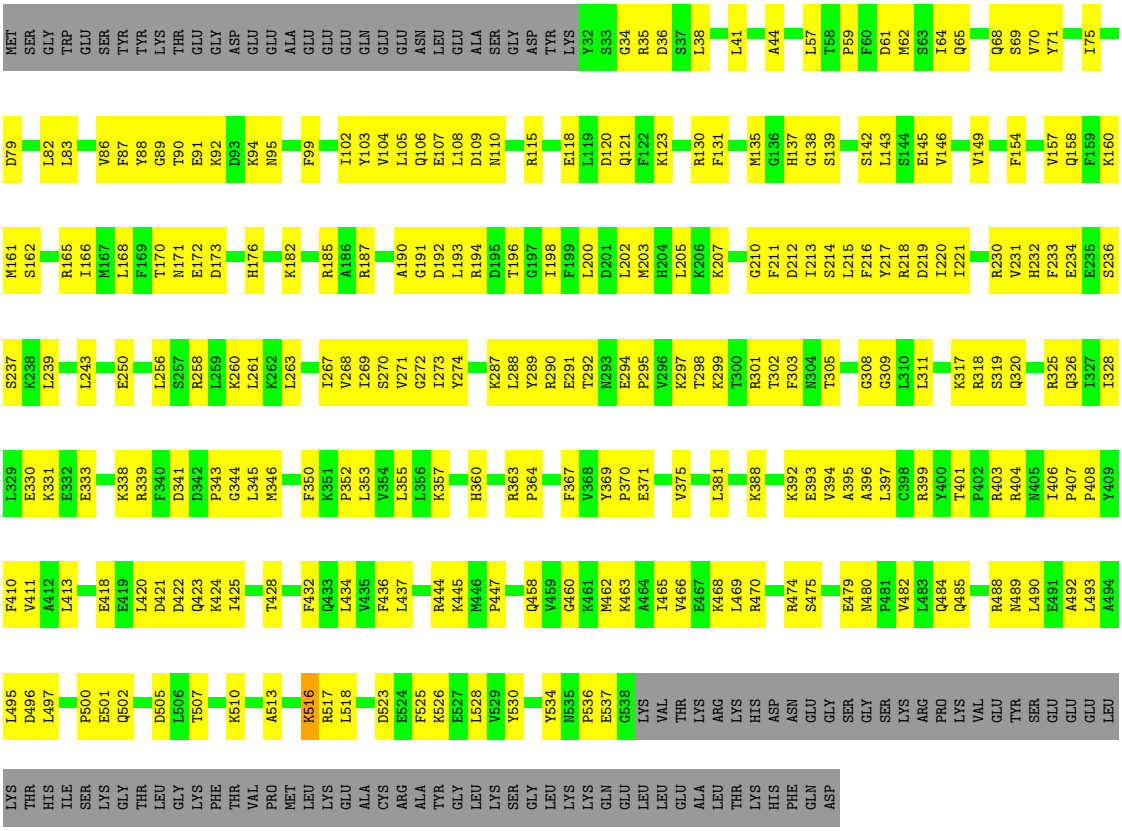
L1571 N1574 L1575 D1576 L1577 A1578 V1579 L1580 E1581 L1582 M1583 S1586 N1589 M1592 V1593 V1596 M1600 L1601 D1602 Q1603 S1604 F1605 R1606 E1607 R1608 Q1611 K1612 H1613 Q1614 K1617 T1620 L1623 Q1624 H1625 W1626 K1627 D1630 W1633 T1641 V1645 L1646 L1649 A1650 K1651 I1652
L1653 Q1654 T1663 S1664 H1665 F1668 P1669 E1670 V1671 F1672 T1673 T1674 Y1675 I1676 L1684 D1685 L1686 H1687 L1688 K1689 V1693 L1696 P1697 F1698 F1699 THR SER LEU THR GLY GLY SER L1707 E1708 E1709 L1710 R1711 R1712 V1713 L1714 E1715 Q1716 L1717 I1718 V1719 A1720 H1721 F1722 P1723 R1727 P1731 F1736
N1737 N1738 Y1739 V1740 D1741 C1742 M1743 K1744 K1745 F1746 L1747 D1748 A1749 L1750 E1751 Q1754 S1755 P1756 M1757 L1758 L1759 E1760 L1761 E1764 E1769 H1772 V1773 E1776 L1777 F1778 Q1779 S1780 S1781 F1782 R1783 R1784 I1785 R1788 T1793 L1797 V1801 M1804 F1805 R1806 LYS ASP ASP PRO ARG LEU
SER PHE T1815 V1820 D1821 R1822 S1823 L1824 L1827 H1830 C1831 R1837 F1840 S1841 V1844 V1845 I1848 D1849 V1850 L1851 K1852 SER ARG PHE THR LYS LEU ASN GLU SER T1862 F1863 D1864 I1867 T1868 K1869 K1870 M1871 G1872 Y1873 I1876 L1877 D1878 V1879 M1880 Y1881 L1884 P1885 LYS ASP
ASP VAL HIS ALA LYS GLU SER LYS ILE ASN GLN VAL PHE HIS GLY SER CYS ILE THR GLU GLY N1909 E1910 L1911 T1912 K1913 T1914 L1915 I1916 K1917 L1918 C1919 Y1920 D1921 A1922 N1926 MET ALA GLY GLU ASN GLN LEU L1934 E1935 R1936 R1937 R1938 L1939 Y1940 C1947 A1948 I1949 S1950 V1951 C1954 V1955
L1959 K1960 F1961 Y1962 Q1963 GLY PHE LEU PHE SER GLU LYS PRO GLU LYS ASN LEU LEU ILE PHE GLU ASN LEU ILE ASP LEU LYS ARG ARG TYR ASN PHE PRO VAL GLU VAL GLU VAL PRO MET GLU ARG LYS LYS LYS TYR ILE GLU ILE ARG LYS GLU ALA ARG GLU ALA ALA ASN GLY
ASP SER ASP GLY PRO SER TYR MET SER SER LEU SER TYR LEU ALA ASP S2034 Q2042 F2043 D2044 G2048 V2049 Q2050 SER TYR SER TYR SER SER GLN ASP PRO ARG PRO ALA THR GLY ARG PHE ARG ARG ARG GLU GLN ARG ASP PRO THR VAL HIS ASP ASP VAL LEU GLU GLU LEU GLU MET
ASP GLU LEU ASN R2090 H2091 E2092 C2093 M2094 L2097 L2100 V2101 K2102 R2106 S2107 L2108 GLY PRO PRO GLN GLY GLU GLU ASP SER SER VAL PRO R2120 D2121 L2122 P2123 S2124 W2125 M2126 K2127 L2133 G2134 N2135 P2136 I2137 V2138 P2139 R2143 L2144 F2145 L2146 L2149 V2150 I2151 N2152 T2153 E2154 E2155 V2156
F2157 R2158 A2161 K2162 H2163 W2164 L2165 S2166 P2167 L2168 L2169 Q2170 L2171 A2172 A2173 S2174 E2175 N2176 ASN GLY G2179 E2180 G2181 I2182 H2183 Y2184 M2185 V2186 V2187 E2188 I2189 V2190 A2191 T2192 I2193 L2194 S2195 W2196 L2199 A2200 T2201 P2202 T2203 P2206 K2207 D2208 E2209 V2210 L2211 R2214 L2215 L2216 N2217 F2218 L2219 M2220
V2223 F2224 H2225 P2226 K2227 F2231 R2232 H2233 N2234 L2235 E2236 I2237 I2238 L2241 W2245 K2246 D2247 C2248 L2249 P2252 Y2253 R2254 L2255 I2256 F2257 F2260 S2261 N2270 S2271 V2272 G2273 I2274 Q2275 L2276 L2277 G2278 I2279 V2280 M2281 A2282 N2283 D2284 L2285 P2286 P2287 Q2291 C2292 G2293 I2294 Q2295 Y2299
N2305 N2306 M2307 S2308 F2309 Y2312 K2313 E2314 V2315 Y2316 E2321 V2322 I2326 L2327 R2328 Y2329 V2330 M2331 E2332 R2333 L2337 E2338 E2339 S2340 L2341 L2344 V2345 A2346 K2347 Q2348 L2349 K2350 Q2351 H2352 Q2353 N2354 T2355 M2356 E2357 D2358 K2359 F2360 N2365 K2366 V2367 T2368 K2369 S2370 F2371 P2372 P2373 L2374 A2375
D2376 R2377 F2378 M2379 V2382 F2383 F2384 L2385 L2386 P2387 K2388 F2389 V2392 T2395 L2396 C2397 L2398 E2399 V2400 V2401 L2402 C2403 R2404 V2405 E2406 G2407 M2408 T2409 E2410 L2411 Y2412 F2413 Q2414 L2415 K2416 S2417 K2418 V2421 M2424 R2425 H2426 R2427 E2430 R2431 Q2432 K2433 V2434 C2435 L2436 D2437 I2438 I2439 Y2440 K2441
M2442 M2443 P2444 E2450 L2451 R2452 L2455 N2456 P2457 E2460 H2464 P2465 S2466 C2469 R2470 E2471 Q2472 M2473 I2476 H2481 D2482 N2483 Y2484 R2485 D2486 PRO GLU SER GLU T2491 S2495 Q2496 E2497 I2498 F2499 K2500 V2505 L2506 I2507 Q2508 G2509 L2510 I2511 D2512 E2513 N2514 L2517 Q2518 L2519 I2520
I2521 R2522 W2525 S2526 L2531 P2532 S2533 N2534 D2537 R2538 S2547 P2548 K2549 I2550 L2555 F2561 L2562 L2563 E2564 S2569 P2570 D2571 Y2572 P2573 N2574 P2575 M2576 F2577 L2581 F2586 Q2587 W2595 R2596 F2597 T2603 PRO MET PHE VAL GLU THR GLN ALA SER GLN GLY THR LEU GLN





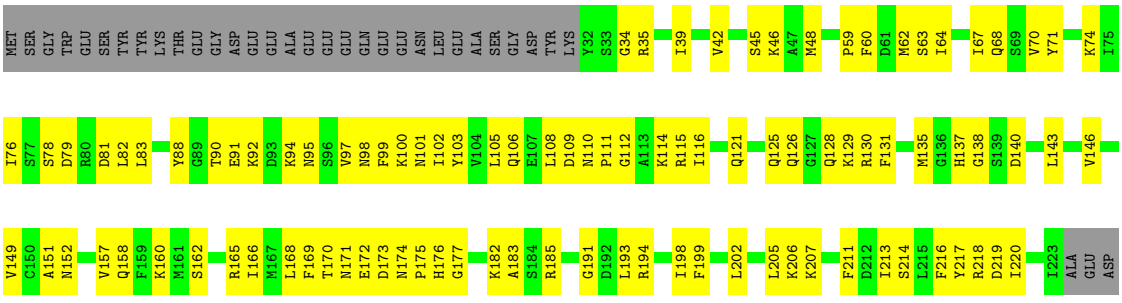
• Molecule 2: X-ray repair cross-complementing protein 6

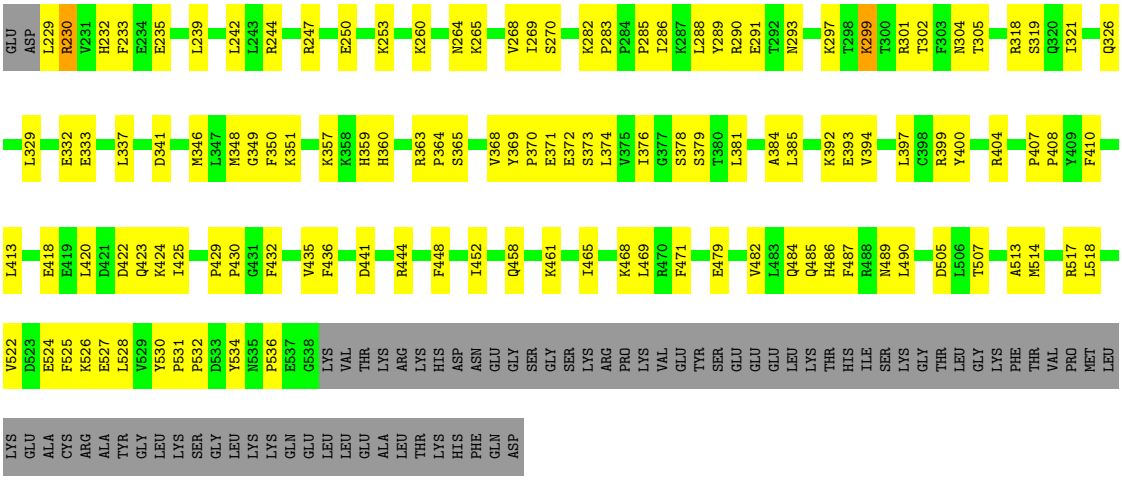
Chain B:



• Molecule 2: X-ray repair cross-complementing protein 6

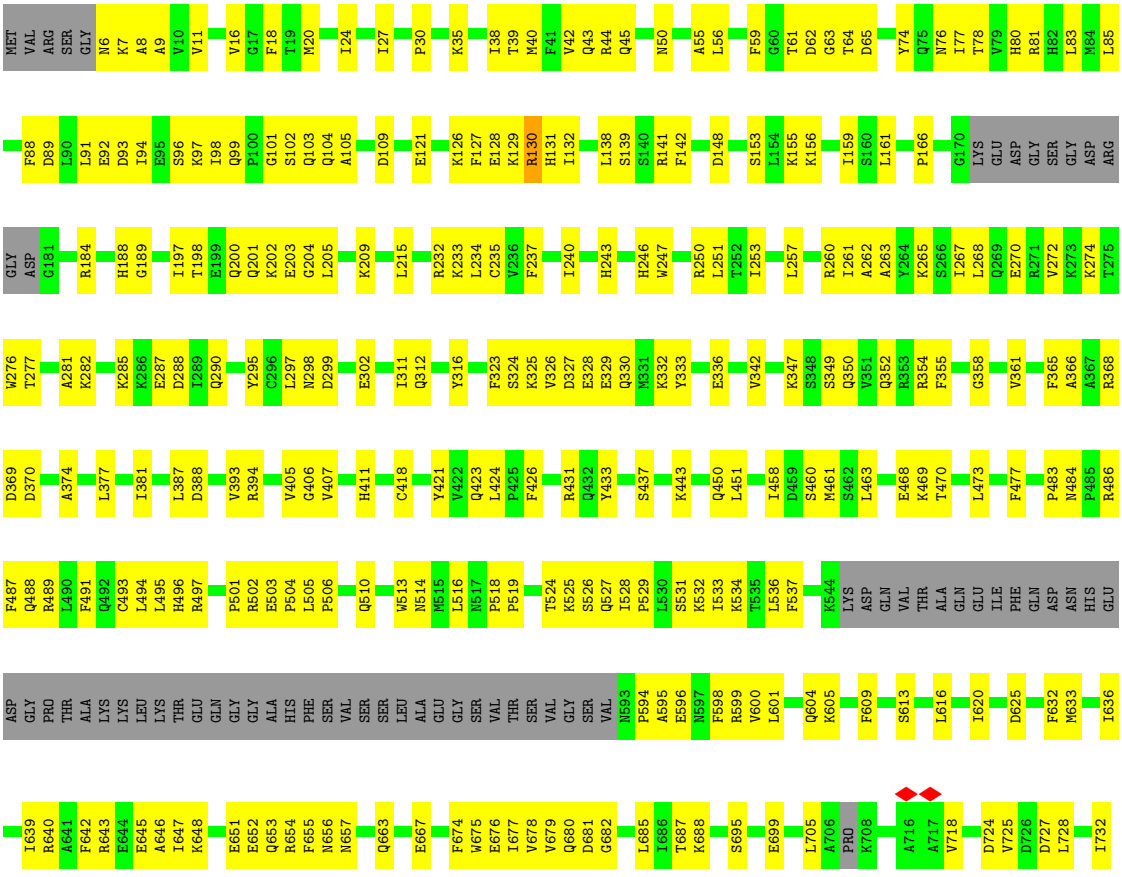
Chain T:





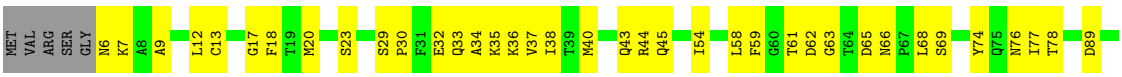
• Molecule 3: X-ray repair cross-complementing protein 5

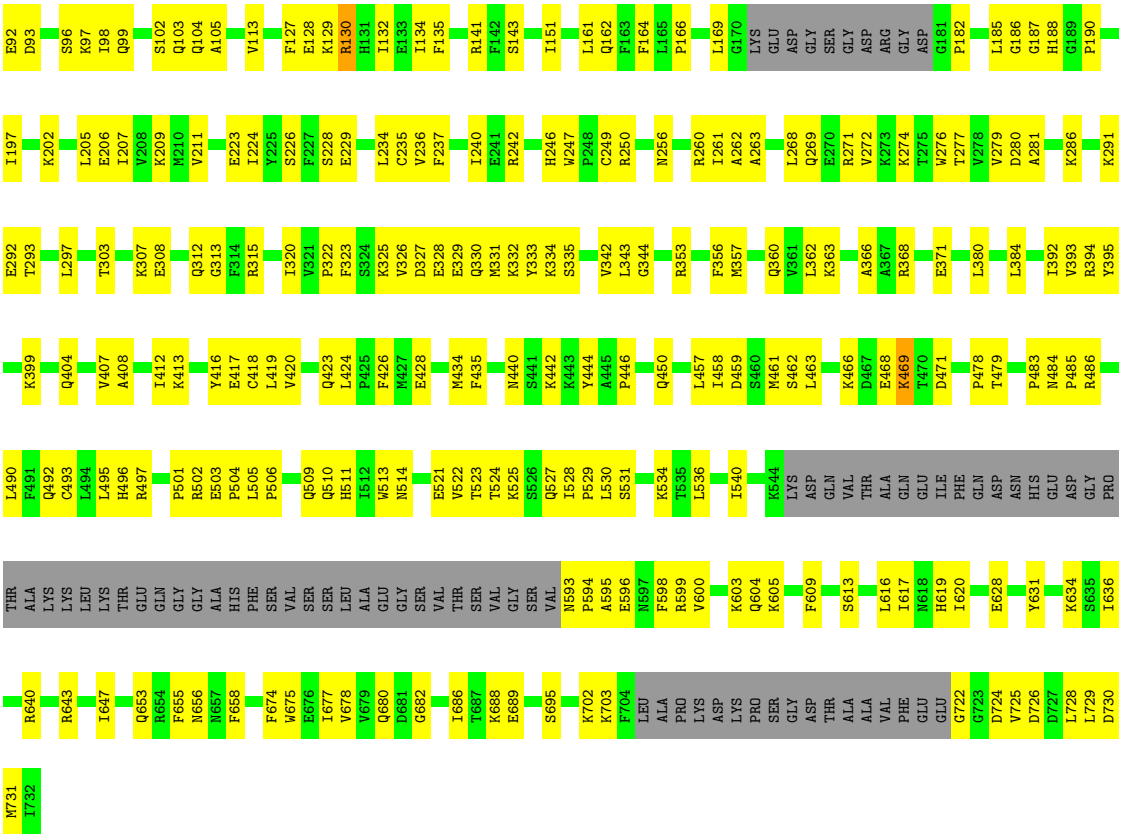
Chain C:



• Molecule 3: X-ray repair cross-complementing protein 5

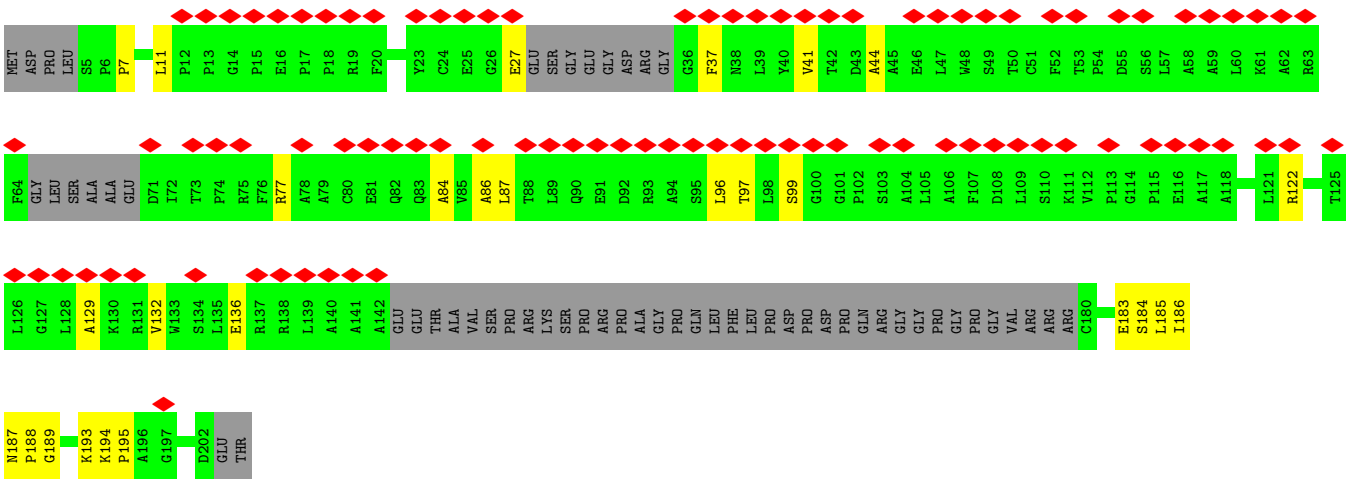
Chain L:





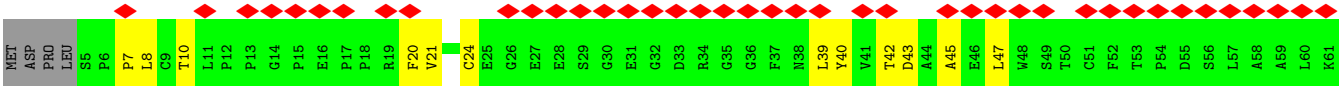
• Molecule 4: Protein PAXX

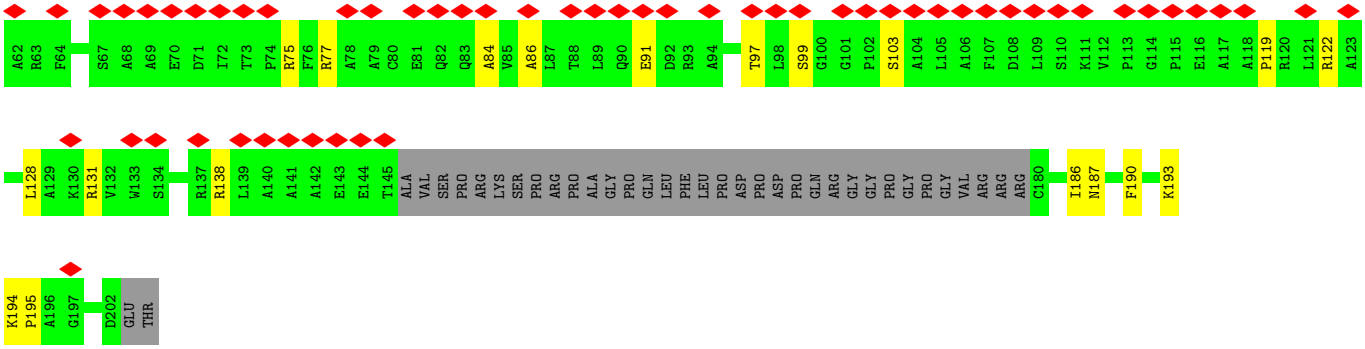
Chain D:



• Molecule 4: Protein PAXX

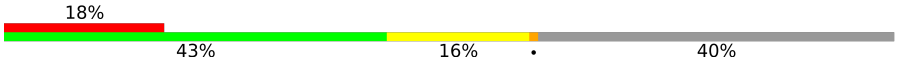
Chain M:

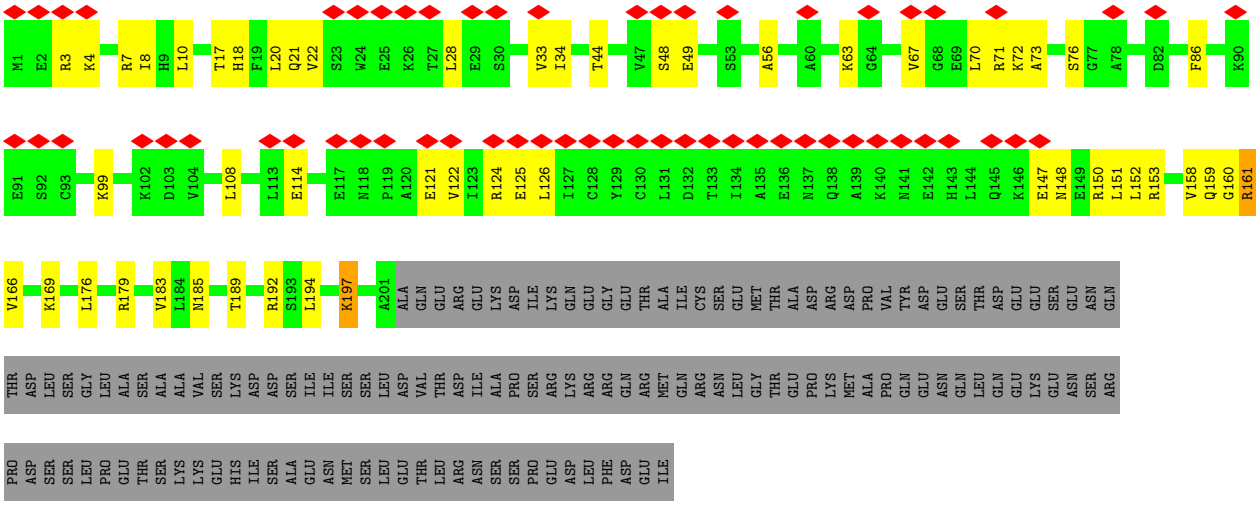




• Molecule 5: DNA repair protein XRCC4

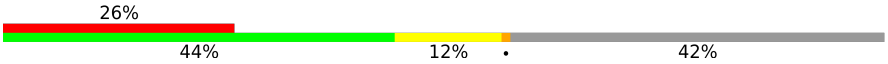
Chain G:

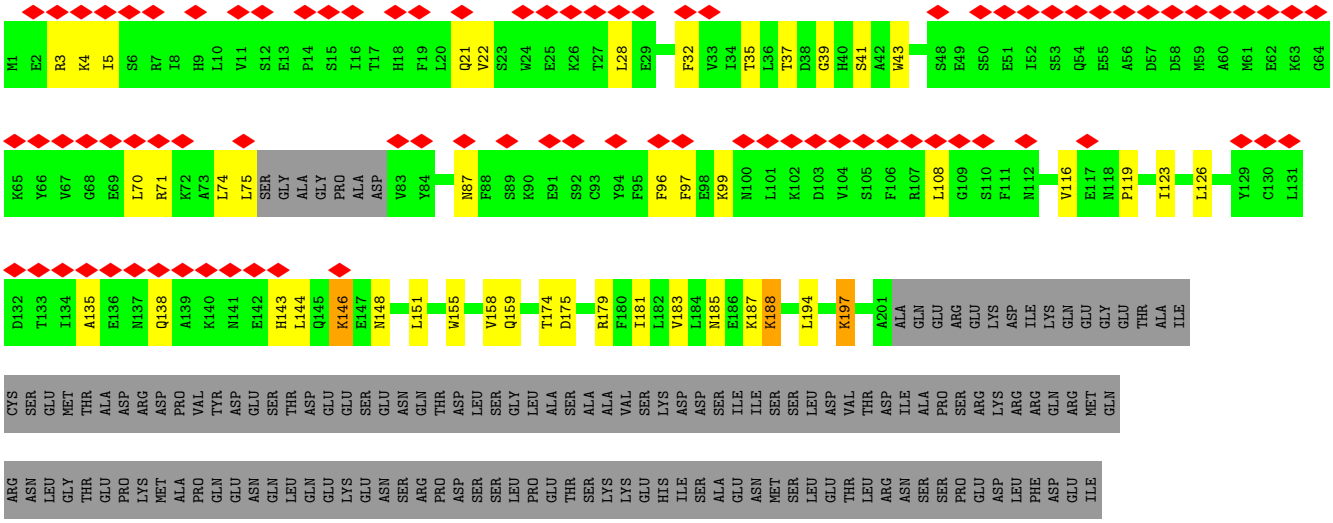




• Molecule 5: DNA repair protein XRCC4

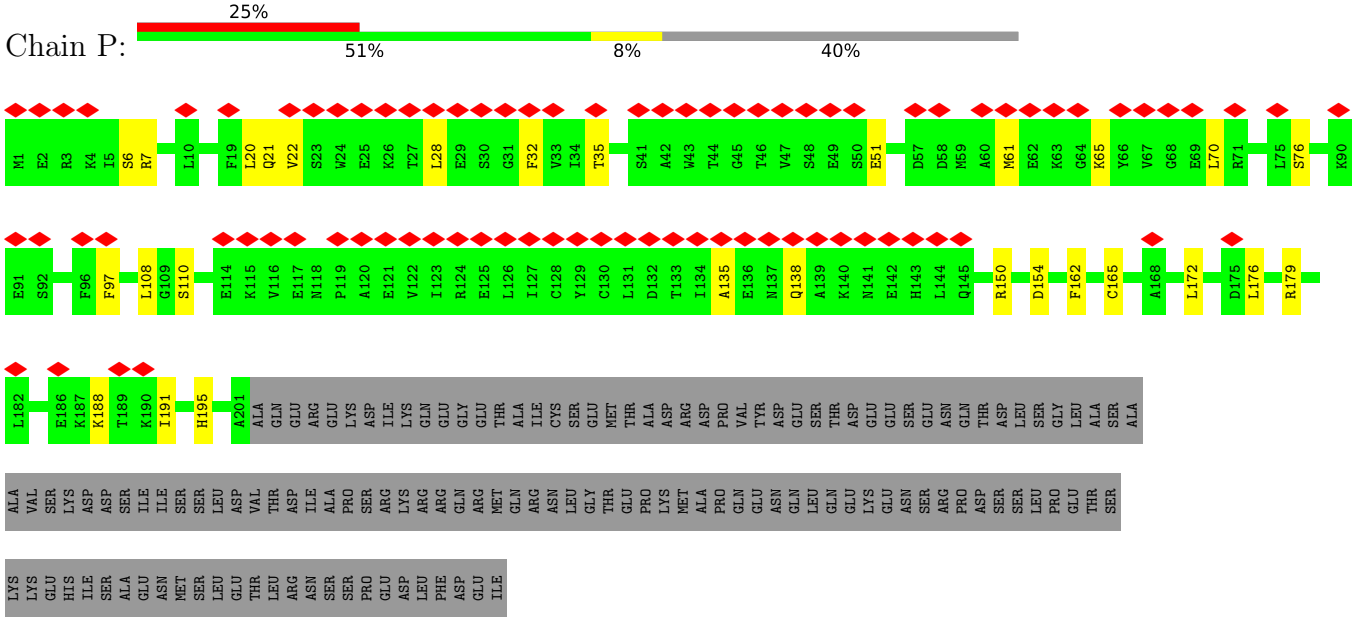
Chain H:





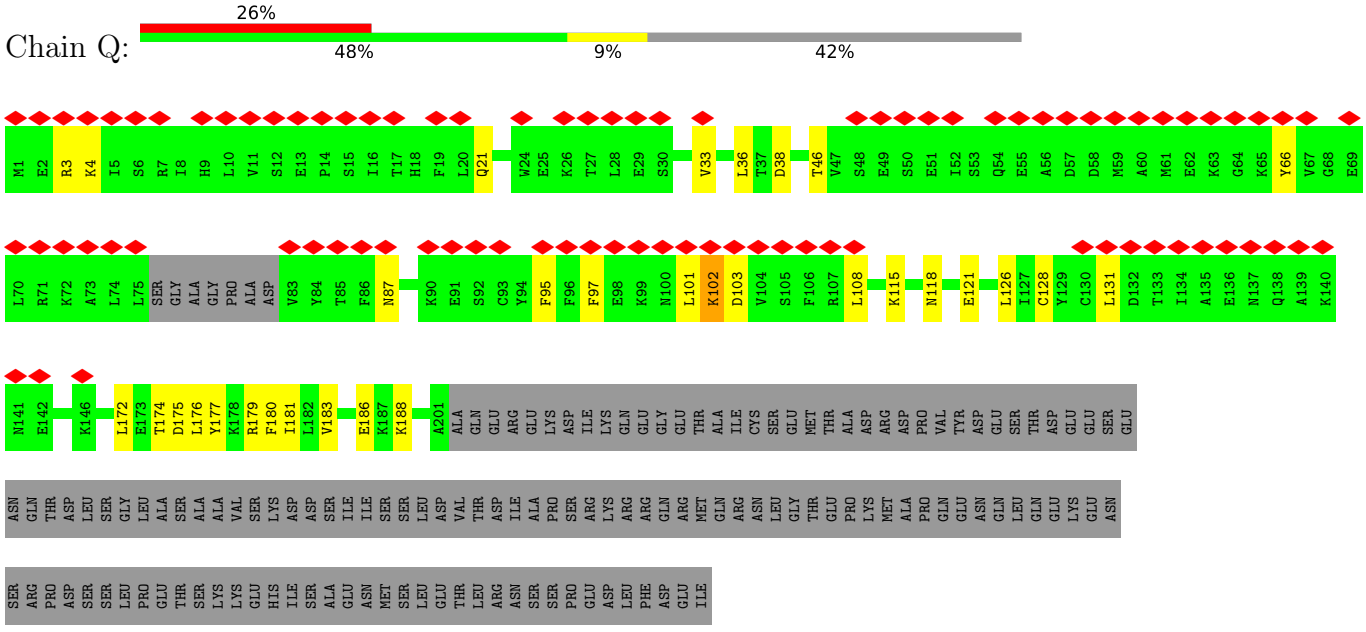
• Molecule 5: DNA repair protein XRCC4

Chain P:



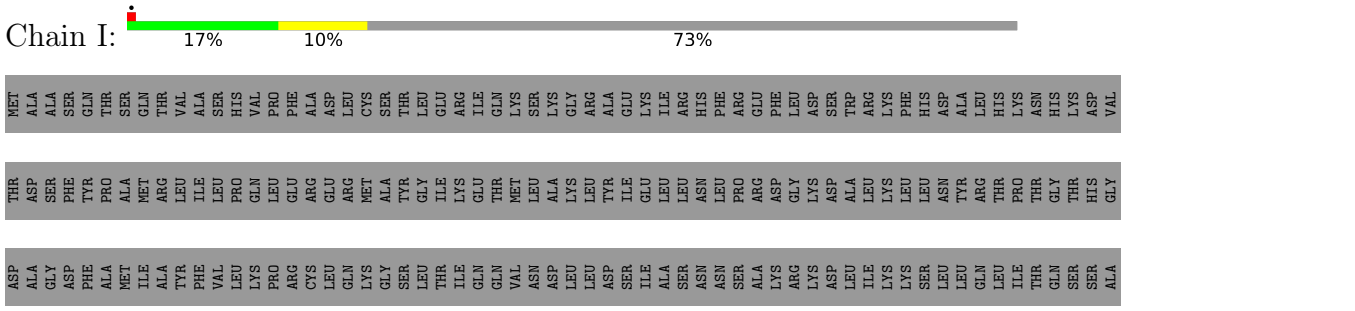
• Molecule 5: DNA repair protein XRCC4

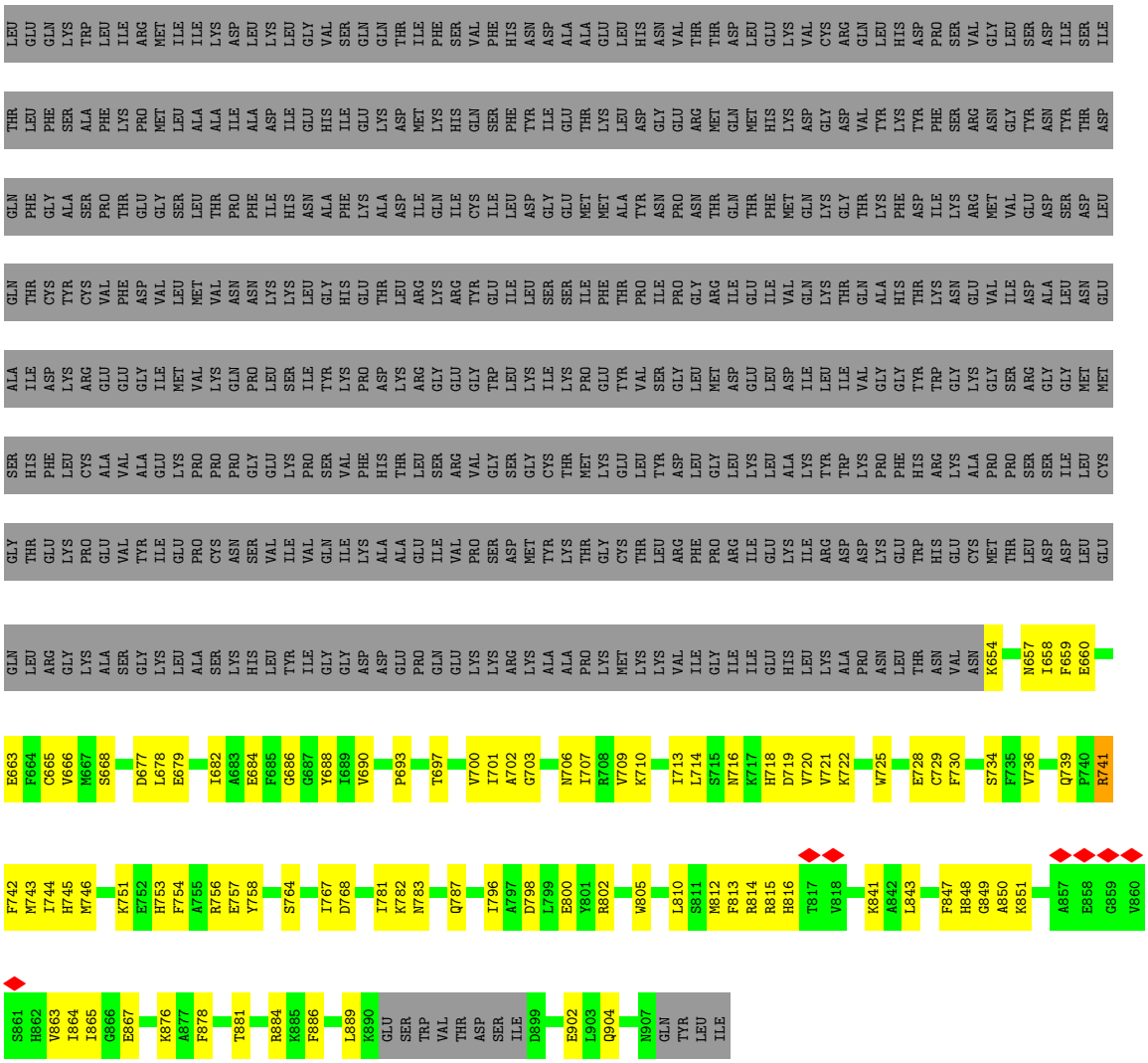
Chain Q:



• Molecule 6: DNA ligase 4

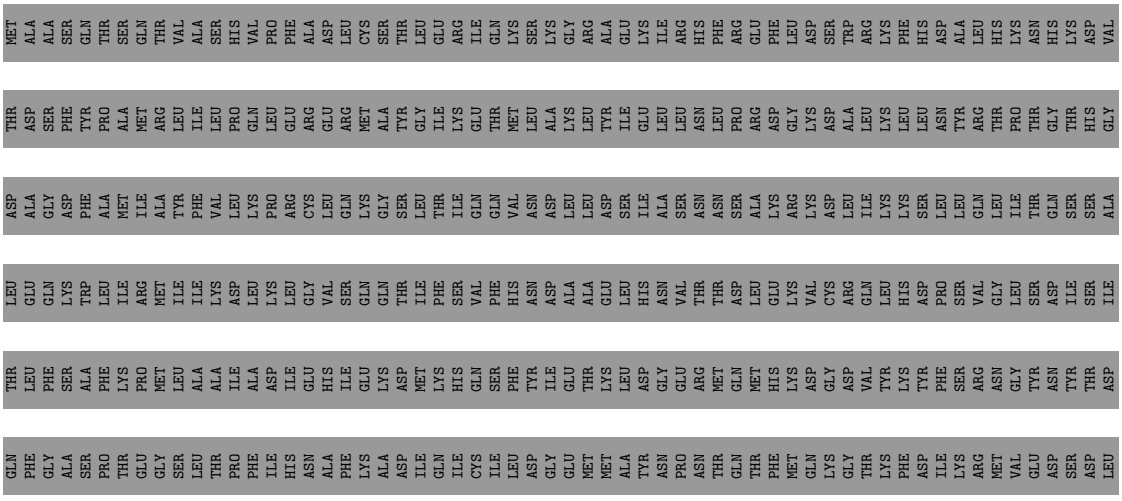
Chain I:

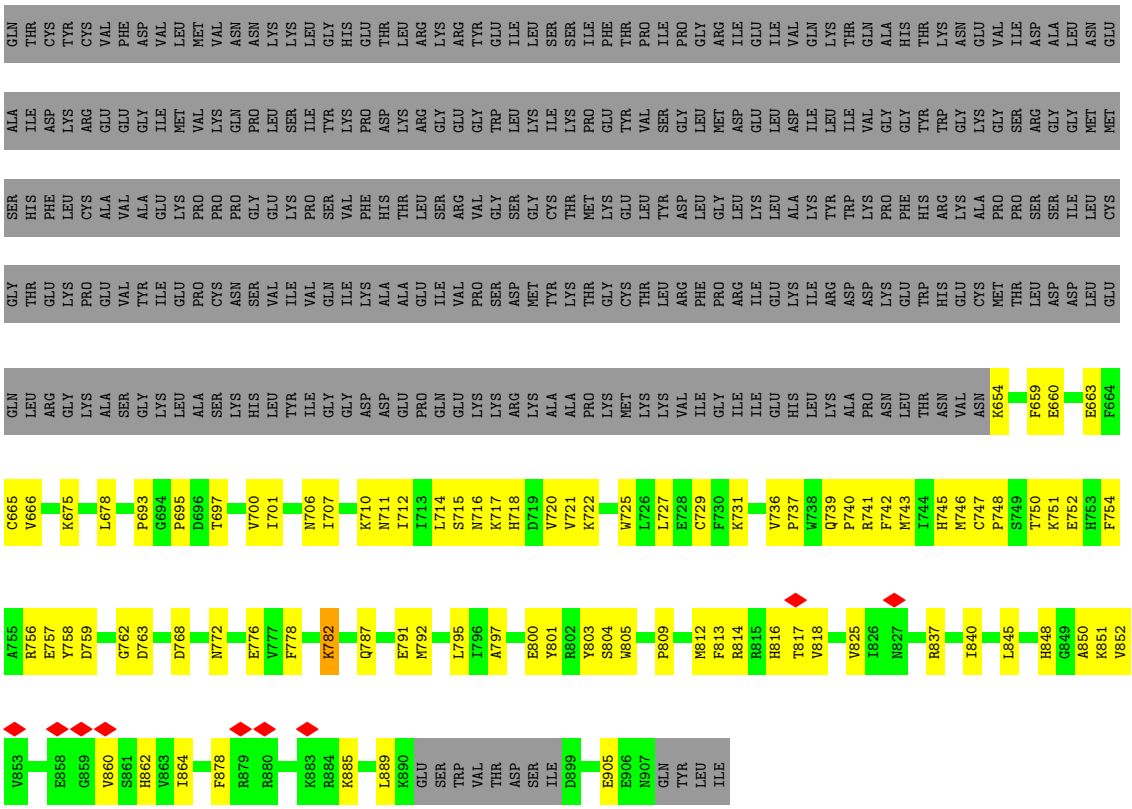




• Molecule 6: DNA ligase 4

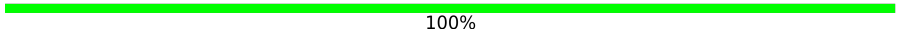
Chain R:





• Molecule 7: DNA (25-MER)

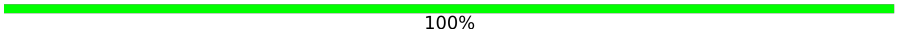
Chain j:



There are no outlier residues recorded for this chain.

• Molecule 8: DNA (27-MER)

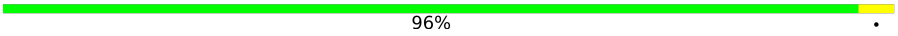
Chain i:



There are no outlier residues recorded for this chain.

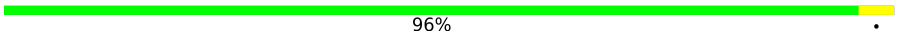
• Molecule 9: DNA (26-MER)

Chain d:



• Molecule 10: DNA (28-MER)

Chain e:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	35211	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 ($e^-/Å^2$)	52.1	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.940	Depositor
Minimum map value	-0.499	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.061	Depositor
Map size (Å)	704.16003, 704.16003, 704.16003	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.304, 1.304, 1.304	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.27	0/28471	0.50	0/38509
1	S	0.26	0/28549	0.49	0/38591
2	B	0.27	0/4118	0.50	0/5556
2	T	0.26	0/4092	0.50	0/5516
3	C	0.25	0/5393	0.46	0/7273
3	L	0.25	0/5272	0.47	0/7107
4	D	0.25	0/1101	0.47	0/1500
4	M	0.27	0/1223	0.51	0/1665
5	G	0.24	0/1657	0.47	0/2228
5	H	0.24	0/1616	0.45	0/2170
5	P	0.24	0/1657	0.46	0/2228
5	Q	0.24	0/1616	0.45	0/2170
6	I	0.25	0/2021	0.49	0/2727
6	R	0.24	0/1999	0.49	0/2697
7	j	0.53	0/570	1.03	0/876
8	i	0.60	0/620	0.99	0/953
9	d	0.63	0/591	1.05	1/908 (0.1%)
10	e	0.56	0/644	0.96	1/990 (0.1%)
All	All	0.27	0/91210	0.51	2/123664 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	e	39	DA	O4'-C4'-C3'	-5.48	102.31	104.50
9	d	19	DA	O4'-C4'-C3'	-5.10	102.46	104.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	27927	0	27803	1226	0
1	S	27999	0	28062	1170	0
2	B	4038	0	4071	210	0
2	T	4014	0	4065	180	0
3	C	5292	0	5264	222	0
3	L	5174	0	5164	215	0
4	D	1075	0	1060	20	0
4	M	1195	0	1157	21	0
5	G	1628	0	1620	45	0
5	H	1589	0	1587	35	0
5	P	1628	0	1620	22	0
5	Q	1589	0	1587	23	0
6	I	1977	0	1923	91	0
6	R	1958	0	1905	72	0
7	j	509	0	271	0	0
8	i	552	0	301	0	0
9	d	528	0	282	0	0
10	e	573	0	312	0	0
All	All	89245	0	88054	3398	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 20.

All (3398) 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)
6:R:814:ARG:H	6:R:850:ALA:H	1.08	0.95
2:T:318:ARG:HB2	2:T:329:LEU:O	1.68	0.94
1:A:174:VAL:O	1:A:177:LEU:HB2	1.69	0.92
2:T:400:TYR:O	2:T:408:PRO:HA	1.68	0.92
1:A:67:VAL:HB	1:A:85:ILE:HD13	1.54	0.89
1:A:3510:GLN:HB3	1:A:3515:GLN:HE22	1.38	0.86
1:S:73:LEU:H	1:S:82:ARG:HH22	1.21	0.86
1:S:4090:ARG:HH22	1:S:4106:CYS:HA	1.40	0.86
1:A:2254:ARG:NH2	1:A:2292:CYS:SG	2.49	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3464:LYS:HD2	1:A:3997:LEU:HD11	1.60	0.84
1:S:3580:ASN:H	1:S:3734:ARG:HH22	1.23	0.84
1:A:1228:GLY:HA2	1:A:1256:TRP:HE1	1.42	0.83
1:A:2121:ASP:HB3	1:A:2127:LYS:HG2	1.59	0.83
1:S:2225:HIS:HB2	1:S:2231:PHE:HB2	1.61	0.82
6:I:814:ARG:H	6:I:850:ALA:H	1.24	0.82
1:S:380:ASP:O	1:S:383:PHE:HB3	1.80	0.82
6:R:814:ARG:H	6:R:850:ALA:N	1.77	0.81
2:B:407:PRO:HG2	3:C:486:ARG:HE	1.46	0.80
2:T:260:LYS:HG2	2:T:268:VAL:HG12	1.64	0.80
1:A:1076:LEU:HB3	1:A:1123:THR:HG22	1.64	0.80
1:S:3266:SER:HB3	1:S:3273:LEU:HA	1.63	0.80
1:S:360:SER:HA	1:S:363:ILE:HD12	1.64	0.80
1:S:71:LYS:HB3	1:S:82:ARG:HH21	1.47	0.79
1:S:2254:ARG:HE	1:S:2294:ILE:HG13	1.45	0.79
2:T:171:ASN:HB3	2:T:205:LEU:HB3	1.65	0.79
1:S:901:MET:HG2	1:S:903:PRO:HD3	1.63	0.79
1:A:1848:ILE:HG12	1:A:1915:LEU:HD11	1.65	0.78
4:M:7:PRO:HB3	4:M:77:ARG:HE	1.48	0.78
1:A:2291:GLN:NE2	1:A:2292:CYS:SG	2.57	0.78
2:B:291:GLU:HB3	6:I:690:VAL:HG23	1.64	0.78
3:L:297:LEU:HD12	3:L:303:THR:HB	1.66	0.78
1:S:1104:LEU:HD23	1:S:1134:LEU:HD13	1.66	0.78
1:A:972:LEU:HD22	1:A:984:TYR:HE2	1.48	0.78
1:A:1917:LYS:HE3	3:L:726:ASP:HA	1.65	0.78
1:A:4008:GLU:HG3	1:A:4011:PHE:HB2	1.66	0.77
1:S:2785:ILE:HD12	1:S:2790:LEU:HD21	1.67	0.77
1:S:2399:GLU:HA	1:S:2402:LEU:HD23	1.66	0.77
1:A:114:VAL:HA	1:A:119:ARG:HH21	1.49	0.76
1:A:1017:ILE:HG21	1:A:1066:LEU:HD21	1.67	0.76
1:S:3809:THR:OG1	1:S:3929:MET:SD	2.41	0.76
1:A:1261:LEU:HD11	1:A:1337:VAL:HG22	1.67	0.76
1:S:1848:ILE:HG12	1:S:1915:LEU:HD11	1.67	0.76
1:S:3915:HIS:HB2	1:S:3920:ILE:HB	1.68	0.76
1:S:3090:TYR:HB3	1:S:3095:ASP:HB2	1.67	0.76
5:H:159:GLN:HG3	6:I:843:LEU:HD21	1.68	0.76
1:S:1300:SER:HA	1:S:1304:HIS:HB2	1.66	0.75
1:A:3929:MET:HG2	1:A:3940:ILE:HG13	1.68	0.75
6:R:800:GLU:HA	6:R:805:TRP:HB2	1.68	0.75
2:B:95:ASN:HD21	2:B:99:PHE:H	1.34	0.75
1:A:1201:ASN:HD21	1:A:1206:LEU:HB2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:736:LEU:HB3	1:S:740:ILE:HD11	1.69	0.74
2:B:213:ILE:HG12	2:B:231:VAL:HA	1.69	0.74
1:S:364:ARG:HA	1:S:415:GLN:HE22	1.52	0.74
3:L:689:GLU:HA	3:L:695:SER:HB3	1.69	0.74
3:L:20:MET:HB2	3:L:30:PRO:HB2	1.70	0.74
1:S:531:PHE:HA	1:S:534:LEU:HB2	1.70	0.74
1:A:1145:LEU:HB3	1:A:1165:LEU:HB2	1.70	0.74
1:S:1023:SER:HA	1:S:1026:ARG:HE	1.51	0.74
1:A:990:GLN:HB3	1:A:2781:PRO:HD3	1.70	0.74
1:A:1196:PRO:HG3	1:A:1203:SER:HB2	1.68	0.74
2:B:230:ARG:HG3	2:B:232:HIS:H	1.51	0.74
1:S:2424:MET:O	1:S:2432:GLN:NE2	2.20	0.74
1:A:935:HIS:HD2	1:A:987:LEU:HD11	1.54	0.73
1:S:753:GLN:NE2	1:S:791:ASP:O	2.21	0.73
2:T:34:GLY:HA2	2:T:160:LYS:HG3	1.69	0.73
2:B:318:ARG:HH22	2:B:331:LYS:HA	1.53	0.73
2:T:74:LYS:HZ3	2:T:81:ASP:H	1.36	0.73
1:S:67:VAL:HB	1:S:71:LYS:HD3	1.71	0.73
1:S:4055:ASN:HB2	1:S:4095:GLU:HA	1.71	0.73
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.22	0.72
1:S:3357:ARG:O	1:S:3360:LEU:HB3	1.88	0.72
6:I:800:GLU:HA	6:I:805:TRP:HB2	1.70	0.72
2:T:218:ARG:HH22	2:T:229:LEU:HA	1.53	0.72
3:C:139:SER:HB3	3:C:201:GLN:HE21	1.54	0.72
1:A:76:ILE:O	1:A:79:ARG:N	2.22	0.72
1:S:1107:TYR:HD2	1:S:1134:LEU:HD11	1.54	0.72
2:T:173:ASP:HB2	2:T:216:PHE:HB3	1.69	0.72
1:A:2317:ALA:HA	1:A:2366:LYS:HE3	1.72	0.72
1:S:1372:LEU:O	1:S:1375:THR:HB	1.89	0.72
1:A:2380:ASN:ND2	2:B:192:ASP:OD1	2.21	0.72
1:A:128:LEU:HA	1:A:173:LYS:HZ1	1.55	0.71
3:L:328:GLU:OE2	2:T:486:HIS:ND1	2.23	0.71
2:B:474:ARG:NH1	2:B:475:SER:OG	2.23	0.71
5:Q:33:VAL:HG22	5:Q:46:THR:HG22	1.71	0.71
1:S:3835:PRO:HA	1:S:3839:TYR:HB2	1.70	0.71
1:S:1915:LEU:HD13	1:S:1918:LEU:HD12	1.71	0.71
1:S:3506:LEU:HD21	1:S:3554:PHE:HB2	1.72	0.71
1:A:82:ARG:HA	1:A:85:ILE:HD12	1.71	0.71
6:I:814:ARG:H	6:I:850:ALA:N	1.87	0.71
1:A:879:MET:HG3	1:A:881:LYS:H	1.55	0.71
1:S:754:MET:HA	1:S:757:LYS:HG2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1368:LEU:HB3	1:S:1372:LEU:HD23	1.71	0.71
2:B:346:MET:HB3	2:B:399:ARG:HB3	1.71	0.71
1:A:1514:LEU:HA	1:A:1517:LEU:HD12	1.72	0.71
2:B:263:LEU:HB2	2:B:267:ILE:HB	1.72	0.71
1:A:1452:VAL:HG22	1:A:1517:LEU:HD11	1.71	0.71
1:A:2228:ARG:HA	1:A:2231:PHE:HB3	1.71	0.71
1:S:3677:PRO:HB2	1:S:3682:GLU:HB2	1.73	0.70
1:S:2375:ALA:HB3	1:S:2404:ARG:HD3	1.71	0.70
1:A:469:ALA:HA	1:A:475:LEU:HD12	1.74	0.70
1:A:1915:LEU:HD13	1:A:1918:LEU:HD12	1.73	0.70
1:A:3493:TRP:H	1:A:3709:GLY:HA2	1.57	0.70
5:H:99:LYS:HE2	5:H:108:LEU:HB3	1.73	0.70
1:S:131:LEU:HD22	1:S:177:LEU:HD11	1.73	0.70
1:A:972:LEU:HD22	1:A:984:TYR:CE2	2.27	0.70
1:A:2287:PRO:HB3	1:A:2326:ILE:HD12	1.73	0.70
1:S:863:GLY:HA3	1:S:3168:TYR:HB2	1.71	0.70
1:A:3171:ALA:HA	1:A:3179:TRP:HZ2	1.57	0.70
1:S:1184:ARG:NH2	1:S:1262:ALA:O	2.24	0.70
1:S:867:ASN:HB3	1:S:3129:LEU:HD13	1.74	0.70
1:S:3236:PHE:HD2	1:S:3269:ARG:HH22	1.40	0.70
1:S:1000:LYS:HG3	1:S:1004:GLN:HE21	1.56	0.70
2:B:299:LYS:HB2	2:B:301:ARG:HH21	1.56	0.69
1:S:2776:ARG:NH2	1:S:2782:ASP:OD2	2.25	0.69
1:S:3796:MET:H	1:S:3801:GLY:HA2	1.55	0.69
1:A:2514:ASN:HD22	1:A:2517:LEU:HG	1.58	0.69
5:G:161:ARG:HH22	6:I:847:PHE:HB3	1.57	0.69
1:A:3281:CYS:O	1:A:3285:HIS:ND1	2.25	0.69
3:C:680:GLN:NE2	3:C:681:ASP:OD2	2.25	0.69
3:L:188:HIS:HE1	3:L:478:PRO:HD2	1.57	0.69
3:L:327:ASP:OD1	6:R:711:ASN:ND2	2.21	0.69
1:S:2254:ARG:HH22	1:S:2292:CYS:HB2	1.55	0.69
3:C:647:ILE:HA	3:C:652:GLU:HG2	1.75	0.69
3:L:605:LYS:HB2	3:L:609:PHE:HZ	1.57	0.69
1:A:755:ALA:O	1:A:759:GLY:N	2.25	0.69
1:A:3444:ALA:HB1	1:A:3482:LEU:HD21	1.74	0.69
1:A:3838:GLU:HG2	1:A:4122:GLU:HB3	1.74	0.69
1:S:36:ARG:O	1:S:40:GLN:NE2	2.26	0.69
2:T:171:ASN:HB2	2:T:207:LYS:HB2	1.74	0.69
1:S:2278:GLY:O	1:S:2282:ALA:N	2.25	0.69
1:A:741:ILE:HG23	1:A:748:TYR:HD2	1.58	0.69
5:P:179:ARG:NH2	6:R:804:SER:OG	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2869:LEU:HB2	1:S:2899:ARG:HH21	1.58	0.69
1:S:2962:ARG:NH2	1:S:2967:GLU:OE1	2.26	0.69
5:G:147:GLU:OE1	5:H:148:ASN:ND2	2.25	0.69
1:S:645:TRP:O	1:S:649:PHE:HB3	1.92	0.69
1:A:998:ASN:OD1	1:A:999:LYS:NZ	2.26	0.69
6:R:666:VAL:HA	6:R:701:ILE:HB	1.73	0.69
1:S:3244:ASP:OD1	1:S:3282:ARG:NH2	2.26	0.69
1:S:2893:LEU:HD22	1:S:2926:LEU:HG	1.75	0.68
5:G:161:ARG:NH1	5:G:165:CYS:SG	2.66	0.68
1:A:935:HIS:CD2	1:A:987:LEU:HD11	2.28	0.68
1:A:1685:ASP:HB3	1:A:1688:LEU:HG	1.74	0.68
2:T:81:ASP:O	2:T:110:ASN:ND2	2.26	0.68
1:A:2527:HIS:HB3	1:A:2530:ARG:HD3	1.75	0.68
6:I:665:CYS:HB3	6:I:700:VAL:HA	1.76	0.68
1:A:38:LEU:HD11	1:A:85:ILE:HG13	1.75	0.68
3:C:93:ASP:HA	3:C:97:LYS:HG2	1.76	0.68
5:H:41:SER:HA	5:H:123:ILE:HD11	1.74	0.68
1:A:3256:MET:SD	1:A:3287:ARG:NH2	2.66	0.68
1:A:2391:GLY:O	1:A:2431:ARG:NH2	2.27	0.68
1:A:3266:SER:HA	1:A:3272:TRP:CD1	2.29	0.68
6:R:695:PRO:HA	6:R:717:LYS:HZ1	1.59	0.68
1:S:916:GLU:HA	1:S:919:LEU:HB3	1.74	0.68
1:A:1477:HIS:HB3	1:A:1481:THR:HG23	1.76	0.68
3:L:18:PHE:HB2	3:L:102:SER:HA	1.76	0.68
1:A:1183:CYS:SG	1:A:1186:LYS:NZ	2.67	0.68
1:A:2278:GLY:O	1:A:2282:ALA:N	2.24	0.68
1:S:2354:ASN:ND2	1:S:2357:GLU:OE2	2.26	0.68
1:A:919:LEU:HD22	1:A:972:LEU:HD12	1.75	0.67
1:S:2383:PHE:HB3	1:S:2418:LYS:HE3	1.76	0.67
6:I:666:VAL:HA	6:I:701:ILE:HB	1.76	0.67
1:A:1820:VAL:HA	1:A:1824:LEU:HD23	1.77	0.67
1:A:2920:VAL:HG12	1:A:2947:ILE:HG23	1.77	0.67
1:S:2416:LYS:NZ	2:T:97:VAL:O	2.27	0.67
1:A:63:PHE:O	1:A:67:VAL:HG12	1.94	0.67
1:A:2357:GLU:HA	1:A:2360:PHE:HB3	1.75	0.67
3:L:6:ASN:HB3	3:L:128:GLU:HB2	1.76	0.67
1:S:73:LEU:H	1:S:82:ARG:NH2	1.92	0.67
1:S:3110:PHE:HD1	1:S:3128:LYS:HZ3	1.43	0.67
1:A:2375:ALA:HB3	1:A:2404:ARG:HD3	1.77	0.67
1:S:1751:GLU:O	1:S:1754:GLN:NE2	2.27	0.67
2:T:191:GLY:HA2	2:T:194:ARG:HE	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:95:ASN:HD21	2:T:99:PHE:H	1.40	0.67
1:A:10:CYS:SG	1:A:11:SER:N	2.68	0.67
2:B:294:GLU:HB3	3:C:298:ASN:HD21	1.60	0.67
3:C:272:VAL:HG22	3:C:274:LYS:H	1.60	0.67
3:L:423:GLN:NE2	3:L:424:LEU:O	2.28	0.67
1:A:1483:LEU:HD21	1:A:1515:LEU:HD23	1.76	0.67
1:A:3750:PHE:HB3	1:A:3802:LEU:HD11	1.75	0.67
6:I:663:GLU:HB3	6:I:697:THR:HA	1.77	0.67
3:L:7:LYS:O	3:L:128:GLU:N	2.27	0.67
1:S:1750:LEU:HD21	1:S:1759:LEU:HD23	1.77	0.67
6:I:813:PHE:HA	6:I:850:ALA:O	1.95	0.66
4:M:186:ILE:HG13	2:T:242:LEU:HD23	1.77	0.66
1:S:2090:ARG:NH2	1:S:2091:HIS:O	2.28	0.66
1:S:2372:PRO:O	1:S:2404:ARG:NH1	2.28	0.66
1:A:188:GLU:O	1:A:192:ASN:ND2	2.28	0.66
1:A:332:GLU:OE2	1:A:336:ASN:ND2	2.28	0.66
1:S:139:ARG:HA	1:S:142:ARG:HH21	1.59	0.66
1:S:2208:ASP:OD1	1:S:2209:GLU:N	2.28	0.66
1:S:2824:LYS:O	1:S:2829:LYS:NZ	2.27	0.66
1:A:933:LEU:HD22	1:A:2797:VAL:HG21	1.77	0.66
1:A:2362:VAL:HG12	1:A:2366:LYS:HZ2	1.61	0.66
1:A:174:VAL:HA	1:A:177:LEU:HD23	1.78	0.66
3:C:687:THR:HB	3:C:699:GLU:HG3	1.78	0.66
3:L:291:LYS:NZ	3:L:292:GLU:O	2.29	0.66
1:S:1651:LYS:HD2	1:S:1654:GLN:HE21	1.61	0.66
1:A:1725:GLN:HE22	1:A:1769:GLU:HB2	1.61	0.66
5:H:87:ASN:HB3	5:H:97:PHE:HA	1.76	0.66
1:S:3506:LEU:HD22	1:S:3555:VAL:HG13	1.76	0.66
1:A:168:ASP:H	1:A:171:LEU:HD12	1.61	0.66
1:A:3625:LEU:HD22	1:A:3630:ARG:HE	1.61	0.66
3:C:727:ASP:OD2	1:S:1960:LYS:NZ	2.26	0.66
1:A:71:LYS:O	1:A:73:LEU:N	2.29	0.66
1:S:90:CYS:HA	1:S:136:GLN:HE22	1.60	0.66
3:C:368:ARG:HE	3:C:369:ASP:H	1.44	0.66
1:S:50:VAL:HG13	1:S:51:LEU:HG	1.76	0.66
1:A:2395:THR:OG1	1:A:2431:ARG:NE	2.28	0.66
1:S:175:TYR:HB2	1:S:223:CYS:HB3	1.77	0.66
1:A:1000:LYS:HA	1:A:1004:GLN:HE21	1.61	0.66
1:A:3142:ILE:O	1:A:3147:LYS:NZ	2.28	0.66
1:A:3758:LEU:HB2	1:A:3795:PRO:HB3	1.78	0.66
1:A:3806:LEU:HD23	1:A:3808:ASN:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:75:ARG:NH2	4:M:103:SER:O	2.29	0.66
1:A:527:TYR:O	1:A:530:LEU:HB3	1.96	0.65
1:A:1279:LEU:HD22	1:A:1356:TRP:HE1	1.60	0.65
1:A:1727:ARG:HH12	1:A:1772:HIS:HB2	1.61	0.65
2:B:272:GLY:N	2:B:369:TYR:O	2.28	0.65
1:A:1052:SER:O	1:A:1055:ASN:ND2	2.28	0.65
3:C:407:VAL:HB	3:C:424:LEU:HD11	1.78	0.65
4:D:11:LEU:HD13	4:D:87:LEU:HD22	1.77	0.65
1:A:1673:THR:HA	1:A:1676:ILE:HD12	1.78	0.65
1:S:1037:LEU:HD11	1:S:1056:THR:HG22	1.79	0.65
1:A:1326:GLU:HG3	1:A:1329:ARG:HG2	1.78	0.65
1:A:3720:ALA:HB3	1:A:3743:HIS:HA	1.77	0.65
1:S:469:ALA:HA	1:S:475:LEU:HD12	1.76	0.65
1:S:974:CYS:HB3	1:S:1028:PHE:HD2	1.61	0.65
1:A:2331:MET:O	1:A:2334:LYS:NZ	2.28	0.65
2:B:468:LYS:O	2:B:517:ARG:NE	2.29	0.65
3:C:678:VAL:O	3:C:682:GLY:N	2.29	0.65
1:A:1568:ASN:HA	1:A:1600:MET:HE2	1.78	0.65
1:A:2333:ARG:HH12	1:A:2371:PHE:HE1	1.43	0.65
1:A:978:GLN:HE22	1:A:2597:PHE:HA	1.60	0.65
1:A:1382:ILE:HD11	1:A:1385:ASN:HD22	1.62	0.65
1:A:3585:PHE:HE2	1:A:3664:ASN:HA	1.62	0.65
2:B:121:GLN:O	2:B:130:ARG:NH1	2.30	0.65
1:A:1407:LYS:HA	1:A:1412:LYS:HD2	1.78	0.65
1:A:1726:SER:OG	1:A:1727:ARG:NH1	2.29	0.65
3:L:268:LEU:O	2:T:444:ARG:NH2	2.30	0.65
1:S:1910:GLU:O	1:S:1913:LYS:NZ	2.30	0.65
1:S:3163:THR:O	1:S:3167:ARG:NH1	2.29	0.65
2:T:88:TYR:HH	2:T:170:THR:HG1	1.43	0.65
1:A:925:GLN:HG3	1:A:2800:ARG:HH12	1.63	0.65
1:A:3422:GLN:OE1	1:A:3423:GLN:NE2	2.30	0.65
1:S:174:VAL:HA	1:S:177:LEU:HD12	1.79	0.65
1:S:2401:VAL:O	1:S:2441:LYS:NZ	2.30	0.65
1:A:2196:TRP:HB2	1:A:2199:LEU:HB2	1.77	0.64
3:L:313:GLY:N	2:T:286:ILE:O	2.29	0.64
1:S:2252:PRO:O	1:S:2291:GLN:NE2	2.30	0.64
1:S:2388:LYS:NZ	2:T:157:VAL:O	2.28	0.64
1:S:3741:ARG:HA	1:S:3747:GLU:HA	1.79	0.64
1:A:1649:LEU:HD13	1:A:1652:ILE:HD11	1.80	0.64
2:B:218:ARG:HA	2:B:221:ILE:HG12	1.79	0.64
3:C:688:LYS:NZ	3:C:695:SER:OG	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2161:ALA:HA	1:A:2164:TRP:HB2	1.79	0.64
3:L:315:ARG:HH11	3:L:320:ILE:HG13	1.62	0.64
1:S:915:THR:HA	1:S:934:LEU:HD11	1.79	0.64
1:S:2135:ASN:ND2	1:S:2137:ILE:O	2.31	0.64
1:A:1488:TYR:HD1	1:A:1559:PHE:HZ	1.45	0.64
4:M:24:CYS:HB3	4:M:39:LEU:HD23	1.79	0.64
2:T:76:ILE:HG21	2:T:247:ARG:HA	1.77	0.64
1:A:1611:GLN:HE21	1:A:1614:GLN:HG2	1.62	0.64
3:L:308:GLU:O	2:T:290:ARG:NH2	2.29	0.64
1:S:919:LEU:HG	1:S:920:THR:HG23	1.79	0.64
1:A:3380:ARG:O	1:A:3384:HIS:ND1	2.31	0.64
3:C:6:ASN:HB3	3:C:128:GLU:HB2	1.78	0.64
3:L:44:ARG:NH2	3:L:45:GLN:OE1	2.30	0.64
1:S:3675:LYS:NZ	1:S:3676:PRO:O	2.31	0.64
1:S:4083:GLY:HA3	1:S:4088:ASN:HB3	1.77	0.64
1:A:71:LYS:HA	1:A:78:PHE:CG	2.32	0.64
1:A:637:LYS:O	1:A:679:LYS:NZ	2.30	0.64
6:I:814:ARG:N	6:I:850:ALA:H	1.94	0.64
2:T:513:ALA:HB1	2:T:517:ARG:HH12	1.63	0.64
1:A:3958:LEU:HG	1:A:4115:ASN:HD22	1.63	0.64
1:A:2869:LEU:O	1:A:2899:ARG:NH1	2.31	0.64
2:B:210:GLY:HA2	2:B:233:PHE:HA	1.80	0.64
1:S:128:LEU:HD11	1:S:170:VAL:HB	1.80	0.64
1:S:2532:PRO:O	1:S:2538:ARG:NH1	2.30	0.64
1:S:1397:ASP:OD1	1:S:1398:VAL:N	2.30	0.64
1:S:3369:ASP:OD2	1:S:3372:LYS:NZ	2.31	0.64
1:A:2466:SER:OG	1:A:2469:CYS:SG	2.55	0.63
3:C:676:GLU:HG3	3:C:677:ILE:HD12	1.80	0.63
1:S:174:VAL:O	1:S:177:LEU:HB2	1.98	0.63
1:A:675:ARG:NH1	1:A:735:SER:O	2.29	0.63
1:A:3581:PRO:HB3	1:A:3629:ARG:HG3	1.79	0.63
1:A:3822:GLN:HA	1:A:3825:LYS:HB3	1.80	0.63
3:L:522:VAL:HA	3:L:525:LYS:HD2	1.80	0.63
1:S:1425:ALA:HB2	1:S:1467:ILE:HG13	1.79	0.63
1:S:3620:PRO:O	1:S:3630:ARG:NH1	2.31	0.63
1:S:3996:GLY:O	1:S:4000:ASN:ND2	2.31	0.63
2:T:418:GLU:HB2	2:T:430:PRO:HB3	1.80	0.63
1:A:487:LEU:HD11	1:A:575:ILE:HG21	1.79	0.63
1:A:538:ASP:HA	1:A:541:MET:HG3	1.79	0.63
1:A:2168:LEU:HA	1:A:2171:LEU:HD12	1.80	0.63
2:B:173:ASP:HB2	2:B:216:PHE:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:816:HIS:N	6:I:851:LYS:H	1.95	0.63
3:L:497:ARG:HD3	3:L:501:PRO:HA	1.80	0.63
1:S:529:ASP:OD1	1:S:530:LEU:N	2.32	0.63
1:S:2425:ARG:NH1	1:S:2457:PRO:O	2.32	0.63
1:S:2595:TRP:O	1:S:2765:GLN:NE2	2.31	0.63
1:S:3730:ALA:HA	1:S:3734:ARG:HA	1.80	0.63
1:A:406:ARG:O	1:A:409:GLN:NE2	2.31	0.63
3:L:643:ARG:NH2	3:L:656:ASN:OD1	2.31	0.63
1:S:3069:MET:HA	1:S:3075:LYS:HB2	1.79	0.63
1:S:3176:MET:HA	1:S:3179:TRP:HB2	1.79	0.63
1:A:1538:LEU:N	1:A:1553:PHE:O	2.27	0.63
1:A:2935:GLU:HG3	1:A:2938:VAL:HG22	1.81	0.63
5:G:22:VAL:HG21	5:G:71:ARG:HH22	1.61	0.63
6:I:746:MET:O	6:I:751:LYS:NZ	2.30	0.63
3:L:636:ILE:O	3:L:640:ARG:HG2	1.98	0.63
6:R:818:VAL:H	6:R:851:LYS:HB3	1.63	0.63
1:S:4055:ASN:HD21	1:S:4091:ALA:HB1	1.62	0.63
1:A:1949:ILE:HD13	1:A:2096:PRO:HB2	1.80	0.63
1:A:3236:PHE:HD2	1:A:3269:ARG:HH22	1.47	0.63
6:R:715:SER:O	6:R:745:HIS:NE2	2.32	0.63
1:S:28:ALA:O	1:S:32:HIS:ND1	2.32	0.63
1:S:261:ASP:HB3	1:S:265:TYR:HA	1.81	0.63
1:S:2281:MET:HE3	1:S:2329:TYR:HB2	1.80	0.63
1:S:2924:VAL:HG11	1:S:2989:ALA:HB1	1.80	0.63
1:S:3962:ARG:HH22	1:S:4125:GLU:HB3	1.64	0.63
1:A:2376:ASP:OD1	1:A:2377:ARG:NH1	2.31	0.63
1:A:3090:TYR:HB3	1:A:3095:ASP:HB2	1.80	0.63
3:L:250:ARG:HH22	2:T:536:PRO:HB2	1.63	0.63
1:S:2723:THR:HA	1:S:2726:LEU:HD13	1.81	0.63
2:B:91:GLU:OE1	2:B:137:HIS:N	2.32	0.63
5:H:175:ASP:OD2	6:I:783:ASN:ND2	2.32	0.63
3:L:521:GLU:HG3	3:L:525:LYS:HE3	1.80	0.63
1:S:2339:GLU:OE2	1:S:2377:ARG:NH2	2.31	0.63
1:S:3000:ASP:O	1:S:3004:HIS:ND1	2.31	0.63
1:A:2348:GLN:OE1	1:A:2353:GLN:NE2	2.32	0.62
1:S:2253:TYR:H	1:S:2256:ILE:HD13	1.63	0.62
1:A:1795:VAL:HG23	1:A:1835:ALA:HB1	1.81	0.62
1:A:3369:ASP:OD2	1:A:3372:LYS:NZ	2.31	0.62
3:C:65:ASP:HB3	3:C:78:THR:HG23	1.80	0.62
6:I:816:HIS:H	6:I:850:ALA:HA	1.64	0.62
3:L:344:GLY:HA3	2:T:471:PHE:HE1	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:814:ARG:N	6:R:850:ALA:H	1.90	0.62
1:S:893:SER:O	1:S:944:LYS:NZ	2.29	0.62
1:A:736:LEU:HD12	1:A:740:ILE:HG21	1.81	0.62
1:A:1603:GLN:OE1	1:A:1606:ARG:NH2	2.32	0.62
6:R:663:GLU:HB3	6:R:697:THR:HA	1.82	0.62
1:S:1490:GLY:O	1:S:1502:SER:N	2.31	0.62
1:S:3603:LYS:H	1:S:3606:ILE:HB	1.64	0.62
1:A:139:ARG:HA	1:A:142:ARG:HH21	1.64	0.62
1:A:3945:ALA:HB3	1:A:3948:SER:HB3	1.81	0.62
2:B:171:ASN:HB2	2:B:207:LYS:HB2	1.81	0.62
1:S:850:GLU:HB2	1:S:854:ARG:HH21	1.64	0.62
1:S:1583:MET:HG2	1:S:1625:HIS:HB3	1.81	0.62
1:S:2512:ASP:N	1:S:2518:GLN:OE1	2.33	0.62
1:S:3052:LEU:HD11	1:S:3061:LEU:HD21	1.80	0.62
1:S:3239:LYS:HA	1:S:3242:MET:HE2	1.81	0.62
1:S:3266:SER:HA	1:S:3272:TRP:CD1	2.35	0.62
2:T:260:LYS:HG2	2:T:268:VAL:CG1	2.30	0.62
1:A:762:TYR:HD2	1:A:765:LEU:HG	1.64	0.62
1:A:1594:SER:O	1:A:1598:ASN:ND2	2.33	0.62
1:A:3266:SER:HB3	1:A:3273:LEU:HA	1.82	0.62
1:A:3725:ARG:HB3	1:A:3739:ILE:HD12	1.80	0.62
5:H:37:THR:HG22	5:H:39:GLY:H	1.64	0.62
6:I:798:ASP:HB3	6:I:802:ARG:HH12	1.65	0.62
1:S:3193:ILE:HD13	1:S:3196:LYS:HZ3	1.63	0.62
1:A:67:VAL:CB	1:A:85:ILE:HD13	2.26	0.62
1:A:1512:SER:HA	1:A:1515:LEU:HD12	1.82	0.62
3:L:62:ASP:HA	3:L:103:GLN:HG2	1.81	0.62
1:S:2586:PHE:HB3	1:S:2776:ARG:HB3	1.80	0.62
1:A:767:GLU:OE1	1:A:854:ARG:NE	2.33	0.62
1:A:1396:PRO:HB3	1:A:1457:GLN:HE21	1.64	0.62
6:I:884:ARG:HE	6:I:886:PHE:HE1	1.46	0.62
1:S:87:LYS:HE3	1:S:831:LEU:HB2	1.82	0.62
1:A:1605:PHE:O	1:A:1608:ARG:NH2	2.33	0.62
2:B:479:GLU:HA	3:C:426:PHE:HB3	1.82	0.62
3:L:269:GLN:O	3:L:271:ARG:NH1	2.33	0.62
1:S:390:GLN:HE22	1:S:1737:ASN:HB2	1.65	0.62
1:S:782:ARG:HH11	1:S:786:GLN:HB2	1.65	0.62
1:A:645:TRP:HB3	1:A:649:PHE:HB2	1.81	0.62
3:C:246:HIS:HB2	3:C:262:ALA:HB1	1.81	0.62
5:H:4:LYS:HG2	5:H:75:LEU:HA	1.81	0.62
3:L:13:CYS:HB3	3:L:134:ILE:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:91:GLU:N	4:M:91:GLU:OE1	2.32	0.62
6:R:746:MET:O	6:R:751:LYS:NZ	2.33	0.62
1:S:3119:VAL:HA	1:S:3125:ARG:HE	1.64	0.62
1:S:3172:LYS:HD2	1:S:3248:LYS:HB3	1.80	0.62
1:S:3680:LEU:HD12	1:S:3724:GLU:HB3	1.81	0.62
1:A:1019:ASP:O	1:A:1026:ARG:NH2	2.32	0.61
1:A:2365:ASN:HD22	1:A:2396:LEU:HG	1.65	0.61
2:B:59:PRO:HA	2:B:62:MET:SD	2.40	0.61
1:S:1011:GLU:HA	1:S:1014:LEU:HG	1.80	0.61
1:S:4041:ARG:HA	1:S:4044:ILE:HG12	1.80	0.61
1:A:477:ASN:OD1	1:A:478:CYS:N	2.32	0.61
1:A:1412:LYS:O	1:A:1416:GLU:N	2.25	0.61
1:A:2372:PRO:O	1:A:2404:ARG:NH1	2.33	0.61
6:R:654:LYS:N	6:R:660:GLU:OE2	2.33	0.61
1:S:477:ASN:OD1	1:S:478:CYS:N	2.33	0.61
1:S:675:ARG:HA	1:S:678:LYS:HE2	1.82	0.61
1:A:337:LYS:HG2	1:A:369:PHE:HZ	1.66	0.61
1:A:802:THR:OG1	1:A:852:ARG:NH2	2.33	0.61
1:A:1505:LEU:HA	1:A:1508:LYS:HE2	1.82	0.61
1:A:2484:TYR:HB3	1:A:2499:PHE:HB2	1.81	0.61
2:B:165:ARG:NH1	4:D:185:LEU:O	2.33	0.61
1:S:832:LYS:HG3	1:S:834:LEU:H	1.66	0.61
1:A:1102:GLU:HA	1:A:1154:PRO:HB3	1.83	0.61
1:A:1370:ARG:O	1:A:1374:GLN:NE2	2.34	0.61
1:A:2271:SER:HA	1:A:2274:ILE:HD12	1.82	0.61
1:A:3831:ASP:HB3	1:A:3832:PRO:HD3	1.83	0.61
1:S:2548:PRO:HB3	1:S:2847:THR:HA	1.82	0.61
1:A:1849:ASP:OD1	1:A:1850:VAL:N	2.33	0.61
1:A:2322:VAL:O	1:A:2326:ILE:HG12	2.01	0.61
1:A:3996:GLY:O	1:A:4000:ASN:ND2	2.32	0.61
2:B:36:ASP:OD2	2:B:165:ARG:NH2	2.33	0.61
2:B:485:GLN:O	2:B:489:ASN:ND2	2.33	0.61
3:C:81:ARG:NH2	3:C:85:LEU:O	2.34	0.61
2:T:105:LEU:HD23	2:T:106:GLN:HG3	1.83	0.61
1:A:889:GLU:OE2	1:A:3889:ARG:NH2	2.34	0.61
1:A:1751:GLU:O	1:A:1788:ARG:NH1	2.34	0.61
1:A:2389:PHE:HB3	1:A:2393:LEU:HB2	1.82	0.61
2:B:495:LEU:HD23	2:B:497:LEU:HD11	1.81	0.61
6:I:864:ILE:HD12	6:I:904:GLN:HB3	1.82	0.61
1:S:2313:LYS:HA	1:S:2316:TYR:CZ	2.36	0.61
1:A:1919:CYS:O	1:A:1922:ALA:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:716:ASN:HA	6:R:745:HIS:HE2	1.65	0.61
1:S:1415:LEU:O	1:S:1419:LEU:N	2.31	0.61
1:S:2223:VAL:HG22	1:S:2231:PHE:HE1	1.65	0.61
1:A:801:LYS:NZ	1:A:3114:TYR:O	2.34	0.61
1:A:850:GLU:HB2	1:A:854:ARG:HH12	1.65	0.61
2:B:428:THR:HG23	3:C:354:ARG:HH12	1.64	0.61
3:C:643:ARG:NH2	3:C:687:THR:O	2.34	0.61
3:C:687:THR:HG22	3:C:688:LYS:H	1.66	0.61
6:I:812:MET:N	6:I:848:HIS:HB2	2.14	0.61
1:S:1663:THR:HG22	1:S:1664:SER:H	1.65	0.61
1:S:3262:LEU:HD22	1:S:3272:TRP:HZ2	1.66	0.61
1:S:3962:ARG:NH1	1:S:4124:TRP:O	2.32	0.61
2:T:381:LEU:HD23	2:T:385:LEU:HD23	1.83	0.61
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	1.82	0.60
1:A:1156:GLY:O	1:A:1171:TRP:NE1	2.33	0.60
1:A:1722:PHE:O	1:A:1768:ARG:NH1	2.31	0.60
1:A:2367:VAL:O	1:A:2371:PHE:N	2.34	0.60
1:A:3628:PHE:HB2	1:A:3675:LYS:H	1.66	0.60
2:B:339:ARG:HH22	2:B:404:ARG:HB3	1.65	0.60
4:M:119:PRO:HA	4:M:122:ARG:HG2	1.83	0.60
1:A:682:TYR:O	1:A:700:LYS:NZ	2.32	0.60
1:A:2512:ASP:HB2	1:A:2518:GLN:HG2	1.83	0.60
3:C:96:SER:O	3:C:99:GLN:NE2	2.32	0.60
4:D:84:ALA:HB1	4:D:99:SER:HB2	1.82	0.60
3:L:274:LYS:NZ	2:T:321:ILE:O	2.34	0.60
1:S:1406:LEU:HD23	1:S:1415:LEU:HD22	1.83	0.60
1:S:1483:LEU:HD13	1:S:1515:LEU:HD23	1.83	0.60
1:A:1413:ASP:OD1	1:A:1414:ILE:N	2.33	0.60
1:A:1574:ASN:HD21	1:A:1577:LEU:HB2	1.66	0.60
1:A:3879:PRO:O	1:A:3965:ARG:NH1	2.28	0.60
2:B:200:LEU:HD11	2:B:221:ILE:HB	1.82	0.60
5:G:176:LEU:HA	5:G:179:ARG:HD3	1.84	0.60
6:I:660:GLU:HG2	6:I:686:GLY:HA3	1.83	0.60
3:L:261:ILE:HA	3:L:366:ALA:HA	1.83	0.60
3:L:426:PHE:HB3	2:T:479:GLU:HA	1.84	0.60
1:S:2803:ILE:O	1:S:2806:LYS:HG2	2.01	0.60
1:S:3767:LEU:HA	1:S:3770:VAL:HG22	1.82	0.60
1:A:2245:TRP:HB2	1:A:2249:LEU:HD11	1.82	0.60
1:A:2978:LYS:NZ	1:A:2980:ASP:OD1	2.34	0.60
1:S:1592:MET:N	1:S:1592:MET:SD	2.73	0.60
1:S:4121:TRP:HB3	1:S:4124:TRP:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:ASP:HA	1:A:1392:MET:HG2	1.81	0.60
4:M:193:LYS:O	2:T:244:ARG:NH1	2.31	0.60
6:R:845:LEU:HB2	6:R:852:VAL:HG12	1.84	0.60
1:S:625:ASN:O	1:S:628:GLU:HG2	2.02	0.60
1:S:1820:VAL:HA	1:S:1824:LEU:HD23	1.84	0.60
1:S:3867:THR:HA	1:S:4118:GLY:HA2	1.83	0.60
1:A:28:ALA:O	1:A:32:HIS:ND1	2.34	0.60
1:A:1650:ALA:HA	1:A:1695:LEU:HD11	1.82	0.60
1:A:2512:ASP:N	1:A:2518:GLN:OE1	2.34	0.60
1:S:29:LEU:O	1:S:33:GLN:NE2	2.34	0.60
1:S:2287:PRO:HG2	1:S:2330:VAL:HA	1.84	0.60
1:A:196:LEU:HB3	1:A:200:PHE:CZ	2.37	0.60
1:A:2371:PHE:HD2	1:A:2374:LEU:HD23	1.67	0.60
1:A:3590:ASN:OD1	1:A:3593:ARG:NH2	2.35	0.60
3:C:524:THR:HA	3:C:527:GLN:HG2	1.83	0.60
5:G:148:ASN:ND2	5:H:144:LEU:O	2.34	0.60
1:S:295:GLU:OE1	1:S:299:LYS:NZ	2.35	0.60
1:S:493:LYS:HD2	1:S:524:TYR:HD1	1.66	0.60
1:A:332:GLU:HB2	1:A:335:LYS:HD2	1.84	0.60
1:A:658:THR:OG1	1:A:659:ARG:NH1	2.35	0.60
2:B:59:PRO:HB3	2:B:205:LEU:HD23	1.84	0.60
2:B:86:VAL:HG22	2:B:104:VAL:HG23	1.84	0.60
3:C:643:ARG:NH1	3:C:656:ASN:OD1	2.30	0.60
3:L:688:LYS:HG3	3:L:695:SER:HA	1.83	0.60
1:S:1118:GLU:HG3	1:S:1121:LEU:HB2	1.84	0.60
1:A:3136:THR:HG23	1:A:3139:GLN:HE21	1.66	0.60
2:B:261:LEU:HA	2:B:345:LEU:HB2	1.84	0.60
6:R:693:PRO:HB2	6:R:718:HIS:CE1	2.36	0.60
1:S:1039:TRP:NE1	1:S:1043:GLN:OE1	2.33	0.60
1:S:1184:ARG:HH22	1:S:1265:GLU:HB3	1.67	0.60
2:B:420:LEU:HB3	2:B:424:LYS:HA	1.84	0.59
3:C:7:LYS:O	3:C:128:GLU:N	2.31	0.59
3:L:12:LEU:HD23	3:L:54:ILE:HD11	1.84	0.59
3:L:128:GLU:OE1	3:L:242:ARG:NH1	2.34	0.59
3:L:628:GLU:HG3	3:L:631:TYR:HB3	1.83	0.59
1:S:1299:GLU:O	1:S:1304:HIS:ND1	2.34	0.59
1:S:2495:SER:HA	1:S:2498:ILE:HD12	1.83	0.59
1:S:3686:TRP:HH2	1:S:3719:ILE:HG22	1.67	0.59
1:A:1369:MET:SD	1:A:1418:HIS:NE2	2.76	0.59
1:A:2310:VAL:HG21	1:A:2359:LYS:HD2	1.84	0.59
1:A:3675:LYS:NZ	1:A:3676:PRO:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:59:PHE:HB2	3:L:77:ILE:HG12	1.83	0.59
3:L:509:GLN:OE1	3:L:511:HIS:NE2	2.31	0.59
1:S:128:LEU:HD13	1:S:173:LYS:HZ1	1.67	0.59
1:S:1413:ASP:OD1	1:S:1414:ILE:N	2.33	0.59
1:A:1017:ILE:HG23	1:A:1077:GLY:HA3	1.84	0.59
1:A:1357:LYS:O	1:A:1360:LYS:HB3	2.02	0.59
1:A:1583:MET:O	1:A:1586:SER:OG	2.21	0.59
1:A:2168:LEU:HD23	1:A:2171:LEU:HD12	1.84	0.59
1:A:4086:ASP:HA	1:A:4089:ILE:HG12	1.84	0.59
2:B:34:GLY:HA3	2:B:162:SER:HB3	1.83	0.59
2:B:353:LEU:HD23	2:B:395:ALA:HB2	1.84	0.59
3:L:613:SER:O	3:L:617:ILE:HG12	2.02	0.59
1:S:763:THR:HB	1:S:851:ILE:HG13	1.83	0.59
1:S:1646:LEU:HD23	1:S:1649:LEU:HD21	1.83	0.59
1:S:3874:ARG:HD3	1:S:4126:PRO:HB2	1.84	0.59
1:A:326:MET:O	1:A:330:ASN:ND2	2.36	0.59
1:A:1675:TYR:HA	1:A:1678:LEU:HD12	1.83	0.59
1:A:1824:LEU:HD13	1:A:1827:LEU:HD21	1.83	0.59
3:L:291:LYS:NZ	2:T:301:ARG:O	2.32	0.59
5:Q:102:LYS:HD2	5:Q:103:ASP:HB2	1.85	0.59
1:S:76:ILE:O	1:S:79:ARG:N	2.34	0.59
1:S:114:VAL:HA	1:S:119:ARG:HH21	1.67	0.59
1:S:958:MET:O	1:S:962:TYR:N	2.34	0.59
1:A:225:LYS:HG2	1:A:274:LEU:HB2	1.84	0.59
1:A:635:PRO:HB3	1:A:672:ILE:HD11	1.85	0.59
1:A:863:GLY:HA3	1:A:3168:TYR:HB2	1.84	0.59
1:A:2348:GLN:OE1	1:A:2352:HIS:NE2	2.34	0.59
1:S:449:TYR:O	1:S:454:GLN:NE2	2.36	0.59
1:S:887:ASP:OD2	1:S:891:ARG:NE	2.34	0.59
1:A:420:VAL:O	1:A:424:LEU:N	2.33	0.59
1:A:1840:PHE:O	1:A:1844:VAL:HG23	2.02	0.59
1:A:2211:LEU:HD23	1:A:2214:ARG:HH22	1.67	0.59
2:B:352:PRO:HA	2:B:394:VAL:HA	1.84	0.59
1:S:1412:LYS:O	1:S:1416:GLU:N	2.27	0.59
1:S:2161:ALA:HA	1:S:2164:TRP:HB2	1.84	0.59
2:T:76:ILE:HD13	2:T:247:ARG:HG3	1.84	0.59
1:A:1066:LEU:HD23	1:A:1078:ALA:HB2	1.83	0.59
1:A:1834:ASP:OD1	1:A:1835:ALA:N	2.36	0.59
2:B:94:LYS:HE2	2:B:104:VAL:HG13	1.83	0.59
1:S:898:PHE:HB2	1:S:901:MET:O	2.02	0.59
1:S:1101:PHE:HA	1:S:1104:LEU:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2737:GLU:HB3	1:S:2740:SER:HB2	1.84	0.59
1:S:2940:ARG:HH22	1:S:3981:TYR:HB3	1.67	0.59
1:S:3311:ASN:HB2	1:S:3314:SER:HA	1.85	0.59
2:T:101:ASN:ND2	2:T:140:ASP:O	2.36	0.59
1:A:1083:ASN:O	1:A:1087:ARG:NH1	2.36	0.59
1:A:1178:ARG:HH21	1:A:1184:ARG:HA	1.68	0.59
1:A:1331:ASN:HA	1:A:1334:LYS:HE3	1.84	0.59
1:A:2574:ASN:O	1:A:2787:HIS:ND1	2.36	0.59
2:B:320:GLN:HG3	3:C:276:TRP:CE3	2.38	0.59
2:B:399:ARG:HG2	2:B:408:PRO:HB2	1.85	0.59
1:S:3930:VAL:HA	1:S:3937:VAL:HA	1.85	0.59
1:A:105:VAL:HG23	1:A:108:LYS:HE2	1.84	0.59
1:A:417:VAL:HA	1:A:420:VAL:HG12	1.85	0.59
1:A:901:MET:HG2	1:A:903:PRO:HD3	1.85	0.59
1:A:3736:LYS:HB2	1:A:3752:VAL:HB	1.84	0.59
1:S:1389:VAL:HG23	1:S:1391:VAL:HG22	1.85	0.59
1:A:1798:LEU:HD22	1:A:1827:LEU:HD13	1.85	0.59
2:B:302:THR:HG22	2:B:311:LEU:HD12	1.83	0.59
3:L:688:LYS:NZ	3:L:695:SER:OG	2.36	0.59
1:S:2986:PRO:O	1:S:2991:LYS:NZ	2.35	0.59
1:A:984:TYR:CD1	1:A:987:LEU:HD12	2.38	0.58
1:A:3949:ALA:HB1	1:A:3957:GLU:HB3	1.84	0.58
6:I:709:VAL:O	6:I:713:ILE:HG12	2.03	0.58
1:S:225:LYS:HG2	1:S:274:LEU:HB2	1.85	0.58
1:S:1693:VAL:HG13	1:S:1696:LEU:HD12	1.85	0.58
1:A:958:MET:HB3	1:A:961:LEU:HB2	1.86	0.58
1:A:1238:GLN:HE21	1:A:1296:PHE:HZ	1.52	0.58
1:S:1776:GLU:O	1:S:1779:GLN:NE2	2.37	0.58
1:S:3593:ARG:NH2	1:S:3661:ASP:OD1	2.36	0.58
2:T:126:GLN:HA	2:T:129:LYS:HE2	1.84	0.58
1:A:993:HIS:ND1	1:A:2779:ASP:OD1	2.34	0.58
1:A:2965:TYR:HB3	1:A:3001:CYS:HB2	1.86	0.58
2:B:397:LEU:HD22	3:C:463:LEU:HD12	1.85	0.58
5:G:121:GLU:HA	5:G:124:ARG:HE	1.67	0.58
6:I:812:MET:H	6:I:848:HIS:HB2	1.69	0.58
3:L:249:CYS:SG	3:L:250:ARG:N	2.72	0.58
1:S:3575:LEU:HD13	1:S:3578:LEU:HD12	1.85	0.58
2:T:217:TYR:HA	2:T:220:ILE:HG22	1.86	0.58
1:A:2824:LYS:O	1:A:2829:LYS:NZ	2.37	0.58
3:L:450:GLN:NE2	3:L:536:LEU:O	2.32	0.58
3:L:596:GLU:HA	3:L:599:ARG:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:793:LEU:HD21	1:S:866:ILE:HG22	1.84	0.58
1:S:2470:ARG:NH1	1:S:2513:GLU:OE2	2.27	0.58
1:A:1069:HIS:HD2	1:A:1074:LYS:HG2	1.68	0.58
2:B:170:THR:OG1	2:B:172:GLU:OE1	2.22	0.58
2:B:396:ALA:HB3	2:B:413:LEU:HB2	1.85	0.58
3:C:596:GLU:OE2	3:C:599:ARG:NH1	2.36	0.58
6:I:810:LEU:HD22	6:I:848:HIS:HD2	1.69	0.58
2:T:74:LYS:HD2	2:T:111:PRO:HG3	1.85	0.58
1:A:848:LEU:HD21	1:A:852:ARG:HH21	1.69	0.58
1:A:2090:ARG:NH2	1:A:2091:HIS:O	2.36	0.58
1:A:3510:GLN:HB3	1:A:3515:GLN:NE2	2.15	0.58
5:H:43:TRP:HD1	5:H:116:VAL:HG12	1.68	0.58
6:I:654:LYS:N	6:I:660:GLU:OE2	2.37	0.58
6:I:728:GLU:OE1	6:I:741:ARG:NH2	2.36	0.58
1:S:131:LEU:HB2	1:S:173:LYS:HD2	1.86	0.58
1:S:1538:LEU:N	1:S:1553:PHE:O	2.34	0.58
1:S:1583:MET:O	1:S:1586:SER:OG	2.22	0.58
1:A:3617:LEU:HA	1:A:3633:ILE:HG22	1.85	0.58
3:L:141:ARG:HH22	3:L:143:SER:HB3	1.69	0.58
1:S:933:LEU:HD13	1:S:2793:PRO:HB2	1.86	0.58
1:S:2322:VAL:O	1:S:2326:ILE:HG12	2.03	0.58
1:S:2330:VAL:HG13	1:S:2333:ARG:HH22	1.68	0.58
1:S:3113:ASN:HB3	1:S:3128:LYS:HZ2	1.69	0.58
2:T:67:ILE:HA	2:T:70:VAL:HG22	1.85	0.58
1:A:337:LYS:HG2	1:A:369:PHE:CZ	2.38	0.58
2:B:297:LYS:H	3:C:298:ASN:HB3	1.68	0.58
1:S:435:LEU:HA	1:S:438:LEU:HD12	1.86	0.58
1:S:1080:LEU:HB3	1:S:1126:GLN:HG3	1.84	0.58
1:S:1082:PHE:HA	1:S:1085:ILE:HG12	1.86	0.58
1:S:2350:LYS:HA	1:S:2354:ASN:OD1	2.04	0.58
1:S:3506:LEU:HD11	1:S:3554:PHE:HB3	1.86	0.58
1:S:3666:LEU:HA	1:S:3669:LYS:HZ3	1.69	0.58
1:A:24:ARG:NH1	1:A:25:CYS:HB3	2.19	0.58
3:C:620:ILE:HD13	3:C:639:ILE:HD11	1.86	0.58
3:C:728:LEU:HD13	1:S:1917:LYS:HG2	1.85	0.58
3:L:129:LYS:NZ	3:L:130:ARG:O	2.36	0.58
1:S:2532:PRO:HD2	1:S:2538:ARG:HA	1.84	0.58
1:S:2806:LYS:HB2	1:S:2857:CYS:HB2	1.85	0.58
1:S:2819:GLU:O	1:S:2822:LYS:NZ	2.33	0.58
1:S:2999:LEU:HD22	1:S:3014:CYS:HA	1.86	0.58
2:T:230:ARG:HD3	2:T:232:HIS:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2353:GLN:HB3	1:A:2360:PHE:HB2	1.84	0.58
2:B:447:PRO:HD3	3:C:243:HIS:HB2	1.86	0.58
3:C:595:ALA:HB1	3:C:599:ARG:HH22	1.69	0.58
6:I:746:MET:HE3	6:I:751:LYS:HG2	1.86	0.58
1:S:275:PHE:HE2	1:S:319:PHE:HB2	1.69	0.58
1:S:582:THR:HG23	1:S:615:ALA:HB3	1.86	0.58
1:S:2452:ARG:HB2	1:S:2498:ILE:HD11	1.86	0.58
1:S:3254:LEU:HD23	1:S:3287:ARG:HH12	1.69	0.58
1:S:3628:PHE:HB2	1:S:3675:LYS:HB3	1.85	0.58
1:S:3793:VAL:HG23	1:S:3803:ILE:HG22	1.83	0.58
1:A:18:THR:O	1:A:22:ALA:N	2.34	0.57
1:A:305:ASN:O	1:A:308:LEU:N	2.36	0.57
1:A:983:LEU:HB3	1:A:2591:ILE:HD11	1.85	0.57
1:A:993:HIS:NE2	1:A:1035:GLU:OE2	2.37	0.57
1:A:1322:THR:O	1:A:1326:GLU:N	2.37	0.57
1:A:2928:LYS:O	1:A:2931:ARG:HD3	2.03	0.57
2:B:34:GLY:HA2	2:B:160:LYS:HG3	1.86	0.57
3:C:104:GLN:O	3:C:141:ARG:NH1	2.36	0.57
3:C:184:ARG:NH2	3:C:514:ASN:O	2.36	0.57
1:S:305:ASN:O	1:S:308:LEU:N	2.37	0.57
1:S:925:GLN:HA	1:S:2769:VAL:HG13	1.85	0.57
1:S:1231:GLN:HE21	1:S:1235:ILE:HD11	1.67	0.57
1:S:3580:ASN:H	1:S:3734:ARG:NH2	1.97	0.57
1:S:3870:SER:OG	1:S:4117:LEU:O	2.22	0.57
1:A:947:GLN:HB2	1:A:2577:PHE:HE1	1.69	0.57
1:A:2246:LYS:NZ	1:A:2284:ASP:OD1	2.37	0.57
2:B:458:GLN:HE21	2:B:528:LEU:HB3	1.68	0.57
2:B:507:THR:OG1	3:C:394:ARG:NH1	2.37	0.57
4:D:27:GLU:HA	4:D:37:PHE:HB2	1.86	0.57
1:S:248:ILE:HA	1:S:251:PHE:HD2	1.69	0.57
1:S:1249:SER:OG	1:S:1312:CYS:SG	2.58	0.57
1:S:1841:SER:HA	1:S:1844:VAL:HG13	1.86	0.57
1:S:2392:VAL:O	1:S:2395:THR:HB	2.04	0.57
1:A:649:PHE:CE2	1:A:653:LEU:HD11	2.39	0.57
1:A:2243:GLU:HA	1:A:2246:LYS:HE3	1.87	0.57
1:S:1095:LEU:O	1:S:1099:PHE:N	2.35	0.57
1:S:2291:GLN:OE1	1:S:2291:GLN:N	2.37	0.57
1:S:2937:ASP:HB2	1:S:3979:LEU:HD23	1.86	0.57
1:A:955:ALA:O	1:A:957:PRO:HD3	2.04	0.57
1:A:1115:HIS:HD2	1:A:1182:GLU:HB3	1.70	0.57
1:A:1354:GLU:HB3	1:A:1357:LYS:HD3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2935:GLU:OE2	1:A:2936:TYR:N	2.38	0.57
1:A:3723:ASP:HB2	1:A:3741:ARG:HB2	1.86	0.57
2:B:82:LEU:HB3	2:B:108:LEU:HD22	1.85	0.57
2:B:168:LEU:HG	2:B:202:LEU:HD13	1.85	0.57
3:L:65:ASP:HB3	3:L:78:THR:HG23	1.86	0.57
1:S:2326:ILE:O	1:S:2330:VAL:N	2.36	0.57
1:S:2577:PHE:HB2	1:S:2783:ILE:HB	1.86	0.57
1:S:2891:ARG:HH12	1:S:3897:PHE:HB3	1.70	0.57
1:A:105:VAL:O	1:A:108:LYS:HB3	2.05	0.57
1:A:3304:VAL:HG21	1:A:3333:THR:HG21	1.86	0.57
2:B:305:THR:HB	3:C:288:ASP:HA	1.85	0.57
3:L:6:ASN:N	3:L:128:GLU:OE1	2.37	0.57
1:S:888:ARG:HH12	1:S:3889:ARG:HG3	1.70	0.57
1:S:2225:HIS:HB3	1:S:2227:LYS:HE2	1.87	0.57
1:S:2234:ASN:HA	1:S:2237:ILE:HD12	1.85	0.57
1:S:2331:MET:HE2	1:S:2338:GLU:HG2	1.86	0.57
2:T:82:LEU:HB3	2:T:108:LEU:HD22	1.86	0.57
2:T:304:ASN:OD1	2:T:305:THR:N	2.35	0.57
1:A:217:LEU:HB2	1:A:220:LEU:HB2	1.86	0.57
1:A:880:MET:HG2	1:A:3934:THR:HB	1.87	0.57
1:A:898:PHE:H	1:A:902:LYS:HE3	1.69	0.57
1:A:1147:LYS:HG3	1:A:1149:LYS:HG2	1.87	0.57
1:A:3444:ALA:HA	1:A:3482:LEU:HD11	1.85	0.57
2:B:462:MET:HE2	2:B:465:ILE:HD12	1.87	0.57
3:L:59:PHE:HA	3:L:77:ILE:HA	1.87	0.57
3:L:368:ARG:NH1	2:T:448:PHE:O	2.35	0.57
3:L:497:ARG:NH2	3:L:503:GLU:O	2.36	0.57
1:S:895:ALA:HA	1:S:904:VAL:HA	1.85	0.57
1:S:2460:GLU:OE1	1:S:2460:GLU:N	2.38	0.57
1:S:3170:ASP:HB3	1:S:3174:ASP:HB2	1.86	0.57
1:S:3483:MET:HE1	1:S:3512:VAL:HG22	1.87	0.57
3:C:18:PHE:HB2	3:C:102:SER:HA	1.87	0.57
3:C:643:ARG:HD3	3:C:655:PHE:CD2	2.40	0.57
6:I:865:ILE:HG12	6:I:889:LEU:HD13	1.86	0.57
1:S:801:LYS:NZ	1:S:3114:TYR:O	2.37	0.57
1:S:1062:ARG:NH1	1:S:1065:SER:OG	2.37	0.57
1:S:1282:LEU:HD13	1:S:1359:LEU:HB3	1.85	0.57
6:I:693:PRO:HB2	6:I:718:HIS:CE1	2.40	0.57
3:L:293:THR:O	3:L:307:LYS:NZ	2.34	0.57
5:Q:183:VAL:O	5:Q:186:GLU:HG3	2.05	0.57
1:S:1849:ASP:OD1	1:S:1850:VAL:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:HD11	1:A:183:GLU:HB2	1.86	0.57
1:A:1458:LEU:HD13	1:A:1467:ILE:HG21	1.86	0.57
1:A:3227:ILE:HA	1:A:3230:LEU:HD12	1.86	0.57
2:B:484:GLN:OE1	2:B:488:ARG:NH1	2.38	0.57
6:I:782:LYS:NZ	6:I:783:ASN:O	2.38	0.57
3:L:325:LYS:HZ3	3:L:328:GLU:HB3	1.70	0.57
1:S:709:LYS:NZ	1:S:1332:TYR:OH	2.30	0.57
1:S:2158:ARG:HH21	1:S:2196:TRP:HB3	1.70	0.57
1:S:2531:LEU:HD22	1:S:2538:ARG:HG3	1.87	0.57
1:A:793:LEU:HB3	1:A:870:LEU:HA	1.87	0.57
1:A:1149:LYS:O	1:A:1151:ARG:NH1	2.38	0.57
6:I:665:CYS:HB2	6:I:697:THR:HG21	1.87	0.57
1:S:760:LEU:HD11	1:S:798:GLY:HA3	1.87	0.57
1:S:1709:GLU:HA	1:S:1712:ARG:HG2	1.87	0.57
1:S:1878:ASP:HB3	1:S:1947:CYS:HA	1.87	0.57
1:S:2367:VAL:O	1:S:2371:PHE:N	2.37	0.57
1:A:720:GLN:OE1	1:A:720:GLN:N	2.36	0.56
1:A:4006:VAL:HG11	1:A:4009:PRO:HB3	1.86	0.56
2:B:469:LEU:HD21	2:B:518:LEU:HG	1.86	0.56
1:S:18:THR:O	1:S:22:ALA:N	2.35	0.56
1:S:3617:LEU:HA	1:S:3633:ILE:HG22	1.87	0.56
2:T:39:ILE:HB	2:T:166:ILE:HG12	1.87	0.56
1:A:1440:ASP:HB2	1:A:1445:ARG:HH21	1.69	0.56
1:A:3609:MET:HA	1:A:3612:ARG:HE	1.70	0.56
5:P:21:GLN:NE2	5:P:35:THR:OG1	2.38	0.56
5:P:51:GLU:HG2	5:P:110:SER:HB3	1.87	0.56
1:S:1570:GLU:HG3	1:S:1571:LEU:HD22	1.87	0.56
1:S:2261:SER:O	1:S:2270:ASN:ND2	2.32	0.56
1:S:2365:ASN:ND2	1:S:2399:GLU:OE2	2.27	0.56
1:S:3069:MET:HG3	1:S:3075:LYS:HD3	1.86	0.56
2:T:423:GLN:HG3	2:T:425:ILE:HG12	1.86	0.56
1:A:240:GLU:HB2	1:A:242:PRO:HD2	1.86	0.56
1:A:895:ALA:HA	1:A:904:VAL:HA	1.86	0.56
1:A:1058:SER:HA	1:A:1061:LYS:HE2	1.87	0.56
1:A:2215:LEU:HA	1:A:2218:PHE:HD2	1.71	0.56
1:A:2274:ILE:HD13	1:A:2319:ALA:HB2	1.87	0.56
1:A:3236:PHE:HE2	1:A:3269:ARG:HH12	1.53	0.56
2:B:488:ARG:HG3	2:B:501:GLU:HB3	1.87	0.56
3:C:468:GLU:O	3:C:469:LYS:HG2	2.05	0.56
6:I:814:ARG:N	6:I:849:GLY:HA2	2.20	0.56
5:Q:181:ILE:HG12	6:R:795:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:348:ILE:HG22	1:S:349:ILE:HG13	1.87	0.56
1:S:1626:TRP:HZ2	1:S:1674:THR:HG21	1.70	0.56
1:S:2234:ASN:O	1:S:2238:ILE:HG12	2.06	0.56
1:S:2830:ASN:OD1	1:S:2834:GLN:NE2	2.39	0.56
2:T:48:MET:SD	2:T:48:MET:N	2.70	0.56
2:T:121:GLN:O	2:T:130:ARG:NH1	2.39	0.56
1:A:345:PHE:HB3	1:A:366:TYR:CZ	2.40	0.56
1:A:979:VAL:HA	1:A:982:GLN:HG2	1.87	0.56
1:A:1793:THR:O	1:A:1797:LEU:HG	2.05	0.56
1:A:3130:GLN:HB3	1:A:3178:ILE:HG12	1.87	0.56
1:A:3789:ARG:NH1	1:A:3936:GLY:O	2.38	0.56
2:B:444:ARG:NH2	3:C:268:LEU:O	2.36	0.56
1:S:1614:GLN:HA	1:S:1617:LYS:HE2	1.87	0.56
1:S:3472:ILE:HG12	1:S:3479:THR:HB	1.85	0.56
1:A:436:GLU:HA	1:A:439:VAL:HG22	1.87	0.56
1:A:1095:LEU:O	1:A:1099:PHE:N	2.29	0.56
1:A:1104:LEU:HD13	1:A:1134:LEU:HD13	1.87	0.56
1:A:2304:VAL:O	1:A:2348:GLN:NE2	2.38	0.56
1:A:2526:SER:O	1:A:2538:ARG:NH2	2.39	0.56
2:B:352:PRO:HD2	2:B:355:LEU:HD12	1.87	0.56
3:L:74:TYR:HB3	3:L:77:ILE:HD12	1.87	0.56
3:L:328:GLU:HA	3:L:331:MET:HG2	1.88	0.56
1:S:1782:PHE:HA	1:S:1785:ILE:HG12	1.87	0.56
1:S:2930:TYR:HB2	1:S:2939:LEU:HD21	1.88	0.56
1:A:71:LYS:C	1:A:73:LEU:N	2.56	0.56
1:A:650:SER:HA	1:A:653:LEU:HD12	1.88	0.56
3:L:312:GLN:HB2	2:T:285:PRO:HB2	1.88	0.56
1:S:734:LEU:HA	1:S:776:TRP:HH2	1.70	0.56
1:S:1423:ILE:HG13	1:S:1425:ALA:H	1.71	0.56
1:S:1606:ARG:HA	1:S:1608:ARG:HH21	1.71	0.56
1:A:638:GLN:HG3	1:A:640:GLU:H	1.71	0.56
1:A:1108:MET:SD	1:A:1178:ARG:NH1	2.76	0.56
1:A:2495:SER:HA	1:A:2498:ILE:HD12	1.87	0.56
1:S:168:ASP:H	1:S:171:LEU:HD12	1.71	0.56
1:S:1205:ASN:HB3	1:S:1275:THR:HA	1.88	0.56
1:S:1649:LEU:HA	1:S:1652:ILE:HD12	1.88	0.56
1:S:2094:MET:HB2	1:S:2097:LEU:HD12	1.88	0.56
1:S:2283:ASN:HB3	1:S:2285:LEU:HG	1.87	0.56
1:S:2353:GLN:HA	1:S:2356:MET:HG3	1.87	0.56
1:A:117:LYS:NZ	3:C:302:GLU:OE1	2.39	0.56
1:A:386:VAL:HG22	1:A:431:TYR:HE2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1684:LEU:O	1:A:1689:LYS:NZ	2.39	0.56
6:I:677:ASP:OD1	6:I:678:LEU:N	2.38	0.56
1:A:166:ILE:HG13	1:A:167:PRO:HD3	1.88	0.56
1:A:3756:GLU:N	1:A:3798:SER:O	2.39	0.56
1:S:3912:CYS:HA	1:S:3915:HIS:CD2	2.41	0.56
1:A:938:VAL:HA	1:A:941:MET:HG3	1.88	0.56
1:A:2302:ALA:O	1:A:2306:ASN:ND2	2.39	0.56
2:B:217:TYR:O	2:B:221:ILE:N	2.28	0.56
2:B:298:THR:HG1	3:C:295:TYR:HD2	1.54	0.56
2:B:534:TYR:OH	3:C:260:ARG:NH2	2.37	0.56
3:C:724:ASP:O	3:C:728:LEU:N	2.39	0.56
6:I:725:TRP:HA	6:I:741:ARG:HH22	1.70	0.56
3:L:9:ALA:HB3	3:L:130:ARG:HG3	1.87	0.56
6:R:860:VAL:HG22	6:R:862:HIS:H	1.70	0.56
1:S:880:MET:HG2	1:S:3934:THR:HB	1.87	0.56
1:S:1687:HIS:O	1:S:1745:LYS:NZ	2.39	0.56
1:A:770:LEU:HD23	1:A:773:LEU:HD21	1.88	0.55
2:B:44:ALA:O	2:B:138:GLY:N	2.38	0.55
3:C:9:ALA:N	3:C:129:LYS:O	2.38	0.55
5:G:44:THR:O	5:G:114:GLU:N	2.36	0.55
6:I:668:SER:HB3	6:I:702:ALA:HA	1.88	0.55
3:L:484:ASN:OD1	3:L:486:ARG:HG2	2.05	0.55
3:L:725:VAL:HG13	3:L:729:LEU:HD13	1.87	0.55
1:A:2227:LYS:O	1:A:2228:ARG:HG3	2.06	0.55
1:A:3550:LYS:O	1:A:3553:GLU:HG2	2.06	0.55
1:A:3967:PHE:O	1:A:3970:LEU:HD22	2.07	0.55
2:B:41:LEU:HB3	2:B:88:TYR:HE1	1.71	0.55
2:B:297:LYS:NZ	3:C:297:LEU:O	2.40	0.55
3:L:640:ARG:HH12	3:L:682:GLY:HA2	1.72	0.55
1:S:1338:VAL:O	1:S:1342:MET:HG2	2.06	0.55
1:S:1769:GLU:H	1:S:1772:HIS:CE1	2.24	0.55
1:S:3183:ILE:HG13	1:S:3242:MET:SD	2.46	0.55
1:A:163:LYS:HG2	2:B:301:ARG:HA	1.88	0.55
1:A:643:GLU:HG3	1:A:644:PRO:HD3	1.87	0.55
1:A:1034:ARG:HG3	1:A:1085:ILE:HA	1.87	0.55
1:A:1639:LEU:HA	1:A:1642:LYS:HD2	1.88	0.55
1:A:3259:LEU:O	1:A:3276:TRP:NE1	2.39	0.55
5:G:8:ILE:HD11	5:G:18:HIS:HB2	1.89	0.55
5:H:179:ARG:NH2	6:I:782:LYS:O	2.38	0.55
6:I:703:GLY:O	6:I:722:LYS:NZ	2.39	0.55
1:S:36:ARG:HD3	1:S:2426:HIS:CD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2395:THR:HA	1:S:2398:LEU:HD12	1.87	0.55
1:S:2563:LEU:HD13	1:S:2795:GLN:HB3	1.87	0.55
1:A:1150:LYS:HA	1:A:1162:SER:HA	1.89	0.55
1:A:2981:TRP:HB2	1:A:2984:GLY:H	1.71	0.55
1:A:3142:ILE:HA	1:A:3145:ILE:HG12	1.89	0.55
2:B:38:LEU:HD11	2:B:165:ARG:NH2	2.22	0.55
6:R:816:HIS:H	6:R:850:ALA:CA	2.20	0.55
1:S:955:ALA:C	1:S:957:PRO:HD3	2.27	0.55
1:S:1780:SER:HB2	1:S:1784:ARG:HH12	1.70	0.55
1:S:2279:ILE:O	1:S:2283:ASN:ND2	2.39	0.55
1:A:128:LEU:HD21	1:A:170:VAL:HG23	1.89	0.55
1:A:616:LYS:NZ	1:A:2033:ASP:O	2.37	0.55
1:A:1662:ASN:OD1	1:A:1663:THR:N	2.39	0.55
2:B:160:LYS:NZ	2:B:161:MET:O	2.40	0.55
2:B:290:ARG:NH2	6:I:693:PRO:O	2.40	0.55
3:C:732:ILE:HA	1:S:1913:LYS:HZ2	1.71	0.55
6:R:812:MET:H	6:R:848:HIS:HB2	1.71	0.55
1:S:486:GLY:O	1:S:490:ILE:HG12	2.06	0.55
1:S:835:LYS:HA	1:S:838:LYS:HG2	1.88	0.55
1:S:2575:PRO:HA	1:S:2786:LYS:HA	1.89	0.55
1:S:4086:ASP:OD1	1:S:4087:HIS:N	2.39	0.55
1:A:1181:THR:HG22	1:A:1262:ALA:HB2	1.88	0.55
1:A:2547:SER:HB3	1:A:2550:ILE:HG12	1.89	0.55
1:A:4121:TRP:HD1	1:A:4123:GLY:H	1.55	0.55
5:G:99:LYS:HG2	5:G:108:LEU:HD13	1.89	0.55
3:L:619:HIS:HD1	3:L:620:ILE:HD13	1.70	0.55
3:L:643:ARG:HD2	3:L:655:PHE:HD2	1.72	0.55
5:P:150:ARG:NH1	5:P:154:ASP:OD2	2.39	0.55
1:S:958:MET:HB3	1:S:961:LEU:HB2	1.89	0.55
1:S:1048:GLN:OE1	1:S:1051:LYS:NZ	2.30	0.55
1:S:2287:PRO:HB3	1:S:2326:ILE:HD12	1.88	0.55
1:S:3048:LYS:HB3	1:S:3061:LEU:HD22	1.88	0.55
1:S:3369:ASP:HB3	1:S:3372:LYS:HG2	1.88	0.55
1:A:2532:PRO:O	1:A:2538:ARG:NH1	2.40	0.55
1:A:3072:GLU:HA	1:A:3075:LYS:HE2	1.89	0.55
1:A:3755:GLY:HA2	1:A:3799:ARG:HA	1.89	0.55
2:B:492:ALA:O	2:B:496:ASP:N	2.40	0.55
3:L:468:GLU:O	3:L:469:LYS:HG3	2.07	0.55
1:S:1296:PHE:O	1:S:1300:SER:N	2.39	0.55
1:S:2773:ARG:HG3	1:S:2789:SER:HB2	1.89	0.55
1:S:3259:LEU:HG	1:S:3276:TRP:CZ2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:GLN:HG3	1:A:1460:ARG:NH2	2.22	0.55
1:A:1663:THR:O	1:A:1665:HIS:ND1	2.39	0.55
1:A:1871:MET:HE1	1:A:1940:TYR:N	2.22	0.55
1:A:2850:PHE:HB3	1:A:2883:SER:HB2	1.88	0.55
1:A:3321:LEU:HB3	1:A:3324:ARG:HH21	1.72	0.55
2:B:305:THR:OG1	3:C:290:GLN:HG3	2.07	0.55
3:C:327:ASP:OD1	3:C:328:GLU:N	2.40	0.55
3:L:643:ARG:HE	3:L:647:ILE:HD11	1.72	0.55
1:S:73:LEU:HG	1:S:75:SER:H	1.69	0.55
1:S:1406:LEU:HD11	1:S:1411:TYR:HB2	1.89	0.55
1:S:3898:LEU:HG	1:S:3901:ARG:HH21	1.71	0.55
2:T:45:SER:OG	2:T:46:LYS:N	2.40	0.55
2:T:346:MET:HB2	2:T:399:ARG:HB3	1.88	0.55
1:A:978:GLN:NE2	1:A:2596:ARG:O	2.40	0.55
1:A:1564:SER:O	1:A:1568:ASN:ND2	2.40	0.55
1:S:2330:VAL:HG22	1:S:2331:MET:HG3	1.88	0.55
1:S:3806:LEU:HD21	1:S:3938:ILE:HD12	1.88	0.55
2:T:363:ARG:HB3	2:T:436:PHE:CD2	2.42	0.55
1:A:1417:THR:O	1:A:1421:GLU:N	2.32	0.54
1:A:1570:GLU:HG3	1:A:1571:LEU:HD22	1.88	0.54
1:A:3516:HIS:O	1:A:3519:GLU:HG3	2.07	0.54
1:A:3806:LEU:HD22	1:A:3809:THR:HB	1.89	0.54
5:G:28:LEU:HB3	5:G:67:VAL:HG22	1.89	0.54
3:L:29:SER:HB3	3:L:32:GLU:HG2	1.89	0.54
3:L:486:ARG:HD2	2:T:407:PRO:HB3	1.89	0.54
4:M:10:THR:HG22	4:M:21:VAL:HG22	1.89	0.54
4:M:86:ALA:HB3	4:M:97:THR:HB	1.89	0.54
1:S:358:GLU:HA	1:S:361:ILE:HD12	1.89	0.54
1:S:3559:LYS:HA	1:S:3562:LEU:HG	1.89	0.54
1:A:1697:PRO:HA	1:A:1753:SER:HB3	1.89	0.54
1:A:3693:GLU:HG2	1:A:3695:LEU:H	1.72	0.54
3:L:394:ARG:NH1	2:T:507:THR:OG1	2.39	0.54
1:S:414:LEU:HB2	1:S:460:ALA:HB1	1.89	0.54
1:A:1661:PHE:HD1	1:A:1665:HIS:HB2	1.72	0.54
1:A:2383:PHE:HB3	1:A:2418:LYS:HE3	1.89	0.54
1:A:3493:TRP:CZ3	1:A:3521:ILE:HA	2.42	0.54
3:C:287:GLU:OE1	3:C:287:GLU:N	2.40	0.54
5:G:28:LEU:HD21	5:G:70:LEU:HD23	1.89	0.54
1:S:169:THR:HA	1:S:172:GLU:HG2	1.89	0.54
1:A:463:LYS:HB3	1:A:544:ILE:HD13	1.89	0.54
1:A:1117:ASP:OD1	1:A:1118:GLU:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:LEU:HB2	1:A:1372:LEU:HD23	1.87	0.54
1:A:2253:TYR:H	1:A:2256:ILE:HD12	1.73	0.54
1:A:2261:SER:O	1:A:2270:ASN:ND2	2.39	0.54
1:A:2986:PRO:O	1:A:2991:LYS:NZ	2.39	0.54
1:A:3114:TYR:HB2	1:A:3128:LYS:HG2	1.90	0.54
6:I:902:GLU:OE1	6:I:904:GLN:NE2	2.41	0.54
1:S:1164:CYS:SG	1:S:1165:LEU:N	2.81	0.54
1:S:2090:ARG:N	1:S:2180:GLU:OE1	2.41	0.54
1:S:2791:ILE:HA	1:S:2794:LEU:HD12	1.89	0.54
1:A:169:THR:HA	1:A:172:GLU:HG2	1.89	0.54
1:A:3657:SER:N	1:A:3660:ASN:OD1	2.41	0.54
5:G:10:LEU:HD13	5:G:17:THR:HA	1.89	0.54
5:P:179:ARG:NH2	6:R:803:TYR:O	2.30	0.54
6:R:747:CYS:O	6:R:751:LYS:N	2.34	0.54
1:S:2162:LYS:HG3	1:S:2163:HIS:ND1	2.22	0.54
1:A:1868:THR:O	1:A:1871:MET:HB2	2.08	0.54
1:A:3604:LYS:NZ	1:A:3605:ASN:OD1	2.38	0.54
2:B:62:MET:HA	2:B:65:GLN:HG3	1.89	0.54
3:C:270:GLU:OE2	3:C:484:ASN:ND2	2.35	0.54
3:C:347:LYS:HB3	3:C:350:GLN:HG3	1.90	0.54
6:I:764:SER:OG	6:I:767:ILE:O	2.25	0.54
6:I:796:ILE:O	6:I:800:GLU:HG2	2.07	0.54
1:S:1146:ASN:HB3	1:S:1199:PRO:HB3	1.89	0.54
1:S:1322:THR:O	1:S:1326:GLU:N	2.41	0.54
1:S:3580:ASN:ND2	1:S:3582:GLU:OE1	2.40	0.54
2:T:42:VAL:HA	2:T:169:PHE:HB2	1.89	0.54
1:A:888:ARG:HH21	1:A:3889:ARG:HB3	1.72	0.54
1:A:3110:PHE:CD2	1:A:3135:LEU:HD11	2.43	0.54
2:B:469:LEU:HD11	2:B:518:LEU:HD11	1.90	0.54
6:I:814:ARG:H	6:I:849:GLY:HA2	1.71	0.54
6:R:889:LEU:HD13	6:R:905:GLU:H	1.72	0.54
1:S:1017:ILE:HG23	1:S:1077:GLY:HA3	1.90	0.54
1:S:1444:ASP:OD1	1:S:1445:ARG:N	2.40	0.54
1:S:3172:LYS:O	1:S:3173:MET:HE2	2.08	0.54
1:A:356:ASN:HB3	1:A:358:GLU:HG2	1.90	0.54
1:A:584:GLU:N	1:A:613:HIS:O	2.38	0.54
1:A:1164:CYS:SG	1:A:1165:LEU:N	2.81	0.54
1:A:1257:LEU:HA	1:A:1260:LEU:HD12	1.88	0.54
1:A:2578:GLU:OE1	1:A:2578:GLU:N	2.41	0.54
1:A:2924:VAL:HG11	1:A:2989:ALA:HB1	1.90	0.54
1:A:3011:LEU:HD12	1:A:3050:LYS:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:260:ARG:NH2	3:C:370:ASP:OD2	2.41	0.54
1:S:196:LEU:HB3	1:S:200:PHE:CZ	2.43	0.54
1:S:1379:PRO:O	1:S:1382:ILE:HG12	2.08	0.54
1:S:3312:VAL:O	1:S:3316:LEU:N	2.34	0.54
1:S:4086:ASP:HA	1:S:4089:ILE:HG12	1.89	0.54
1:A:928:VAL:HB	1:A:2769:VAL:HG11	1.88	0.54
1:A:984:TYR:HD1	1:A:987:LEU:HD12	1.73	0.54
1:A:1228:GLY:HA2	1:A:1256:TRP:NE1	2.17	0.54
1:A:2876:VAL:HG11	1:A:2892:LEU:HD11	1.90	0.54
1:A:3159:ARG:HG2	1:A:3230:LEU:HD13	1.89	0.54
2:B:120:ASP:HA	2:B:123:LYS:HB3	1.90	0.54
3:C:62:ASP:HA	3:C:103:GLN:HG2	1.90	0.54
3:C:643:ARG:HH21	3:C:685:LEU:HD22	1.73	0.54
1:S:635:PRO:HB3	1:S:672:ILE:HD11	1.89	0.54
1:S:864:GLY:HA3	1:S:3170:ASP:OD1	2.08	0.54
1:S:936:SER:HB2	1:S:2790:LEU:HD22	1.90	0.54
1:S:1603:GLN:OE1	1:S:1606:ARG:NH1	2.41	0.54
1:S:3506:LEU:O	1:S:3551:ASN:ND2	2.40	0.54
1:S:3614:TYR:O	1:S:3619:ASP:N	2.34	0.54
1:A:1690:GLY:HA2	1:A:1693:VAL:HG22	1.88	0.54
1:A:2388:LYS:NZ	2:B:154:PHE:O	2.41	0.54
1:S:785:MET:HA	1:S:788:TYR:CZ	2.42	0.54
1:A:960:GLN:HA	1:A:963:LYS:HE2	1.90	0.53
1:A:1172:LEU:HD11	1:A:1187:SER:HB2	1.89	0.53
1:A:1231:GLN:H	1:A:1232:PRO:HD2	1.73	0.53
1:A:3190:LEU:HD21	1:A:3231:ILE:HD12	1.91	0.53
4:D:132:VAL:HG11	4:M:8:LEU:HD21	1.90	0.53
5:G:56:ALA:HB1	5:G:63:LYS:HE3	1.90	0.53
3:L:185:LEU:O	3:L:514:ASN:ND2	2.34	0.53
1:S:1029:CYS:HA	1:S:1032:CYS:SG	2.47	0.53
1:S:1331:ASN:HA	1:S:1334:LYS:HE3	1.90	0.53
1:S:2470:ARG:O	1:S:2473:MET:HG2	2.08	0.53
2:T:270:SER:HB3	2:T:374:LEU:HB2	1.89	0.53
2:T:465:ILE:HG12	2:T:518:LEU:HD22	1.90	0.53
1:A:702:SER:O	1:A:706:LEU:HG	2.08	0.53
1:A:3938:ILE:HG13	1:A:3940:ILE:HD11	1.89	0.53
3:L:162:GLN:HG2	3:L:223:GLU:HB3	1.90	0.53
3:L:462:SER:HA	2:T:350:PHE:HB2	1.89	0.53
1:S:1426:GLN:NE2	1:S:1468:LEU:HD13	2.23	0.53
1:S:2195:SER:O	1:S:2722:ARG:NH1	2.42	0.53
1:S:2831:ASN:O	1:S:2835:LYS:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2965:TYR:HD2	1:S:3253:SER:HB2	1.73	0.53
1:S:3158:LYS:HG3	1:S:3159:ARG:HD3	1.89	0.53
1:S:3450:MET:HG3	1:S:3468:LEU:HD11	1.90	0.53
1:S:3719:ILE:HA	1:S:3742:GLY:HA2	1.90	0.53
1:A:634:LEU:HD23	1:A:672:ILE:HG13	1.91	0.53
1:A:3483:MET:HA	1:A:3486:GLU:HG3	1.90	0.53
2:B:234:GLU:OE1	2:B:234:GLU:N	2.40	0.53
3:L:277:THR:O	2:T:319:SER:N	2.34	0.53
3:L:524:THR:HA	3:L:527:GLN:HG2	1.91	0.53
3:L:686:ILE:HD12	3:L:702:LYS:HG3	1.91	0.53
6:R:737:PRO:O	6:R:739:GLN:NE2	2.41	0.53
1:S:670:LEU:HB2	1:S:732:PHE:HZ	1.73	0.53
1:S:1959:LEU:HD12	1:S:2123:PRO:HG2	1.90	0.53
1:S:4055:ASN:ND2	1:S:4091:ALA:O	2.42	0.53
2:T:239:LEU:HA	2:T:242:LEU:HD12	1.89	0.53
1:A:71:LYS:O	1:A:72:SER:C	2.45	0.53
1:A:433:PRO:O	1:A:436:GLU:HG3	2.08	0.53
1:A:720:GLN:HE21	1:A:1122:GLY:N	2.07	0.53
1:A:850:GLU:HG3	1:A:854:ARG:HH22	1.72	0.53
1:A:978:GLN:NE2	1:A:2597:PHE:HA	2.24	0.53
1:A:1436:LEU:HD12	1:A:1445:ARG:HG2	1.89	0.53
1:A:2548:PRO:HB2	1:A:2848:PHE:CD1	2.44	0.53
1:A:2563:LEU:HD22	1:A:2795:GLN:HB3	1.91	0.53
2:B:165:ARG:HH22	4:D:188:PRO:HD3	1.74	0.53
2:B:525:PHE:HA	2:B:528:LEU:HB2	1.90	0.53
3:C:61:THR:OG1	3:C:63:GLY:O	2.27	0.53
3:L:23:SER:HB3	3:L:29:SER:HA	1.90	0.53
1:S:1115:HIS:NE2	1:S:1182:GLU:HB3	2.23	0.53
1:S:1673:THR:HA	1:S:1676:ILE:HD12	1.90	0.53
1:S:2482:ASP:HA	1:S:2485:ARG:CZ	2.39	0.53
1:S:2893:LEU:HD21	1:S:2922:ARG:HB2	1.91	0.53
1:S:3684:SER:HB3	1:S:3687:MET:HB2	1.90	0.53
1:A:13:LEU:HB2	1:A:59:PHE:CZ	2.43	0.53
1:A:1270:PHE:HB3	1:A:1276:VAL:HG12	1.91	0.53
1:A:1645:VAL:HA	1:A:1648:LEU:HG	1.91	0.53
1:A:3883:LEU:HD13	1:A:3966:GLN:HB3	1.91	0.53
1:S:1190:LEU:HA	1:S:1193:LYS:HG2	1.90	0.53
1:S:1686:LEU:HD11	1:S:1738:ASN:HB3	1.90	0.53
1:S:3686:TRP:CH2	1:S:3719:ILE:HG22	2.44	0.53
1:S:4073:ALA:HB1	1:S:4076:ASP:HB3	1.90	0.53
1:A:3058:ASP:OD1	1:A:3059:GLN:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3228:SER:HA	1:A:3231:ILE:HG12	1.91	0.53
1:S:1420:ARG:HH22	1:S:1469:PRO:HD3	1.74	0.53
1:S:1754:GLN:HE21	1:S:1785:ILE:HG22	1.73	0.53
1:S:2466:SER:OG	1:S:2469:CYS:SG	2.61	0.53
1:S:2824:LYS:HE3	1:S:2828:GLU:HB3	1.91	0.53
1:S:3236:PHE:HB3	1:S:3272:TRP:CH2	2.44	0.53
2:T:357:LYS:HB2	2:T:360:HIS:CG	2.44	0.53
1:A:3633:ILE:HG13	1:A:3634:GLN:H	1.73	0.53
1:A:4006:VAL:HB	1:A:4009:PRO:HD3	1.90	0.53
5:H:5:ILE:HG13	5:H:21:GLN:HB3	1.91	0.53
3:L:333:TYR:HD2	2:T:482:VAL:HG22	1.73	0.53
3:L:459:ASP:OD1	2:T:392:LYS:NZ	2.36	0.53
1:S:107:ILE:O	1:S:111:CYS:N	2.34	0.53
1:S:2122:LEU:HB2	1:S:2126:MET:CE	2.38	0.53
1:A:450:SER:O	1:A:454:GLN:HG3	2.09	0.53
1:A:2361:ILE:HD11	1:A:2393:LEU:HD22	1.90	0.53
1:A:2532:PRO:HD2	1:A:2538:ARG:HA	1.90	0.53
2:B:363:ARG:NH1	2:B:364:PRO:O	2.42	0.53
5:G:99:LYS:HB2	5:G:108:LEU:HB2	1.91	0.53
1:S:304:THR:OG1	1:S:305:ASN:OD1	2.27	0.53
1:S:789:TYR:HD1	1:S:792:ILE:HD12	1.74	0.53
1:S:1282:LEU:HB3	1:S:1359:LEU:HD22	1.91	0.53
1:S:1684:LEU:HB2	1:S:1689:LYS:HE3	1.89	0.53
1:S:2173:ALA:HB1	1:S:2214:ARG:HH12	1.74	0.53
1:S:2184:TYR:CZ	1:S:2734:ARG:HD2	2.43	0.53
1:A:67:VAL:HB	1:A:85:ILE:CD1	2.32	0.53
1:A:207:GLN:HB3	1:A:217:LEU:HD22	1.90	0.53
1:A:415:GLN:HA	1:A:463:LYS:HD2	1.90	0.53
1:A:1595:ALA:HA	1:A:1598:ASN:HD21	1.74	0.53
1:A:2414:GLN:OE1	1:A:2414:GLN:N	2.40	0.53
1:A:2440:TYR:HA	1:A:2443:MET:CE	2.39	0.53
1:A:2485:ARG:NH2	1:A:2529:THR:O	2.42	0.53
1:A:3699:LEU:HB2	1:A:3719:ILE:HD12	1.91	0.53
1:A:3974:MET:SD	1:A:3976:GLU:N	2.75	0.53
2:B:250:GLU:HG3	4:D:187:ASN:HD21	1.73	0.53
2:B:274:TYR:HB2	2:B:367:PHE:HD2	1.73	0.53
3:L:531:SER:HA	3:L:534:LYS:HG2	1.90	0.53
1:S:994:TRP:CD1	1:S:2581:LEU:HD21	2.44	0.53
1:S:1063:LEU:HG	1:S:1078:ALA:HB1	1.91	0.53
1:S:1769:GLU:O	1:S:1822:ARG:NH1	2.41	0.53
1:S:2897:LEU:HD23	1:S:3973:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3676:PRO:HB3	1:S:3726:VAL:HG11	1.90	0.53
1:S:3924:HIS:CE1	1:S:3926:ASN:HB2	2.44	0.53
2:T:218:ARG:NH2	2:T:229:LEU:HA	2.23	0.53
1:A:348:ILE:HG21	1:A:362:ALA:HB2	1.91	0.53
1:A:1128:CYS:HA	1:A:1131:ILE:HG12	1.90	0.53
1:A:2260:PHE:HE1	1:A:2302:ALA:HB3	1.73	0.53
1:A:3718:ARG:H	1:A:3743:HIS:HB3	1.74	0.53
2:B:94:LYS:H	2:B:103:TYR:HA	1.73	0.53
6:I:889:LEU:HD23	6:I:904:GLN:HA	1.91	0.53
3:L:96:SER:O	3:L:99:GLN:NE2	2.38	0.53
1:S:831:LEU:HD12	1:S:833:HIS:H	1.73	0.53
1:S:1117:ASP:OD1	1:S:1118:GLU:N	2.40	0.53
1:A:741:ILE:HG22	1:A:745:VAL:HG12	1.90	0.52
1:A:914:VAL:O	1:A:918:ALA:N	2.34	0.52
1:A:1134:LEU:O	1:A:1138:ILE:HG12	2.09	0.52
1:A:1586:SER:HB2	1:A:1632:TRP:HH2	1.74	0.52
1:A:3173:MET:CE	1:A:3174:ASP:H	2.21	0.52
1:A:3496:ILE:HA	1:A:3499:ILE:HG23	1.91	0.52
2:B:350:PHE:CE2	3:C:458:ILE:HG12	2.44	0.52
3:C:328:GLU:O	3:C:332:LYS:N	2.42	0.52
1:S:1196:PRO:O	1:S:1202:ARG:NH1	2.42	0.52
1:S:2356:MET:HE1	1:S:2359:LYS:H	1.75	0.52
1:S:3262:LEU:O	1:S:3266:SER:N	2.42	0.52
1:A:64:GLY:O	1:A:67:VAL:HG13	2.07	0.52
1:A:71:LYS:O	1:A:73:LEU:HB2	2.09	0.52
1:A:384:MET:HE3	1:A:388:LEU:HD11	1.90	0.52
1:A:2817:LEU:HD23	1:A:2865:HIS:CE1	2.44	0.52
1:A:3049:LEU:HD22	1:A:3085:GLU:HB2	1.91	0.52
1:A:3992:ARG:NH1	1:A:4051:LEU:O	2.43	0.52
2:B:422:ASP:N	2:B:422:ASP:OD1	2.42	0.52
5:G:21:GLN:HG2	5:G:21:GLN:O	2.09	0.52
1:S:986:PRO:HB3	1:S:2777:HIS:CD2	2.44	0.52
1:S:2371:PHE:HB3	1:S:2374:LEU:HD23	1.92	0.52
1:S:3125:ARG:O	1:S:3129:LEU:HG	2.10	0.52
1:S:3949:ALA:HB1	1:S:3957:GLU:HB3	1.91	0.52
1:A:857:GLN:CD	1:A:3139:GLN:HE22	2.12	0.52
1:A:2830:ASN:OD1	1:A:2834:GLN:NE2	2.42	0.52
1:A:2865:HIS:HB2	1:A:2868:LEU:HG	1.91	0.52
1:A:3170:ASP:HB3	1:A:3174:ASP:HB2	1.90	0.52
3:C:265:LYS:HD2	3:C:268:LEU:HD21	1.92	0.52
6:I:725:TRP:NE1	6:I:736:VAL:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:928:VAL:HB	1:S:2769:VAL:HG11	1.91	0.52
1:A:1255:CYS:HA	1:A:1258:ASP:OD2	2.10	0.52
1:A:1949:ILE:HA	1:A:2100:LEU:HD11	1.90	0.52
2:B:271:VAL:HG12	2:B:370:PRO:HA	1.91	0.52
2:B:500:PRO:O	2:B:502:GLN:NE2	2.39	0.52
3:C:261:ILE:HA	3:C:366:ALA:HA	1.91	0.52
3:L:616:LEU:O	3:L:620:ILE:HG12	2.08	0.52
4:M:7:PRO:HB3	4:M:77:ARG:NE	2.23	0.52
1:S:2547:SER:HB3	1:S:2550:ILE:HG12	1.89	0.52
1:A:236:LYS:O	1:A:281:GLN:NE2	2.42	0.52
1:A:362:ALA:O	1:A:366:TYR:HD1	1.92	0.52
1:A:1963:GLN:HB2	1:A:2125:TRP:CE3	2.45	0.52
1:A:2405:VAL:HG22	1:A:2441:LYS:HD2	1.91	0.52
2:B:107:GLU:O	2:B:115:ARG:NH2	2.42	0.52
5:H:87:ASN:ND2	5:H:96:PHE:O	2.34	0.52
3:L:490:LEU:HA	2:T:337:LEU:HD23	1.92	0.52
6:R:665:CYS:HB2	6:R:697:THR:HG21	1.92	0.52
1:S:167:PRO:HA	1:S:171:LEU:HD12	1.92	0.52
1:S:392:CYS:HB2	1:S:438:LEU:HD22	1.92	0.52
1:S:2233:HIS:CE1	1:S:2728:LEU:HA	2.45	0.52
1:A:710:PHE:O	1:A:714:VAL:HG22	2.10	0.52
1:A:2920:VAL:HA	1:A:2923:TRP:HB2	1.92	0.52
1:A:3179:TRP:HZ3	1:A:3241:LYS:HB3	1.74	0.52
2:B:102:ILE:HD12	2:B:146:VAL:HG12	1.91	0.52
3:C:679:VAL:HG21	3:C:705:LEU:HD21	1.90	0.52
5:G:152:LEU:HA	5:H:151:LEU:HD21	1.91	0.52
6:R:675:LYS:HA	6:R:678:LEU:HD12	1.90	0.52
1:S:417:VAL:HA	1:S:420:VAL:HG12	1.91	0.52
1:S:955:ALA:O	1:S:957:PRO:HD3	2.10	0.52
1:S:1426:GLN:HE22	1:S:1468:LEU:HD13	1.75	0.52
1:S:2349:LEU:O	1:S:2353:GLN:HB2	2.09	0.52
2:T:458:GLN:HB3	2:T:525:PHE:HE1	1.75	0.52
1:A:786:GLN:HA	1:A:789:TYR:CE2	2.45	0.52
1:A:3337:ILE:HG21	1:A:3360:LEU:HD22	1.91	0.52
2:B:187:ARG:HH21	2:B:220:ILE:HD11	1.74	0.52
2:B:510:LYS:HB3	2:B:513:ALA:HB3	1.91	0.52
3:C:9:ALA:HB3	3:C:130:ARG:HG3	1.91	0.52
5:G:192:ARG:NH2	6:I:768:ASP:OD1	2.43	0.52
5:H:183:VAL:O	5:H:187:LYS:HG2	2.10	0.52
3:L:326:VAL:O	3:L:329:GLU:HG3	2.10	0.52
3:L:678:VAL:O	3:L:682:GLY:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:327:VAL:HA	1:S:330:ASN:HB2	1.92	0.52
1:S:420:VAL:O	1:S:424:LEU:N	2.39	0.52
1:S:956:PRO:HA	1:S:959:TYR:HB2	1.91	0.52
1:S:1098:GLN:OE1	1:S:1152:ARG:N	2.43	0.52
1:S:1447:ARG:HH12	1:S:1448:LEU:HG	1.75	0.52
1:S:2133:LEU:HG	1:S:2171:LEU:HD11	1.91	0.52
1:S:3720:ALA:HB3	1:S:3743:HIS:HA	1.92	0.52
2:T:214:SER:HB3	2:T:218:ARG:CZ	2.39	0.52
1:A:752:LEU:HD22	1:A:776:TRP:CZ3	2.45	0.52
2:B:319:SER:N	3:C:277:THR:O	2.40	0.52
6:I:741:ARG:NH1	6:I:742:PHE:HB3	2.24	0.52
3:L:61:THR:HG21	3:L:78:THR:HB	1.91	0.52
3:L:418:CYS:SG	3:L:419:LEU:N	2.83	0.52
1:S:533:HIS:O	1:S:537:SER:OG	2.25	0.52
1:S:893:SER:HA	1:S:906:PHE:HA	1.92	0.52
1:S:3110:PHE:CD2	1:S:3135:LEU:HD11	2.45	0.52
1:S:3966:GLN:HA	1:S:3969:ASN:HB2	1.90	0.52
2:T:45:SER:HA	2:T:138:GLY:HA2	1.91	0.52
1:A:14:ARG:HH12	1:A:3070:HIS:HA	1.73	0.52
1:A:181:LEU:HB2	1:A:230:LEU:HD11	1.92	0.52
1:A:498:PRO:HG2	1:A:2596:ARG:HB2	1.92	0.52
1:A:1111:LEU:HD13	1:A:1186:LYS:HE3	1.92	0.52
1:A:1296:PHE:HA	1:A:1299:GLU:HG3	1.92	0.52
1:A:3278:GLN:HA	1:A:3281:CYS:SG	2.49	0.52
1:A:3389:VAL:O	1:A:3393:GLU:HG3	2.08	0.52
1:A:3500:SER:HA	1:A:3503:VAL:HG12	1.92	0.52
1:A:3964:THR:HG22	1:A:3967:PHE:CD2	2.45	0.52
2:B:94:LYS:HB2	2:B:103:TYR:CD2	2.45	0.52
3:L:182:PRO:HG2	3:L:190:PRO:HD2	1.91	0.52
1:S:214:GLU:OE2	2:T:404:ARG:NH2	2.42	0.52
1:S:3718:ARG:H	1:S:3743:HIS:HB3	1.75	0.52
2:T:213:ILE:HG13	2:T:218:ARG:HH21	1.75	0.52
1:A:723:ASP:C	1:A:725:LEU:H	2.12	0.52
1:A:1452:VAL:O	1:A:1456:LYS:HG2	2.10	0.52
1:A:2394:LYS:HB2	1:A:2431:ARG:NH2	2.25	0.52
1:A:3490:VAL:HG23	1:A:3494:GLN:HG2	1.91	0.52
3:C:45:GLN:OE1	3:C:50:ASN:ND2	2.42	0.52
3:C:489:ARG:NH1	3:C:506:PRO:O	2.39	0.52
3:C:497:ARG:HD3	3:C:501:PRO:HA	1.90	0.52
3:L:272:VAL:HG12	3:L:274:LYS:H	1.75	0.52
3:L:731:MET:SD	3:L:731:MET:N	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2464:HIS:O	1:S:2470:ARG:NE	2.43	0.52
2:T:235:GLU:OE1	2:T:235:GLU:N	2.43	0.52
1:A:934:LEU:HA	1:A:937:MET:HG2	1.91	0.51
1:A:1621:THR:O	1:A:1625:HIS:ND1	2.42	0.51
1:A:1693:VAL:HG21	1:A:1746:PHE:HE1	1.75	0.51
1:A:2429:ASP:OD1	1:A:2430:GLU:N	2.43	0.51
1:A:4085:LYS:O	1:A:4089:ILE:HG23	2.10	0.51
1:S:1096:VAL:O	1:S:1100:VAL:HG13	2.11	0.51
1:S:1306:ILE:HG13	1:S:1307:ILE:HG22	1.91	0.51
1:S:1589:ASN:HB3	1:S:1592:MET:SD	2.50	0.51
1:S:2122:LEU:HB2	1:S:2126:MET:HE2	1.93	0.51
1:S:3359:ILE:HD12	1:S:3362:LEU:HB2	1.91	0.51
1:S:4038:TRP:HE3	1:S:4043:LYS:HE3	1.75	0.51
1:A:542:ASP:OD1	1:A:543:SER:N	2.42	0.51
1:A:1062:ARG:HH22	1:A:3745:GLU:HB3	1.73	0.51
1:A:1923:PHE:HD1	1:A:1941:HIS:HB3	1.74	0.51
1:A:2090:ARG:NE	1:A:2092:GLU:OE2	2.37	0.51
1:A:2575:PRO:HA	1:A:2786:LYS:HA	1.93	0.51
2:B:165:ARG:NH2	4:D:188:PRO:HD3	2.25	0.51
3:C:510:GLN:HA	3:C:513:TRP:HD1	1.74	0.51
3:C:595:ALA:HA	3:C:598:PHE:CZ	2.45	0.51
3:C:687:THR:HG22	3:C:688:LYS:N	2.25	0.51
1:S:1200:GLY:O	1:S:1202:ARG:NH2	2.41	0.51
1:S:3088:LEU:HD23	1:S:3138:ILE:HD12	1.92	0.51
1:S:4087:HIS:C	1:S:4090:ARG:HD2	2.30	0.51
1:A:342:MET:N	1:A:342:MET:SD	2.82	0.51
1:A:456:VAL:HA	1:A:459:ARG:HD2	1.93	0.51
1:A:895:ALA:HB2	1:A:904:VAL:HG22	1.92	0.51
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.92	0.51
1:A:3924:HIS:N	1:A:3927:ASN:OD1	2.33	0.51
3:C:138:LEU:HD22	3:C:204:GLY:HA3	1.91	0.51
3:C:251:LEU:HB2	3:C:261:ILE:HD13	1.91	0.51
6:R:665:CYS:HB3	6:R:700:VAL:HA	1.91	0.51
1:S:640:GLU:HA	1:S:643:GLU:HG3	1.92	0.51
1:S:3114:TYR:HB2	1:S:3128:LYS:HG2	1.92	0.51
2:T:90:THR:HA	2:T:137:HIS:HA	1.92	0.51
1:A:183:GLU:HG2	1:A:184:VAL:H	1.75	0.51
1:A:526:ASP:OD1	1:A:526:ASP:N	2.42	0.51
1:A:865:GLN:OE1	1:A:3171:ALA:N	2.43	0.51
1:A:2866:ALA:HA	1:A:2869:LEU:HD12	1.93	0.51
1:A:3828:TYR:HE2	1:A:3879:PRO:HD3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:706:ASN:O	6:I:710:LYS:NZ	2.40	0.51
1:S:425:ASP:N	1:S:425:ASP:OD1	2.42	0.51
1:S:702:SER:O	1:S:706:LEU:HG	2.11	0.51
1:S:3268:THR:OG1	1:S:3269:ARG:NH1	2.43	0.51
1:S:3496:ILE:HD12	1:S:3707:GLY:HA3	1.91	0.51
1:A:3364:GLY:HA3	1:A:3373:VAL:HA	1.92	0.51
1:A:3588:TRP:NE1	1:A:3609:MET:O	2.34	0.51
1:A:3626:GLY:HA2	1:A:3677:PRO:HD3	1.92	0.51
3:C:640:ARG:HH12	3:C:685:LEU:HB2	1.75	0.51
6:I:743:MET:HG3	6:I:754:PHE:HE2	1.74	0.51
3:L:23:SER:HB3	3:L:30:PRO:HD3	1.93	0.51
3:L:76:ASN:HB2	3:L:105:ALA:HB2	1.92	0.51
1:S:681:LYS:NZ	1:S:739:ASN:OD1	2.44	0.51
1:S:2341:LEU:HD13	1:S:2344:LEU:HD12	1.92	0.51
1:S:3100:LYS:HA	1:S:3103:ILE:HG22	1.93	0.51
1:S:3570:ASP:HB3	1:S:3685:PRO:HG3	1.92	0.51
1:A:414:LEU:HB2	1:A:460:ALA:HB1	1.90	0.51
1:A:730:LEU:HA	1:A:733:LEU:HD12	1.93	0.51
1:A:2295:GLN:NE2	1:A:2298:GLU:HG2	2.25	0.51
1:A:2466:SER:HG	1:A:2469:CYS:HG	1.52	0.51
3:L:197:ILE:HG13	3:L:202:LYS:HE2	1.93	0.51
1:S:360:SER:HB2	1:S:364:ARG:HH12	1.76	0.51
1:S:664:SER:HA	1:S:667:TYR:CD1	2.45	0.51
1:S:675:ARG:NH1	1:S:679:LYS:HB2	2.25	0.51
1:S:801:LYS:HZ3	1:S:3125:ARG:HH12	1.59	0.51
1:S:978:GLN:HA	1:S:981:ARG:HH21	1.76	0.51
1:S:2321:GLU:HA	1:S:2366:LYS:HD2	1.92	0.51
2:T:143:LEU:HA	2:T:146:VAL:HG22	1.92	0.51
1:A:528:VAL:HB	1:A:633:ILE:HD11	1.92	0.51
1:A:2197:THR:H	1:A:2722:ARG:NH2	2.09	0.51
1:A:2753:ARG:O	1:A:2756:GLU:HG3	2.10	0.51
1:A:2823:PHE:HD1	1:A:2824:LYS:HE3	1.76	0.51
1:A:3046:ARG:NE	1:A:3046:ARG:HA	2.26	0.51
6:R:740:PRO:HG2	6:R:762:GLY:HA2	1.92	0.51
1:S:385:TYR:HA	1:S:388:LEU:HD12	1.93	0.51
1:S:664:SER:HA	1:S:667:TYR:HD1	1.75	0.51
1:S:1837:ARG:NH2	1:S:1884:LEU:HB2	2.25	0.51
1:S:2430:GLU:HA	1:S:2433:LYS:HE2	1.92	0.51
1:S:2522:ARG:NH2	1:S:2564:GLU:HB2	2.26	0.51
1:A:65:LEU:O	1:A:69:VAL:HG22	2.11	0.51
1:A:1296:PHE:O	1:A:1300:SER:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:ASP:O	1:A:1508:LYS:N	2.39	0.51
1:A:2257:PHE:HA	1:A:2260:PHE:CE2	2.45	0.51
1:A:2791:ILE:HA	1:A:2794:LEU:HD12	1.92	0.51
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.44	0.51
1:A:3425:ARG:HH11	1:A:3996:GLY:HA3	1.75	0.51
1:A:3493:TRP:HZ3	1:A:3521:ILE:HA	1.76	0.51
1:S:631:ARG:NH1	1:S:632:GLU:HB3	2.26	0.51
1:S:881:LYS:HZ1	1:S:3934:THR:HG1	1.54	0.51
1:S:3324:ARG:O	1:S:3328:ILE:HG12	2.10	0.51
1:S:3842:TRP:HB3	1:S:3855:TYR:CD1	2.45	0.51
1:S:3874:ARG:NH2	1:S:4117:LEU:O	2.44	0.51
2:T:91:GLU:HG2	2:T:137:HIS:H	1.75	0.51
1:A:2382:VAL:O	1:A:2386:LEU:HG	2.11	0.51
3:C:59:PHE:HD2	3:C:105:ALA:HB3	1.75	0.51
5:G:158:VAL:HG21	5:H:155:TRP:NE1	2.26	0.51
1:S:994:TRP:CG	1:S:2581:LEU:HD21	2.46	0.51
1:S:1124:ILE:HG13	1:S:1125:GLN:N	2.26	0.51
1:S:1297:PHE:HA	1:S:1301:ILE:HG12	1.93	0.51
1:S:1341:ILE:HD12	1:S:1368:LEU:HD21	1.93	0.51
1:S:2102:LYS:NZ	1:S:2152:ASN:O	2.44	0.51
1:S:2435:CYS:HA	1:S:2438:ILE:HD12	1.93	0.51
1:S:2572:TYR:HE1	1:S:2791:ILE:HD11	1.75	0.51
1:S:3454:LEU:HD22	1:S:3461:ALA:HB1	1.92	0.51
1:S:3789:ARG:HE	1:S:3938:ILE:HD11	1.76	0.51
1:A:410:MET:HA	1:A:413:PHE:HD2	1.75	0.51
1:A:1294:VAL:O	1:A:1367:HIS:NE2	2.41	0.51
1:A:1558:TYR:O	1:A:1562:LEU:HG	2.10	0.51
1:A:1606:ARG:HA	1:A:1608:ARG:HH21	1.76	0.51
1:A:2572:TYR:HE1	1:A:2791:ILE:HD11	1.75	0.51
1:A:3144:PHE:HA	1:A:3147:LYS:HD3	1.93	0.51
1:A:4073:ALA:HB1	1:A:4076:ASP:HB3	1.92	0.51
2:B:203:MET:HE3	2:B:237:SER:HB2	1.92	0.51
2:B:480:ASN:HB2	3:C:426:PHE:CE2	2.45	0.51
3:C:155:LYS:HE2	3:C:215:LEU:HA	1.92	0.51
3:C:265:LYS:HE3	3:C:268:LEU:HD11	1.93	0.51
3:C:732:ILE:H	1:S:1913:LYS:HD3	1.75	0.51
5:G:151:LEU:HD12	5:H:148:ASN:OD1	2.11	0.51
6:I:658:ILE:HD11	6:I:734:SER:HA	1.93	0.51
3:L:412:ILE:HG23	3:L:417:GLU:HG2	1.93	0.51
3:L:440:ASN:O	3:L:442:LYS:NZ	2.33	0.51
1:S:73:LEU:HB3	1:S:78:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:73:LEU:N	1:S:82:ARG:HH22	2.01	0.51
1:S:129:ASP:HA	1:S:132:ILE:HG12	1.92	0.51
1:S:3034:PRO:O	1:S:3038:GLU:N	2.41	0.51
1:S:3171:ALA:HA	1:S:3179:TRP:HZ2	1.76	0.51
1:A:923:ASP:O	1:A:926:THR:N	2.42	0.50
1:A:2440:TYR:HA	1:A:2443:MET:HE1	1.93	0.50
1:A:3880:ALA:O	1:A:3885:ARG:NH2	2.40	0.50
5:P:7:ARG:H	5:P:76:SER:HB2	1.76	0.50
6:R:725:TRP:NE1	6:R:736:VAL:O	2.42	0.50
1:S:356:ASN:HB3	1:S:358:GLU:HG2	1.93	0.50
1:S:2414:GLN:OE1	1:S:2414:GLN:N	2.42	0.50
1:S:2508:GLN:NE2	1:S:2549:LYS:HE2	2.26	0.50
1:S:2737:GLU:O	1:S:2741:LEU:N	2.37	0.50
2:T:106:GLN:HB3	2:T:115:ARG:HH21	1.76	0.50
1:A:128:LEU:HA	1:A:173:LYS:NZ	2.25	0.50
1:A:2773:ARG:HH22	1:A:2785:ILE:HG21	1.75	0.50
1:A:3046:ARG:NH1	1:A:3085:GLU:OE2	2.43	0.50
1:A:3898:LEU:HD23	1:A:3901:ARG:HH12	1.76	0.50
1:A:4113:ASP:O	1:A:4117:LEU:HG	2.11	0.50
3:C:205:LEU:HG	3:C:209:LYS:HD2	1.92	0.50
1:S:923:ASP:O	1:S:926:THR:N	2.44	0.50
1:S:2921:LEU:O	1:S:2925:GLU:HG3	2.10	0.50
1:S:3913:ILE:HD13	1:S:3987:ALA:HB3	1.92	0.50
1:A:1916:ILE:HG13	1:A:1917:LYS:N	2.27	0.50
1:A:2893:LEU:HB3	1:A:2926:LEU:HD13	1.92	0.50
1:A:3700:GLU:OE2	1:A:3716:HIS:ND1	2.45	0.50
5:G:21:GLN:HG2	5:G:33:VAL:HG13	1.92	0.50
5:G:158:VAL:HG21	5:H:155:TRP:HE1	1.77	0.50
1:S:667:TYR:HA	1:S:732:PHE:CE2	2.46	0.50
1:S:726:LEU:HD12	1:S:729:CYS:HB2	1.93	0.50
1:S:1474:ASP:N	1:S:1474:ASP:OD1	2.44	0.50
1:S:1750:LEU:HD21	1:S:1759:LEU:HA	1.93	0.50
1:S:1827:LEU:O	1:S:1831:CYS:N	2.45	0.50
1:S:2133:LEU:HD22	1:S:2146:LEU:HB3	1.93	0.50
1:S:3239:LYS:HB3	1:S:3262:LEU:HD11	1.93	0.50
1:S:3420:CYS:HB2	1:S:3446:VAL:HG11	1.93	0.50
1:A:1171:TRP:O	1:A:1175:HIS:ND1	2.44	0.50
1:A:1675:TYR:O	1:A:1678:LEU:HB2	2.12	0.50
1:A:2090:ARG:HH21	1:A:2092:GLU:HG3	1.77	0.50
1:A:2271:SER:O	1:A:2274:ILE:HB	2.11	0.50
1:A:3912:CYS:HA	1:A:3915:HIS:NE2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:ILE:O	3:C:202:LYS:NZ	2.44	0.50
5:G:148:ASN:ND2	5:H:148:ASN:HB2	2.26	0.50
3:L:656:ASN:HB3	3:L:688:LYS:HB2	1.94	0.50
5:P:176:LEU:HD23	6:R:805:TRP:CH2	2.46	0.50
5:Q:177:TYR:O	5:Q:181:ILE:HD12	2.11	0.50
6:R:746:MET:HG2	6:R:751:LYS:HG3	1.94	0.50
1:S:1326:GLU:HB3	1:S:1329:ARG:NE	2.26	0.50
1:S:2440:TYR:HA	1:S:2443:MET:CE	2.42	0.50
2:T:59:PRO:HB3	2:T:205:LEU:HD11	1.93	0.50
3:C:405:VAL:O	3:C:423:GLN:NE2	2.44	0.50
6:I:722:LYS:HB2	6:I:742:PHE:HB2	1.93	0.50
1:S:432:THR:OG1	1:S:433:PRO:HD3	2.11	0.50
1:S:2209:GLU:HB2	1:S:2248:CYS:HB2	1.94	0.50
1:S:3940:ILE:HG22	1:S:3941:ASP:H	1.76	0.50
2:T:74:LYS:HE2	2:T:81:ASP:HB2	1.94	0.50
2:T:282:LYS:HD2	2:T:283:PRO:HD2	1.91	0.50
1:A:192:ASN:O	1:A:196:LEU:HG	2.12	0.50
1:A:409:GLN:HG2	1:A:413:PHE:CE2	2.46	0.50
1:A:1115:HIS:HB3	1:A:1180:GLN:HG3	1.93	0.50
2:B:295:PRO:O	3:C:298:ASN:ND2	2.45	0.50
3:C:654:ARG:HA	3:C:657:ASN:HD21	1.76	0.50
3:L:186:GLY:N	3:L:228:SER:OG	2.43	0.50
3:L:353:ARG:HA	3:L:356:PHE:CD2	2.46	0.50
4:M:195:PRO:HG3	2:T:244:ARG:HD3	1.94	0.50
1:S:110:THR:O	1:S:114:VAL:N	2.36	0.50
1:S:897:PRO:HA	1:S:902:LYS:HE3	1.93	0.50
1:S:2254:ARG:NE	1:S:2294:ILE:HG13	2.21	0.50
1:A:1389:VAL:HG22	1:A:1390:GLN:H	1.77	0.50
1:A:2737:GLU:O	1:A:2741:LEU:N	2.41	0.50
3:C:496:HIS:CG	3:C:506:PRO:HD3	2.47	0.50
6:I:666:VAL:HG11	6:I:679:GLU:HG2	1.94	0.50
1:S:542:ASP:OD1	1:S:543:SER:N	2.42	0.50
1:S:573:LEU:HD21	1:S:649:PHE:HD1	1.75	0.50
1:S:861:SER:N	1:S:3136:THR:HG21	2.26	0.50
1:S:2207:LYS:HA	1:S:2210:VAL:HG12	1.94	0.50
1:S:2331:MET:HE1	1:S:2337:LEU:H	1.77	0.50
1:S:3258:LEU:O	1:S:3261:GLU:HG3	2.12	0.50
1:A:125:ILE:H	1:A:125:ILE:HD12	1.77	0.50
1:A:887:ASP:HB2	1:A:961:LEU:HD21	1.92	0.50
1:A:1457:GLN:HG3	1:A:1460:ARG:HH21	1.77	0.50
1:A:2269:ASP:O	1:A:2272:VAL:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2430:GLU:N	1:A:2430:GLU:OE1	2.45	0.50
1:A:2544:SER:HA	1:A:2842:ARG:HH12	1.77	0.50
1:A:3506:LEU:HG	1:A:3515:GLN:HG3	1.93	0.50
3:C:44:ARG:HH12	3:C:488:GLN:HG3	1.77	0.50
3:C:88:PHE:HA	3:C:91:LEU:HD12	1.94	0.50
3:L:599:ARG:O	3:L:603:LYS:NZ	2.31	0.50
3:L:725:VAL:O	3:L:729:LEU:N	2.43	0.50
6:R:722:LYS:HB2	6:R:742:PHE:HB2	1.94	0.50
1:S:360:SER:HB2	1:S:364:ARG:NH1	2.26	0.50
1:S:571:SER:O	1:S:574:LYS:HG2	2.12	0.50
1:S:1055:ASN:OD1	1:S:1058:SER:N	2.39	0.50
1:S:2196:TRP:HB2	1:S:2199:LEU:HD13	1.94	0.50
1:S:2257:PHE:HA	1:S:2260:PHE:CZ	2.46	0.50
1:S:3179:TRP:O	1:S:3183:ILE:HG12	2.11	0.50
1:S:3467:ARG:HH22	1:S:3474:ARG:HH11	1.59	0.50
1:A:741:ILE:HA	1:A:748:TYR:HE2	1.77	0.50
1:A:1066:LEU:HA	1:A:1069:HIS:CD2	2.47	0.50
1:A:1864:ASP:OD1	1:A:1864:ASP:N	2.45	0.50
1:A:1948:ALA:HA	1:A:1951:VAL:HG22	1.93	0.50
3:L:434:MET:O	2:T:253:LYS:NZ	2.44	0.50
1:S:541:MET:SD	1:S:560:LEU:HB2	2.52	0.50
1:S:985:GLU:HG2	1:S:986:PRO:HD3	1.94	0.50
1:S:1873:TYR:O	1:S:1877:LEU:HD23	2.12	0.50
2:T:341:ASP:OD2	2:T:399:ARG:NH1	2.45	0.50
2:T:422:ASP:N	2:T:422:ASP:OD1	2.43	0.50
1:A:789:TYR:HD1	1:A:792:ILE:HD12	1.76	0.49
1:A:1413:ASP:O	1:A:1416:GLU:HB3	2.12	0.49
1:A:1876:ILE:HG13	1:A:1877:LEU:HD22	1.94	0.49
1:A:2094:MET:HB2	1:A:2097:LEU:HD12	1.93	0.49
2:B:399:ARG:NH2	3:C:516:LEU:O	2.45	0.49
5:Q:179:ARG:NH2	6:R:782:LYS:O	2.32	0.49
1:S:1868:THR:O	1:S:1871:MET:HB2	2.12	0.49
1:S:2357:GLU:HA	1:S:2360:PHE:HB3	1.94	0.49
1:A:672:ILE:O	1:A:676:ASN:ND2	2.44	0.49
1:A:1086:TYR:CE1	1:A:1133:HIS:HB3	2.47	0.49
1:A:1407:LYS:HG3	1:A:1412:LYS:HE3	1.94	0.49
1:A:2356:MET:HE1	1:A:2359:LYS:H	1.77	0.49
1:A:2363:CYS:HA	1:A:2366:LYS:HE2	1.94	0.49
1:A:2988:GLU:HA	1:A:2991:LYS:HE2	1.93	0.49
1:A:3160:LEU:O	1:A:3167:ARG:NH2	2.44	0.49
1:A:3178:ILE:O	1:A:3182:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:ARG:O	2:B:162:SER:OG	2.29	0.49
3:C:605:LYS:HB2	3:C:609:PHE:HE2	1.76	0.49
3:L:656:ASN:CG	3:L:689:GLU:H	2.15	0.49
3:L:677:ILE:HA	3:L:680:GLN:HG2	1.94	0.49
1:S:479:ILE:HA	1:S:482:VAL:HG22	1.94	0.49
1:S:939:MET:HE2	1:S:939:MET:HA	1.95	0.49
1:S:1367:HIS:HB2	1:S:1370:ARG:HH22	1.76	0.49
1:S:1949:ILE:HG12	1:S:2100:LEU:HD22	1.94	0.49
1:S:2168:LEU:HA	1:S:2171:LEU:HD12	1.93	0.49
1:S:2439:ILE:O	1:S:2443:MET:HE3	2.12	0.49
1:S:2822:LYS:HZ3	1:S:2823:PHE:HE2	1.60	0.49
1:S:3126:LEU:O	1:S:3130:GLN:NE2	2.45	0.49
1:S:3228:SER:HA	1:S:3231:ILE:HG12	1.94	0.49
1:S:3998:LEU:O	1:S:4002:MET:HG2	2.13	0.49
1:A:418:ALA:HB2	1:A:464:VAL:HG12	1.93	0.49
1:A:989:MET:SD	1:A:990:GLN:HG3	2.52	0.49
1:A:1560:TYR:O	1:A:1564:SER:OG	2.20	0.49
1:A:2422:GLN:HA	1:A:2425:ARG:HG3	1.94	0.49
2:B:102:ILE:HG21	2:B:149:VAL:HG21	1.92	0.49
5:H:143:HIS:O	5:H:146:LYS:HG3	2.12	0.49
6:R:817:THR:H	6:R:851:LYS:HB2	1.78	0.49
1:S:296:VAL:HA	1:S:299:LYS:HG2	1.94	0.49
1:S:1740:VAL:HA	1:S:1743:MET:HG2	1.93	0.49
1:S:1844:VAL:HG23	1:S:1845:VAL:H	1.76	0.49
1:S:2724:ASP:OD1	1:S:2724:ASP:N	2.43	0.49
1:S:3354:ASP:OD1	1:S:3354:ASP:N	2.46	0.49
2:T:365:SER:HB2	2:T:435:VAL:HG12	1.94	0.49
2:T:531:PRO:HD2	2:T:534:TYR:HD2	1.78	0.49
1:A:345:PHE:HB3	1:A:366:TYR:CE1	2.48	0.49
1:A:762:TYR:CD2	1:A:764:PRO:HD2	2.47	0.49
1:A:2455:LEU:HD12	1:A:2458:VAL:HB	1.94	0.49
1:A:3962:ARG:HD2	1:A:4124:TRP:CZ2	2.47	0.49
1:S:2376:ASP:HA	1:S:2379:MET:HG2	1.94	0.49
1:S:2587:GLN:O	1:S:2777:HIS:N	2.46	0.49
1:S:3499:ILE:HA	1:S:3502:MET:SD	2.52	0.49
1:S:3842:TRP:HB3	1:S:3855:TYR:HD1	1.78	0.49
1:A:163:LYS:NZ	2:B:311:LEU:O	2.39	0.49
1:A:371:GLY:HA2	1:A:423:TYR:CE2	2.47	0.49
1:A:1256:TRP:CE2	1:A:1260:LEU:HD11	2.47	0.49
1:A:2402:LEU:HD12	1:A:2441:LYS:HD3	1.95	0.49
2:B:388:LYS:O	2:B:392:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:68:LEU:HD13	3:L:113:VAL:HG22	1.94	0.49
3:L:594:PRO:HG2	3:L:619:HIS:HD2	1.78	0.49
1:S:80:GLU:O	1:S:83:GLU:HG3	2.12	0.49
1:S:540:MET:O	1:S:544:ILE:HG12	2.11	0.49
1:S:1447:ARG:NH1	1:S:1448:LEU:HG	2.27	0.49
1:S:1626:TRP:CZ2	1:S:1674:THR:HG21	2.47	0.49
1:S:1712:ARG:HA	1:S:1715:GLU:OE1	2.13	0.49
1:S:1754:GLN:HE22	1:S:1788:ARG:CZ	2.26	0.49
1:S:3245:SER:O	1:S:3249:GLN:NE2	2.45	0.49
1:A:1851:LEU:HB3	1:A:1852:LYS:HZ2	1.78	0.49
1:A:2216:LEU:HD11	1:A:2249:LEU:HD22	1.95	0.49
1:A:3267:LYS:HA	1:A:3273:LEU:HD22	1.95	0.49
4:D:86:ALA:HB3	4:D:97:THR:HB	1.94	0.49
4:D:184:SER:OG	4:D:187:ASN:O	2.31	0.49
5:Q:36:LEU:HD11	5:Q:95:PHE:HB2	1.94	0.49
6:R:817:THR:N	6:R:851:LYS:HB2	2.27	0.49
6:R:864:ILE:HA	6:R:889:LEU:HD11	1.94	0.49
1:S:740:ILE:HG13	1:S:741:ILE:HG23	1.94	0.49
1:A:460:ALA:O	1:A:464:VAL:HG13	2.12	0.49
1:A:752:LEU:O	1:A:755:ALA:HB3	2.13	0.49
1:A:917:LEU:O	1:A:927:LYS:NZ	2.38	0.49
1:A:1016:GLY:O	1:A:1026:ARG:HG2	2.12	0.49
1:A:2379:MET:HA	1:A:2382:VAL:HG12	1.94	0.49
1:A:3496:ILE:O	1:A:3499:ILE:HG12	2.12	0.49
3:L:344:GLY:HA3	2:T:471:PHE:CE1	2.47	0.49
3:L:492:GLN:HE21	3:L:506:PRO:HB2	1.77	0.49
1:S:297:LEU:HD13	1:S:316:LEU:HA	1.95	0.49
1:S:2512:ASP:HB2	1:S:2518:GLN:HG2	1.93	0.49
1:A:12:LEU:HA	1:A:41:GLU:OE2	2.12	0.49
1:A:785:MET:HA	1:A:788:TYR:CZ	2.48	0.49
1:A:3136:THR:HA	1:A:3139:GLN:HG3	1.94	0.49
1:A:4094:PRO:HB2	1:A:4098:LEU:HD13	1.94	0.49
3:C:645:GLU:HA	3:C:648:LYS:HE2	1.93	0.49
3:L:35:LYS:HA	3:L:38:ILE:HG12	1.94	0.49
3:L:322:PRO:HB3	2:T:288:LEU:HD11	1.94	0.49
1:S:71:LYS:HB3	1:S:82:ARG:NH2	2.23	0.49
1:S:392:CYS:HA	1:S:395:MET:HB3	1.94	0.49
1:S:1419:LEU:HD21	1:S:1467:ILE:HB	1.94	0.49
1:S:2257:PHE:HA	1:S:2260:PHE:CE2	2.47	0.49
1:A:3064:PHE:HA	1:A:3067:LYS:HD2	1.94	0.49
1:A:3419:PHE:O	1:A:3423:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3468:LEU:O	1:A:3472:ILE:HG12	2.12	0.49
1:A:3871:PHE:HB2	1:A:4117:LEU:HA	1.94	0.49
3:L:497:ARG:HH11	3:L:501:PRO:HA	1.77	0.49
1:S:938:VAL:HA	1:S:941:MET:HG3	1.95	0.49
1:S:1034:ARG:HB2	1:S:1085:ILE:HG22	1.95	0.49
1:S:1558:TYR:O	1:S:1562:LEU:HG	2.12	0.49
1:S:3314:SER:OG	1:S:3318:LYS:HG3	2.13	0.49
1:S:3964:THR:HG23	1:S:3966:GLN:H	1.77	0.49
1:A:19:LEU:HD22	1:A:34:LEU:HA	1.94	0.49
1:A:25:CYS:SG	1:A:26:GLY:N	2.85	0.49
1:A:67:VAL:O	1:A:68:PHE:C	2.52	0.49
1:A:72:SER:HA	1:A:119:ARG:HH12	1.78	0.49
1:A:1379:PRO:O	1:A:1382:ILE:HG12	2.13	0.49
1:A:1614:GLN:O	1:A:1618:LEU:HD23	2.13	0.49
1:A:2212:ALA:O	1:A:2216:LEU:HG	2.12	0.49
1:A:2251:ILE:HD11	1:A:2285:LEU:HD13	1.93	0.49
1:A:2752:LYS:HD3	1:A:2755:LYS:HE3	1.95	0.49
1:A:2856:SER:HB3	1:A:2885:GLN:HE21	1.78	0.49
1:A:2916:LEU:HD13	1:A:2946:GLU:OE1	2.13	0.49
2:B:250:GLU:O	2:B:250:GLU:HG2	2.13	0.49
2:B:411:VAL:HG12	2:B:436:PHE:HA	1.95	0.49
3:C:237:PHE:HA	3:C:240:ILE:HG12	1.95	0.49
5:G:7:ARG:H	5:G:76:SER:HB2	1.77	0.49
4:M:20:PHE:CD1	4:M:43:ASP:HB3	2.48	0.49
5:P:20:LEU:HD12	5:P:22:VAL:HG13	1.95	0.49
1:S:1935:GLU:O	1:S:1939:LEU:HG	2.13	0.49
1:S:3097:ASP:OD1	1:S:3098:ARG:N	2.39	0.49
1:S:4113:ASP:O	1:S:4117:LEU:HG	2.13	0.49
1:A:2328:ARG:HB2	1:A:2370:SER:O	2.13	0.48
1:A:2443:MET:SD	1:A:2444:PRO:HD3	2.53	0.48
1:A:3478:GLU:O	1:A:3482:LEU:HG	2.12	0.48
3:C:270:GLU:HG3	3:C:487:PHE:HE2	1.78	0.48
3:L:595:ALA:HA	3:L:598:PHE:CE2	2.48	0.48
1:S:114:VAL:O	1:S:119:ARG:HB2	2.13	0.48
1:S:149:ILE:O	1:S:153:PHE:N	2.38	0.48
1:S:172:GLU:HG3	1:S:220:LEU:HG	1.95	0.48
1:S:738:HIS:O	1:S:742:GLU:HG3	2.13	0.48
1:S:1779:GLN:O	1:S:1783:ARG:HG2	2.13	0.48
1:S:3443:PRO:HA	1:S:3446:VAL:HG22	1.95	0.48
1:A:1348:LEU:O	1:A:1352:SER:OG	2.28	0.48
1:A:1725:GLN:NE2	1:A:1769:GLU:HB2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:TRP:O	1:A:2167:PRO:HD2	2.13	0.48
1:A:2180:GLU:HG3	1:A:2184:TYR:HD2	1.78	0.48
1:A:3496:ILE:HD12	1:A:3707:GLY:N	2.28	0.48
2:B:484:GLN:O	2:B:488:ARG:HD3	2.13	0.48
3:C:324:SER:OG	3:C:325:LYS:N	2.45	0.48
4:M:40:TYR:HD2	4:M:47:LEU:HD11	1.77	0.48
1:S:1015:ASP:OD1	1:S:1016:GLY:N	2.44	0.48
1:S:1630:ASP:HA	1:S:1633:TRP:CZ2	2.48	0.48
1:S:2151:ILE:HG12	1:S:2192:THR:HG21	1.95	0.48
1:S:2233:HIS:CE1	1:S:2237:ILE:HD11	2.48	0.48
1:S:2382:VAL:O	1:S:2386:LEU:HG	2.13	0.48
1:S:2497:GLU:HA	1:S:2500:LYS:HD2	1.94	0.48
1:S:2792:THR:OG1	1:S:2793:PRO:HD3	2.13	0.48
1:S:3771:MET:O	1:S:3775:LEU:HG	2.12	0.48
2:T:64:ILE:O	2:T:68:GLN:HG2	2.13	0.48
1:A:924:ARG:HH21	1:A:2766:ASP:HB3	1.78	0.48
1:A:2981:TRP:HD1	1:A:2984:GLY:HA2	1.77	0.48
1:A:3158:LYS:HG3	1:A:3159:ARG:HD3	1.94	0.48
2:B:460:GLY:HA2	2:B:463:LYS:HD2	1.95	0.48
3:C:674:PHE:HB2	3:C:675:TRP:CE3	2.48	0.48
3:L:363:LYS:NZ	3:L:416:TYR:OH	2.26	0.48
1:S:782:ARG:HD2	1:S:786:GLN:HB2	1.95	0.48
1:S:1038:LYS:HG2	1:S:1042:LYS:HD3	1.95	0.48
1:A:1513:GLY:HA2	1:A:1516:GLU:OE2	2.14	0.48
1:A:2283:ASN:HB3	1:A:2285:LEU:HG	1.96	0.48
1:A:2573:PRO:O	1:A:2786:LYS:NZ	2.30	0.48
1:A:2987:THR:HG23	1:A:2990:GLU:H	1.77	0.48
2:B:203:MET:CE	2:B:239:LEU:HG	2.43	0.48
2:B:434:LEU:HG	2:B:436:PHE:HE1	1.79	0.48
5:H:22:VAL:HG13	5:H:35:THR:H	1.79	0.48
6:R:813:PHE:HA	6:R:850:ALA:HB3	1.94	0.48
1:S:801:LYS:HZ3	1:S:3125:ARG:HH22	1.59	0.48
1:S:848:LEU:O	1:S:852:ARG:HG3	2.14	0.48
1:S:914:VAL:HA	1:S:917:LEU:HD12	1.94	0.48
1:S:2256:ILE:H	1:S:2256:ILE:HD12	1.78	0.48
2:T:168:LEU:HD23	2:T:168:LEU:H	1.77	0.48
1:A:614:PRO:HB2	1:A:617:PRO:HG3	1.95	0.48
1:A:898:PHE:HB2	1:A:901:MET:O	2.12	0.48
1:A:1878:ASP:OD1	1:A:1879:VAL:N	2.47	0.48
1:A:2258:GLU:HA	1:A:2261:SER:OG	2.13	0.48
1:A:3048:LYS:O	1:A:3052:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HB3	2:B:88:TYR:CE1	2.48	0.48
3:L:496:HIS:CD2	3:L:506:PRO:HD3	2.48	0.48
3:L:528:ILE:O	3:L:531:SER:OG	2.25	0.48
1:S:19:LEU:HD22	1:S:34:LEU:HA	1.94	0.48
1:S:358:GLU:HG3	1:S:359:LEU:HD12	1.96	0.48
1:S:898:PHE:O	1:S:902:LYS:NZ	2.36	0.48
1:S:960:GLN:O	1:S:964:ARG:HG2	2.13	0.48
1:S:990:GLN:HG3	1:S:2779:ASP:C	2.34	0.48
1:S:1415:LEU:HA	1:S:1418:HIS:HB2	1.95	0.48
1:S:2257:PHE:HB2	1:S:2299:TYR:HE1	1.78	0.48
1:S:2378:PHE:O	1:S:2382:VAL:N	2.31	0.48
1:S:2531:LEU:HB3	1:S:2538:ARG:NE	2.29	0.48
1:S:3728:VAL:HG22	1:S:3736:LYS:HG3	1.95	0.48
2:T:288:LEU:HD13	2:T:293:ASN:HA	1.94	0.48
2:T:299:LYS:NZ	2:T:301:ARG:HD2	2.29	0.48
1:A:15:LEU:O	1:A:19:LEU:HG	2.14	0.48
1:A:1340:ARG:O	1:A:1343:GLU:HG2	2.14	0.48
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.95	0.48
1:A:1731:PRO:HA	1:A:1736:PHE:CD2	2.49	0.48
1:A:2371:PHE:CD2	1:A:2374:LEU:HD23	2.48	0.48
1:A:3515:GLN:HA	1:A:3518:VAL:HG12	1.95	0.48
2:B:537:GLU:OE1	3:C:250:ARG:NH1	2.47	0.48
3:C:411:HIS:N	3:C:418:CYS:O	2.43	0.48
3:L:493:CYS:HB2	2:T:337:LEU:HD21	1.96	0.48
5:Q:174:THR:HG23	6:R:792:MET:HG2	1.95	0.48
1:S:865:GLN:HA	1:S:868:LYS:HZ3	1.78	0.48
1:S:2167:PRO:O	1:S:2170:GLN:HG3	2.13	0.48
1:S:2187:VAL:HG23	1:S:2728:LEU:HD21	1.96	0.48
1:S:2368:THR:HG21	1:S:2400:VAL:HA	1.95	0.48
1:A:343:GLU:HG2	1:A:344:GLN:N	2.28	0.48
1:A:2187:VAL:HA	1:A:2190:VAL:HG12	1.96	0.48
1:A:2439:ILE:HA	1:A:2442:MET:HG3	1.96	0.48
1:A:2452:ARG:NH1	1:A:2497:GLU:OE1	2.45	0.48
1:A:3126:LEU:O	1:A:3130:GLN:HG2	2.13	0.48
1:A:3172:LYS:NZ	1:A:3248:LYS:O	2.47	0.48
1:A:3181:ASP:O	1:A:3185:ASN:ND2	2.47	0.48
1:A:3263:HIS:HB2	1:A:3276:TRP:CE2	2.48	0.48
3:C:24:ILE:HB	3:C:27:ILE:HB	1.96	0.48
3:C:323:PHE:CE2	3:C:328:GLU:HB3	2.48	0.48
1:S:67:VAL:CB	1:S:71:LYS:HD3	2.41	0.48
1:S:1576:ASP:HA	1:S:1579:VAL:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1718:ILE:HA	1:S:1721:HIS:ND1	2.28	0.48
1:S:1747:LEU:HD21	1:S:1778:PHE:HD1	1.78	0.48
1:S:1778:PHE:CE2	1:S:1782:PHE:HE2	2.32	0.48
1:S:3736:LYS:HB2	1:S:3752:VAL:HG12	1.94	0.48
2:T:59:PRO:HA	2:T:62:MET:HG3	1.95	0.48
2:T:98:ASN:O	2:T:100:LYS:NZ	2.47	0.48
1:A:655:LEU:O	1:A:659:ARG:HG2	2.14	0.48
1:A:1755:SER:HB3	1:A:1758:LEU:HD12	1.96	0.48
1:A:2500:LYS:HA	1:A:2503:LYS:HZ2	1.79	0.48
1:A:3679:ASN:HA	1:A:3726:VAL:HG22	1.96	0.48
2:B:106:GLN:HB3	2:B:115:ARG:HH21	1.79	0.48
3:C:11:VAL:HG23	3:C:55:ALA:HB3	1.95	0.48
3:C:44:ARG:NH1	3:C:488:GLN:HG3	2.29	0.48
3:C:148:ASP:N	3:C:148:ASP:OD1	2.46	0.48
5:H:194:LEU:O	5:H:197:LYS:HG3	2.14	0.48
3:L:593:ASN:HB2	1:S:1723:PRO:HG3	1.95	0.48
1:S:910:PHE:CE1	1:S:2807:GLN:HG3	2.49	0.48
1:A:899:ARG:HH12	1:A:2566:THR:HA	1.77	0.48
1:A:1783:ARG:HE	1:A:1830:HIS:CG	2.32	0.48
1:A:3389:VAL:HG11	1:A:3449:LYS:HD3	1.96	0.48
1:A:3588:TRP:CE2	1:A:3609:MET:HE2	2.49	0.48
3:C:64:THR:OG1	3:C:76:ASN:N	2.46	0.48
3:C:198:THR:HG22	3:C:200:GLN:H	1.79	0.48
3:C:431:ARG:HH21	3:C:433:TYR:HE2	1.62	0.48
3:C:528:ILE:O	3:C:532:LYS:HG3	2.14	0.48
3:L:360:GLN:HE22	3:L:362:LEU:HG	1.79	0.48
3:L:613:SER:O	3:L:616:LEU:HG	2.13	0.48
5:P:22:VAL:HA	5:P:32:PHE:HB2	1.96	0.48
1:S:22:ALA:HA	1:S:24:ARG:HH11	1.79	0.48
1:S:246:ARG:HA	1:S:249:PHE:HD2	1.78	0.48
1:S:847:SER:N	1:S:850:GLU:OE2	2.47	0.48
1:S:978:GLN:NE2	1:S:2597:PHE:HA	2.29	0.48
1:S:1102:GLU:HA	1:S:1154:PRO:HB3	1.95	0.48
1:S:1194:PHE:HA	1:S:1197:LEU:HD23	1.94	0.48
1:S:1416:GLU:O	1:S:1419:LEU:HB3	2.13	0.48
1:S:1878:ASP:OD1	1:S:1879:VAL:N	2.47	0.48
1:S:3831:ASP:HB3	1:S:3832:PRO:HD3	1.96	0.48
2:T:371:GLU:OE2	2:T:373:SER:OG	2.31	0.48
1:A:35:ILE:HD12	1:A:80:GLU:HB3	1.95	0.48
1:A:245:SER:O	1:A:249:PHE:HD1	1.96	0.48
1:A:1231:GLN:O	1:A:1235:ILE:N	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1794:GLN:O	1:A:1798:LEU:HG	2.13	0.48
1:A:1935:GLU:O	1:A:1939:LEU:HG	2.14	0.48
1:A:3629:ARG:O	1:A:3633:ILE:HG12	2.14	0.48
2:B:343:PRO:HA	2:B:401:THR:HB	1.96	0.48
3:C:61:THR:N	3:C:76:ASN:O	2.40	0.48
3:C:189:GLY:HA2	3:C:519:PRO:HB3	1.96	0.48
3:C:347:LYS:HG3	3:C:349:SER:H	1.78	0.48
5:Q:175:ASP:HB3	5:Q:179:ARG:CZ	2.43	0.48
1:S:627:VAL:HG22	1:S:669:LEU:HD23	1.96	0.48
1:S:1000:LYS:HA	1:S:1004:GLN:NE2	2.29	0.48
1:S:1210:ASP:HA	1:S:1213:LYS:HD2	1.96	0.48
1:S:2166:SER:OG	1:S:2167:PRO:HD3	2.13	0.48
1:S:2245:TRP:HE3	1:S:2249:LEU:HD21	1.79	0.48
1:S:2346:ALA:HA	1:S:2349:LEU:HD12	1.96	0.48
1:S:2938:VAL:O	1:S:2942:ILE:HG12	2.14	0.48
2:T:95:ASN:ND2	2:T:99:PHE:H	2.10	0.48
1:A:2281:MET:HE1	1:A:2287:PRO:HG3	1.96	0.47
1:A:2402:LEU:HD13	1:A:2438:ILE:HG13	1.95	0.47
1:A:2799:GLN:OE1	1:A:2799:GLN:N	2.46	0.47
4:D:129:ALA:HA	4:M:128:LEU:HD22	1.96	0.47
6:I:713:ILE:HD13	6:I:720:VAL:HG21	1.96	0.47
3:L:40:MET:O	3:L:43:GLN:HG2	2.14	0.47
3:L:132:ILE:HG23	3:L:161:LEU:HG	1.96	0.47
6:R:837:ARG:HH21	6:R:840:ILE:HG21	1.79	0.47
1:S:1919:CYS:O	1:S:1922:ALA:HB3	2.14	0.47
1:S:2201:THR:HG23	1:S:2203:THR:HG22	1.96	0.47
1:S:2864:GLN:HG3	1:S:2865:HIS:CE1	2.49	0.47
1:A:409:GLN:HG2	1:A:413:PHE:HE2	1.79	0.47
1:A:1099:PHE:HD1	1:A:1152:ARG:HH21	1.63	0.47
1:A:2303:LEU:HA	1:A:2306:ASN:HD22	1.79	0.47
1:A:3634:GLN:HA	1:A:3638:LYS:NZ	2.28	0.47
2:B:411:VAL:HA	2:B:437:LEU:HG	1.96	0.47
2:B:482:VAL:HG13	3:C:333:TYR:HB3	1.95	0.47
1:S:200:PHE:CZ	1:S:227:LEU:HD13	2.49	0.47
1:S:1191:PHE:O	1:S:1195:VAL:HG23	2.14	0.47
1:S:1260:LEU:HD21	1:S:1293:ALA:HB2	1.95	0.47
1:S:1419:LEU:HG	1:S:1467:ILE:HD13	1.96	0.47
1:S:1783:ARG:HE	1:S:1830:HIS:HB2	1.79	0.47
1:S:1844:VAL:HG23	1:S:1845:VAL:N	2.30	0.47
1:S:2412:TYR:CZ	1:S:2450:GLU:HB2	2.49	0.47
1:S:2941:GLY:O	1:S:2944:THR:OG1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3925:LEU:HB2	1:S:3962:ARG:HH21	1.80	0.47
2:T:131:PHE:O	2:T:135:MET:HB3	2.14	0.47
1:A:1428:ILE:O	1:A:1432:CYS:N	2.46	0.47
1:A:2231:PHE:O	1:A:2235:LEU:HG	2.15	0.47
1:A:2354:ASN:ND2	1:A:2357:GLU:OE2	2.45	0.47
1:A:2801:ASP:HB3	1:A:2804:ILE:HG12	1.96	0.47
1:A:2923:TRP:O	1:A:2926:LEU:HB3	2.14	0.47
2:B:413:LEU:HD12	2:B:432:PHE:HB3	1.96	0.47
3:C:16:VAL:HG22	3:C:101:GLY:H	1.79	0.47
3:L:331:MET:SD	2:T:489:ASN:HB3	2.54	0.47
3:L:407:VAL:HB	3:L:424:LEU:HD11	1.95	0.47
3:L:674:PHE:HB2	3:L:675:TRP:CE3	2.50	0.47
1:S:850:GLU:HA	1:S:853:ILE:HG12	1.97	0.47
1:S:959:TYR:O	1:S:963:LYS:HG3	2.15	0.47
1:S:1406:LEU:HD12	1:S:1409:SER:HB3	1.96	0.47
1:S:1484:LEU:HB2	1:S:1531:LEU:HD13	1.95	0.47
1:S:2410:GLU:OE2	1:S:2413:PHE:N	2.33	0.47
1:S:2833:THR:HG21	1:S:2867:ALA:HB1	1.96	0.47
1:S:3967:PHE:O	1:S:3970:LEU:HD22	2.14	0.47
1:A:159:GLU:HA	2:B:301:ARG:HH12	1.80	0.47
1:A:179:GLY:C	1:A:230:LEU:HD23	2.34	0.47
1:A:1215:GLU:HB3	1:A:1218:SER:HB2	1.96	0.47
1:A:2340:SER:O	1:A:2344:LEU:HG	2.14	0.47
1:A:3008:TRP:HB2	1:A:3051:LEU:HD23	1.96	0.47
1:A:3564:GLN:NE2	1:A:3697:ASN:HB3	2.29	0.47
1:A:3915:HIS:HE1	1:A:3961:PHE:HA	1.78	0.47
1:A:4002:MET:SD	1:A:4044:ILE:HG22	2.54	0.47
3:C:43:GLN:NE2	3:C:491:PHE:O	2.40	0.47
3:C:605:LYS:HB2	3:C:609:PHE:CE2	2.49	0.47
5:H:179:ARG:HD3	6:I:781:ILE:HD12	1.95	0.47
1:S:382:ASP:HA	1:S:385:TYR:HB3	1.96	0.47
1:S:2231:PHE:O	1:S:2235:LEU:HG	2.14	0.47
1:S:3863:ASN:H	1:S:3866:GLU:HG3	1.78	0.47
1:S:4090:ARG:NH2	1:S:4106:CYS:HA	2.20	0.47
2:T:206:LYS:N	2:T:235:GLU:HB3	2.30	0.47
2:T:239:LEU:HD23	2:T:242:LEU:HD12	1.95	0.47
1:A:115:TYR:HB2	1:A:130:LEU:HD22	1.96	0.47
1:A:560:LEU:O	1:A:564:LEU:HG	2.14	0.47
1:A:1008:ALA:O	1:A:1011:GLU:HG2	2.14	0.47
1:A:1039:TRP:NE1	1:A:1043:GLN:OE1	2.44	0.47
1:A:1058:SER:O	1:A:1062:ARG:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2141:ASN:O	1:A:2144:LEU:HG	2.14	0.47
1:A:2147:ALA:O	1:A:2151:ILE:HG13	2.14	0.47
1:A:3320:ILE:HG22	1:A:3391:ALA:HB1	1.95	0.47
1:A:4086:ASP:N	1:A:4086:ASP:OD1	2.47	0.47
3:L:93:ASP:HA	3:L:97:LYS:HD3	1.97	0.47
3:L:485:PRO:HG2	3:L:486:ARG:NH2	2.29	0.47
3:L:605:LYS:HB2	3:L:609:PHE:CZ	2.45	0.47
5:P:61:MET:HB2	5:P:65:LYS:HZ1	1.79	0.47
5:Q:21:GLN:HB2	5:Q:126:LEU:HD11	1.95	0.47
5:Q:179:ARG:HH11	6:R:778:PHE:HD1	1.61	0.47
1:S:326:MET:O	1:S:330:ASN:N	2.47	0.47
1:S:921:ALA:H	1:S:927:LYS:HZ2	1.63	0.47
1:S:1715:GLU:HA	1:S:1718:ILE:HG12	1.96	0.47
1:S:2328:ARG:HG2	1:S:2329:TYR:CE1	2.50	0.47
1:S:2385:LEU:HD13	1:S:2389:PHE:HE2	1.79	0.47
1:S:2431:ARG:HA	1:S:2434:VAL:HG22	1.96	0.47
1:S:3306:LEU:O	1:S:3307:LEU:C	2.52	0.47
2:T:461:LYS:NZ	2:T:524:GLU:OE1	2.40	0.47
1:A:80:GLU:HA	1:A:83:GLU:OE1	2.15	0.47
1:A:103:TYR:O	1:A:106:GLU:HB2	2.14	0.47
1:A:981:ARG:O	1:A:984:TYR:N	2.44	0.47
1:A:1208:LEU:HD21	1:A:1276:VAL:HB	1.96	0.47
1:A:1740:VAL:HA	1:A:1743:MET:HG3	1.95	0.47
1:A:2235:LEU:HD13	1:A:2275:GLN:HG2	1.96	0.47
1:A:3814:ASP:OD1	1:A:3815:LEU:N	2.47	0.47
1:A:3985:VAL:HG12	1:A:3989:ARG:NE	2.29	0.47
2:B:338:LYS:HE2	3:C:486:ARG:NH2	2.30	0.47
3:C:83:LEU:HD12	3:C:121:GLU:HB2	1.95	0.47
3:C:496:HIS:NE2	3:C:504:PRO:O	2.47	0.47
3:L:17:GLY:HA2	3:L:103:GLN:O	2.14	0.47
3:L:58:LEU:O	3:L:78:THR:N	2.44	0.47
1:S:114:VAL:O	1:S:119:ARG:NE	2.45	0.47
1:S:220:LEU:HD12	1:S:220:LEU:H	1.79	0.47
1:S:2455:LEU:HD21	1:S:2498:ILE:HG12	1.97	0.47
1:S:3679:ASN:HA	1:S:3726:VAL:HG22	1.97	0.47
1:A:1420:ARG:NH2	1:A:1465:HIS:O	2.47	0.47
1:A:1468:LEU:HD12	1:A:1469:PRO:HD2	1.96	0.47
1:A:1601:LEU:HD23	1:A:1651:LYS:HB3	1.97	0.47
1:A:1872:GLY:HA2	1:A:1875:LYS:HG2	1.95	0.47
1:A:2154:GLU:HA	1:A:2157:PHE:CE1	2.50	0.47
1:A:2786:LYS:O	1:A:2789:SER:OG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2860:ASP:O	1:A:2864:GLN:HG3	2.15	0.47
1:A:2866:ALA:HB1	1:A:2899:ARG:HD2	1.96	0.47
1:A:3190:LEU:HD22	1:A:3235:LYS:HD2	1.96	0.47
1:A:3571:PHE:O	1:A:3575:LEU:HG	2.14	0.47
2:B:357:LYS:HB2	2:B:360:HIS:CG	2.48	0.47
3:C:9:ALA:O	3:C:131:HIS:N	2.41	0.47
3:C:91:LEU:HD13	3:C:495:LEU:HD13	1.97	0.47
3:L:33:GLN:O	3:L:37:VAL:HG23	2.15	0.47
3:L:202:LYS:O	3:L:206:GLU:HG2	2.14	0.47
3:L:246:HIS:HB2	3:L:262:ALA:HB1	1.97	0.47
3:L:323:PHE:CE2	3:L:328:GLU:HB2	2.50	0.47
6:R:727:LEU:O	6:R:731:LYS:HG2	2.14	0.47
1:S:125:ILE:H	1:S:125:ILE:HD12	1.79	0.47
1:S:240:GLU:HG3	1:S:243:GLN:HG2	1.96	0.47
1:S:429:GLU:O	1:S:432:THR:OG1	2.30	0.47
1:S:649:PHE:O	1:S:653:LEU:HB2	2.15	0.47
1:S:1401:ASN:HA	1:S:1404:LYS:HE2	1.97	0.47
1:S:2817:LEU:HD22	1:S:2865:HIS:CD2	2.48	0.47
1:S:2860:ASP:HA	1:S:2863:CYS:SG	2.55	0.47
1:S:3311:ASN:HB3	1:S:3315:TYR:CZ	2.49	0.47
2:T:79:ASP:N	2:T:79:ASP:OD1	2.47	0.47
2:T:172:GLU:HG3	2:T:175:PRO:HD3	1.95	0.47
1:A:1253:THR:O	1:A:1257:LEU:HG	2.14	0.47
1:A:2324:GLY:HA3	1:A:2370:SER:OG	2.15	0.47
1:A:2470:ARG:O	1:A:2473:MET:HG2	2.15	0.47
1:A:2724:ASP:N	1:A:2724:ASP:OD1	2.47	0.47
1:A:2762:LYS:HA	1:A:2765:GLN:HE21	1.79	0.47
1:A:3231:ILE:HG13	1:A:3232:ARG:N	2.30	0.47
1:A:3483:MET:HA	1:A:3486:GLU:CG	2.45	0.47
2:B:367:PHE:CE2	2:B:369:TYR:HB2	2.50	0.47
3:C:312:GLN:NE2	3:C:324:SER:O	2.34	0.47
3:C:377:LEU:O	3:C:381:ILE:HG12	2.14	0.47
3:L:61:THR:OG1	3:L:63:GLY:O	2.33	0.47
6:R:739:GLN:H	6:R:742:PHE:HE2	1.61	0.47
1:S:865:GLN:HE22	1:S:3170:ASP:HA	1.80	0.47
1:S:994:TRP:CZ2	1:S:1000:LYS:HD3	2.50	0.47
1:S:1399:CYS:O	1:S:1403:MET:HG2	2.15	0.47
1:S:1773:VAL:HG12	1:S:1773:VAL:O	2.14	0.47
1:S:1801:VAL:HA	1:S:1804:MET:HG3	1.96	0.47
1:S:2246:LYS:NZ	1:S:2284:ASP:H	2.12	0.47
1:S:2294:ILE:HD12	1:S:2294:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2954:GLN:HA	1:S:2957:LEU:HD12	1.97	0.47
1:S:3525:TYR:OH	1:S:3712:LEU:N	2.36	0.47
2:T:487:PHE:O	2:T:490:LEU:N	2.48	0.47
1:A:344:GLN:O	1:A:348:ILE:HG12	2.15	0.47
1:A:1729:PHE:HB3	1:A:1735:ARG:HG3	1.97	0.47
1:A:3085:GLU:HA	1:A:3088:LEU:HD12	1.96	0.47
1:A:3761:ASP:HB3	1:A:3793:VAL:HG11	1.97	0.47
1:A:3927:ASN:HB3	1:A:3941:ASP:HB2	1.97	0.47
3:C:234:LEU:HD21	3:C:483:PRO:HB3	1.96	0.47
4:D:136:GLU:OE2	4:M:131:ARG:NH1	2.48	0.47
5:H:185:ASN:O	5:H:188:LYS:HG3	2.15	0.47
6:R:818:VAL:HG12	6:R:851:LYS:N	2.29	0.47
1:S:151:GLU:OE1	1:S:151:GLU:N	2.38	0.47
1:S:225:LYS:HE3	1:S:270:ALA:O	2.14	0.47
1:S:2139:PRO:O	1:S:2143:ARG:HG3	2.14	0.47
1:S:2246:LYS:HZ1	1:S:2283:ASN:HA	1.80	0.47
1:S:2443:MET:N	1:S:2444:PRO:HD2	2.30	0.47
1:S:2548:PRO:HB2	1:S:2848:PHE:CD1	2.49	0.47
1:S:3873:LYS:O	1:S:3877:LYS:N	2.46	0.47
2:T:146:VAL:HA	2:T:149:VAL:HG22	1.97	0.47
2:T:351:LYS:HE2	2:T:351:LYS:HB2	1.78	0.47
1:A:209:THR:O	1:A:212:VAL:HG22	2.14	0.47
1:A:1737:ASN:O	1:A:1740:VAL:HG22	2.15	0.47
1:A:2335:ASN:ND2	1:A:2337:LEU:HD23	2.31	0.47
1:A:3075:LYS:O	1:A:3079:GLU:OE1	2.33	0.47
1:A:3793:VAL:HG23	1:A:3803:ILE:HG13	1.97	0.47
1:A:4041:ARG:O	1:A:4044:ILE:HG12	2.15	0.47
2:B:203:MET:CE	2:B:237:SER:HB2	2.45	0.47
2:B:212:ASP:HB3	2:B:215:LEU:HD22	1.97	0.47
3:C:450:GLN:HG2	3:C:536:LEU:HB3	1.97	0.47
3:C:595:ALA:HA	3:C:598:PHE:CE2	2.50	0.47
5:G:48:SER:OG	5:G:49:GLU:N	2.48	0.47
5:H:174:THR:HB	6:I:787:GLN:HE22	1.80	0.47
6:R:710:LYS:O	6:R:714:LEU:HG	2.14	0.47
1:S:127:ALA:O	1:S:131:LEU:HG	2.14	0.47
1:S:1128:CYS:HA	1:S:1131:ILE:HG12	1.97	0.47
1:S:1574:ASN:ND2	1:S:1578:ALA:H	2.13	0.47
1:S:1871:MET:HE3	1:S:1939:LEU:HB2	1.97	0.47
1:S:2953:THR:HG1	1:S:2994:TRP:HE1	1.61	0.47
1:S:2999:LEU:CD2	1:S:3014:CYS:HA	2.45	0.47
1:A:532:ARG:O	1:A:536:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1008:ALA:HA	1:A:1011:GLU:OE2	2.14	0.46
1:A:1504:ASP:HB3	1:A:1507:CYS:HB2	1.97	0.46
1:A:2353:GLN:HG2	1:A:2359:LYS:HZ3	1.80	0.46
1:A:3870:SER:HA	1:A:3873:LYS:HE2	1.97	0.46
6:I:706:ASN:HB2	6:I:709:VAL:HG23	1.96	0.46
3:L:279:VAL:HG12	3:L:286:LYS:N	2.29	0.46
3:L:327:ASP:O	3:L:331:MET:HG2	2.15	0.46
6:R:759:ASP:N	6:R:759:ASP:OD1	2.46	0.46
1:S:1177:GLY:H	1:S:1184:ARG:HG3	1.79	0.46
1:A:1625:HIS:HA	1:A:1628:LYS:HD3	1.97	0.46
1:A:1863:PHE:CD1	3:C:718:VAL:HG23	2.49	0.46
1:A:2735:ASP:N	1:A:2735:ASP:OD1	2.49	0.46
1:A:3011:LEU:O	1:A:3047:SER:OG	2.32	0.46
1:A:3422:GLN:N	1:A:3425:ARG:HH21	2.12	0.46
2:B:303:PHE:HE2	2:B:308:GLY:HA2	1.79	0.46
1:S:156:PHE:O	1:S:159:GLU:HG2	2.15	0.46
1:S:1107:TYR:CD2	1:S:1134:LEU:HD11	2.43	0.46
1:S:3119:VAL:HG13	1:S:3120:LEU:HD23	1.96	0.46
1:S:3589:SER:HB3	1:S:3664:ASN:HD21	1.80	0.46
1:A:69:VAL:O	1:A:70:ARG:C	2.53	0.46
1:A:290:TYR:CE2	1:A:291:VAL:HG13	2.50	0.46
1:A:649:PHE:O	1:A:653:LEU:HG	2.16	0.46
1:A:1333:SER:O	1:A:1337:VAL:HG23	2.15	0.46
1:A:3420:CYS:SG	1:A:3446:VAL:HG11	2.56	0.46
1:A:3428:GLU:OE1	1:A:3474:ARG:NH1	2.49	0.46
1:A:3834:ALA:HB1	1:A:3839:TYR:HE1	1.81	0.46
1:A:3922:ASP:O	1:A:3959:MET:HE1	2.16	0.46
3:C:61:THR:HG21	3:C:78:THR:HB	1.96	0.46
3:L:236:VAL:HG23	3:L:237:PHE:CD2	2.50	0.46
3:L:280:ASP:OD1	3:L:281:ALA:N	2.47	0.46
6:R:748:PRO:HA	6:R:751:LYS:HD2	1.97	0.46
1:S:117:LYS:HG2	1:S:118:ASP:H	1.80	0.46
1:S:2154:GLU:HA	1:S:2157:PHE:CE1	2.50	0.46
1:S:2347:LYS:O	1:S:2351:GLN:N	2.41	0.46
1:S:3454:LEU:HD11	1:S:3462:ARG:HA	1.97	0.46
1:A:1139:GLU:HA	1:A:1197:LEU:HD11	1.96	0.46
1:A:1406:LEU:O	1:A:1412:LYS:HB3	2.16	0.46
1:A:3173:MET:HE3	1:A:3174:ASP:H	1.80	0.46
1:A:4054:ALA:HA	1:A:4096:SER:HA	1.97	0.46
2:B:363:ARG:HD3	2:B:436:PHE:CE2	2.50	0.46
2:B:482:VAL:HG22	3:C:333:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ILE:O	3:C:161:LEU:HA	2.16	0.46
3:C:253:ILE:HB	3:C:257:LEU:HB2	1.97	0.46
6:I:815:ARG:H	6:I:850:ALA:N	2.12	0.46
3:L:151:ILE:HD11	3:L:211:VAL:HG13	1.96	0.46
1:S:382:ASP:O	1:S:385:TYR:HB3	2.16	0.46
1:S:450:SER:HB3	1:S:453:MET:HE3	1.96	0.46
1:S:903:PRO:HB3	1:S:2819:GLU:HB2	1.96	0.46
1:S:943:GLY:O	1:S:946:THR:OG1	2.27	0.46
1:S:1076:LEU:HB3	1:S:1123:THR:OG1	2.16	0.46
1:S:1165:LEU:O	1:S:1169:VAL:HG23	2.15	0.46
1:S:1173:LEU:HB2	1:S:1191:PHE:CE1	2.51	0.46
1:S:1722:PHE:CE1	1:S:1739:TYR:HB3	2.49	0.46
1:S:2133:LEU:HD13	1:S:2146:LEU:HD22	1.96	0.46
1:S:2571:ASP:O	1:S:2787:HIS:ND1	2.48	0.46
1:S:2735:ASP:OD1	1:S:2735:ASP:N	2.46	0.46
1:S:3085:GLU:OE1	1:S:3085:GLU:N	2.41	0.46
1:S:3972:LEU:HB3	1:S:3973:PRO:HD3	1.98	0.46
1:A:391:ARG:NH1	1:A:1737:ASN:OD1	2.49	0.46
1:A:479:ILE:HA	1:A:482:VAL:HG22	1.97	0.46
1:A:523:THR:OG1	1:A:524:TYR:N	2.48	0.46
1:A:719:LYS:HZ1	1:A:1026:ARG:HH22	1.61	0.46
2:B:325:ARG:HB2	3:C:88:PHE:CE1	2.50	0.46
3:C:491:PHE:HD1	3:C:494:LEU:HD12	1.80	0.46
3:C:653:GLN:HA	3:C:656:ASN:ND2	2.30	0.46
5:G:160:GLY:O	5:G:164:LYS:HG2	2.16	0.46
3:L:188:HIS:CE1	3:L:478:PRO:HD2	2.44	0.46
6:R:754:PHE:HA	6:R:757:GLU:HG2	1.98	0.46
1:S:244:THR:O	1:S:248:ILE:HG12	2.15	0.46
1:S:1279:LEU:HD22	1:S:1356:TRP:HE1	1.81	0.46
1:S:1611:GLN:HB2	1:S:1613:HIS:ND1	2.30	0.46
1:S:1737:ASN:HA	1:S:1740:VAL:HG22	1.98	0.46
1:S:1840:PHE:CE2	1:S:1844:VAL:HG12	2.50	0.46
1:S:2395:THR:O	1:S:2398:LEU:HB2	2.15	0.46
1:A:3749:PRO:HB2	1:A:3805:TRP:HB3	1.96	0.46
1:A:4040:PRO:O	1:A:4044:ILE:HG23	2.16	0.46
2:B:158:GLN:OE1	2:B:158:GLN:N	2.49	0.46
2:B:344:GLY:H	2:B:401:THR:HB	1.81	0.46
3:C:233:LYS:HE2	3:C:235:CYS:HB3	1.98	0.46
3:C:461:MET:CE	3:C:526:SER:HB3	2.46	0.46
3:C:528:ILE:O	3:C:531:SER:OG	2.24	0.46
1:S:1023:SER:HA	1:S:1026:ARG:NE	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1135:CYS:HA	1:S:1138:ILE:HG22	1.96	0.46
1:S:2356:MET:SD	1:S:2357:GLU:N	2.89	0.46
1:S:3123:GLN:CD	1:S:3123:GLN:H	2.19	0.46
1:A:2356:MET:SD	1:A:2357:GLU:N	2.89	0.46
1:A:3036:TYR:O	1:A:3039:THR:OG1	2.27	0.46
1:A:3527:GLN:OE1	1:A:3697:ASN:ND2	2.49	0.46
1:A:3675:LYS:HA	1:A:3675:LYS:HD2	1.80	0.46
2:B:530:TYR:CZ	2:B:536:PRO:HB3	2.51	0.46
3:C:460:SER:HA	3:C:525:LYS:HE2	1.98	0.46
3:L:342:VAL:HA	3:L:393:VAL:HA	1.97	0.46
3:L:368:ARG:HD2	3:L:368:ARG:HA	1.80	0.46
3:L:496:HIS:CG	3:L:506:PRO:HD3	2.50	0.46
5:Q:4:LYS:HA	5:Q:4:LYS:HD2	1.83	0.46
5:Q:188:LYS:HD2	5:Q:188:LYS:HA	1.70	0.46
1:S:790:LYS:HA	1:S:869:ASN:HB3	1.96	0.46
1:S:1031:ARG:NH1	1:S:1032:CYS:HB3	2.30	0.46
1:S:1367:HIS:HB2	1:S:1370:ARG:HH12	1.80	0.46
1:S:2439:ILE:HA	1:S:2442:MET:HG3	1.98	0.46
1:S:2894:GLU:HG2	1:S:3973:PRO:HG2	1.98	0.46
1:S:3575:LEU:HD22	1:S:3681:LYS:NZ	2.31	0.46
1:S:3809:THR:OG1	1:S:3930:VAL:O	2.34	0.46
2:T:90:THR:HG23	2:T:92:LYS:O	2.16	0.46
2:T:176:HIS:CD2	2:T:182:LYS:HG2	2.51	0.46
1:A:828:LYS:HB2	1:A:830:VAL:HG22	1.97	0.46
1:A:1290:LEU:O	1:A:1294:VAL:HG23	2.15	0.46
1:A:2595:TRP:CE2	1:A:2762:LYS:HD2	2.50	0.46
1:A:2747:GLY:HA2	1:A:2750:GLU:OE1	2.16	0.46
2:B:318:ARG:HG2	3:C:276:TRP:HB3	1.98	0.46
3:C:16:VAL:O	3:C:101:GLY:N	2.48	0.46
5:H:3:ARG:HD3	5:H:21:GLN:HB2	1.98	0.46
3:L:335:SER:OG	3:L:399:LYS:O	2.34	0.46
5:P:172:LEU:HD13	6:R:809:PRO:HD2	1.98	0.46
6:R:787:GLN:HG3	6:R:791:GLU:OE2	2.16	0.46
1:S:894:PHE:HZ	1:S:2787:HIS:HD2	1.64	0.46
1:S:1075:ARG:NH2	1:S:1117:ASP:OD2	2.48	0.46
1:S:1605:PHE:HE2	1:S:2042:GLN:HA	1.79	0.46
1:S:2187:VAL:HA	1:S:2190:VAL:HG22	1.98	0.46
1:S:3589:SER:HB2	1:S:3593:ARG:CZ	2.45	0.46
1:S:3714:GLU:N	1:S:3714:GLU:OE1	2.49	0.46
2:T:48:MET:HA	2:T:59:PRO:HB2	1.98	0.46
2:T:151:ALA:HB2	2:T:193:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:TRP:CE3	1:A:308:LEU:HD21	2.51	0.46
1:A:389:ILE:HG22	1:A:393:LYS:NZ	2.31	0.46
1:A:923:ASP:O	1:A:926:THR:OG1	2.28	0.46
1:A:1148:ALA:O	1:A:1162:SER:OG	2.24	0.46
1:A:1261:LEU:HD23	1:A:1336:THR:HG22	1.98	0.46
1:A:1715:GLU:HA	1:A:1718:ILE:HG12	1.97	0.46
1:A:3554:PHE:O	1:A:3558:ILE:HG12	2.15	0.46
1:A:3732:LEU:HG	1:A:3733:ARG:HG2	1.97	0.46
1:A:3924:HIS:HD2	1:A:3926:ASN:H	1.64	0.46
1:A:4102:THR:HA	1:A:4105:LYS:HE2	1.97	0.46
2:B:64:ILE:O	2:B:68:GLN:HG2	2.15	0.46
3:C:247:TRP:HB3	3:C:263:ALA:HB3	1.98	0.46
3:C:656:ASN:CG	3:C:688:LYS:HA	2.37	0.46
5:G:185:ASN:O	5:G:189:THR:HG23	2.16	0.46
3:L:89:ASP:O	3:L:92:GLU:HG2	2.15	0.46
3:L:496:HIS:NE2	3:L:504:PRO:O	2.49	0.46
1:S:38:LEU:HD21	1:S:63:PHE:CE2	2.50	0.46
1:S:584:GLU:HB2	1:S:613:HIS:ND1	2.31	0.46
1:S:923:ASP:OD2	1:S:926:THR:OG1	2.28	0.46
1:S:2880:CYS:HB2	1:S:2885:GLN:O	2.15	0.46
1:S:3364:GLY:HA3	1:S:3373:VAL:HA	1.97	0.46
2:T:413:LEU:HD12	2:T:432:PHE:HB3	1.98	0.46
1:A:14:ARG:HH22	1:A:3071:GLY:N	2.13	0.46
1:A:117:LYS:O	1:A:120:ALA:N	2.38	0.46
1:A:475:LEU:O	1:A:479:ILE:HG12	2.15	0.46
1:A:894:PHE:N	1:A:905:ILE:O	2.47	0.46
1:A:1202:ARG:HA	1:A:1202:ARG:HD3	1.76	0.46
1:A:1389:VAL:O	1:A:1392:MET:HG3	2.16	0.46
1:A:1780:SER:O	1:A:1784:ARG:HG3	2.15	0.46
1:A:2313:LYS:HA	1:A:2316:TYR:CZ	2.51	0.46
1:A:2485:ARG:CZ	1:A:2529:THR:HG22	2.46	0.46
1:A:3150:ASN:HD21	1:A:3158:LYS:HE2	1.80	0.46
2:B:287:LYS:HA	3:C:312:GLN:HA	1.97	0.46
2:B:423:GLN:HB2	2:B:425:ILE:HG12	1.98	0.46
3:C:188:HIS:NE2	3:C:232:ARG:HD2	2.31	0.46
6:I:716:ASN:HA	6:I:745:HIS:CE1	2.50	0.46
3:L:250:ARG:HG2	3:L:260:ARG:HA	1.98	0.46
5:Q:118:ASN:HB3	5:Q:121:GLU:HB2	1.98	0.46
1:S:139:ARG:HH22	1:S:230:LEU:HD11	1.81	0.46
1:S:1209:LYS:O	1:S:1213:LYS:HG3	2.16	0.46
1:S:1331:ASN:OD1	1:S:1385:ASN:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1710:LEU:O	1:S:1714:LEU:HG	2.16	0.46
1:S:2232:ARG:HD2	1:S:2235:LEU:HD12	1.96	0.46
1:S:2936:TYR:HE1	1:S:2957:LEU:HB3	1.81	0.46
1:S:3063:THR:O	1:S:3067:LYS:HG2	2.16	0.46
1:A:152:LEU:O	1:A:155:LYS:HG2	2.16	0.45
1:A:238:MET:HA	1:A:243:GLN:HG3	1.98	0.45
1:A:420:VAL:HG13	1:A:421:LEU:HD22	1.97	0.45
1:A:752:LEU:HD22	1:A:776:TRP:HZ3	1.81	0.45
1:A:1023:SER:HA	1:A:1026:ARG:HG3	1.97	0.45
1:A:1776:GLU:HA	1:A:1779:GLN:HG3	1.98	0.45
1:A:3444:ALA:HB2	1:A:3478:GLU:HG3	1.98	0.45
1:A:3585:PHE:CE2	1:A:3664:ASN:HA	2.48	0.45
2:B:399:ARG:HE	2:B:410:PHE:HE1	1.62	0.45
3:C:725:VAL:HG22	1:S:1917:LYS:HE2	1.98	0.45
3:L:127:PHE:O	3:L:130:ARG:NH1	2.49	0.45
3:L:328:GLU:O	3:L:332:LYS:N	2.49	0.45
5:P:188:LYS:HD2	6:R:768:ASP:OD1	2.16	0.45
1:S:560:LEU:O	1:S:564:LEU:HG	2.16	0.45
1:S:1731:PRO:HA	1:S:1736:PHE:CD2	2.51	0.45
1:S:2481:HIS:O	1:S:2485:ARG:NE	2.48	0.45
2:T:289:TYR:CE2	2:T:291:GLU:HB2	2.51	0.45
2:T:513:ALA:HB1	2:T:517:ARG:NH1	2.29	0.45
1:A:865:GLN:HB2	1:A:3168:TYR:CG	2.52	0.45
1:A:2349:LEU:O	1:A:2353:GLN:HB2	2.16	0.45
1:A:3506:LEU:HA	1:A:3515:GLN:HE21	1.80	0.45
1:A:3772:ASN:OD1	1:A:3788:LEU:N	2.48	0.45
1:A:4084:SER:HB3	1:A:4085:LYS:HZ2	1.81	0.45
2:B:106:GLN:NE2	2:B:118:GLU:OE1	2.49	0.45
3:L:276:TRP:CE3	2:T:318:ARG:HB3	2.50	0.45
3:L:521:GLU:O	3:L:525:LYS:HG3	2.15	0.45
1:S:1137:ILE:HG22	1:S:1140:LYS:HZ1	1.81	0.45
1:S:1329:ARG:HA	1:S:1332:TYR:HB2	1.98	0.45
1:S:1574:ASN:HD21	1:S:1578:ALA:H	1.65	0.45
1:S:2440:TYR:HA	1:S:2443:MET:HE1	1.98	0.45
1:S:3778:ASP:HB3	1:S:3781:CYS:HB2	1.99	0.45
1:S:3964:THR:OG1	1:S:4127:TRP:O	2.35	0.45
1:S:4102:THR:O	1:S:4105:LYS:HG3	2.15	0.45
2:T:143:LEU:HG	2:T:176:HIS:CE1	2.52	0.45
2:T:182:LYS:HA	2:T:185:ARG:NE	2.31	0.45
2:T:321:ILE:HG13	2:T:326:GLN:HG3	1.98	0.45
1:A:243:GLN:OE1	1:A:246:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:TYR:O	1:A:389:ILE:HG12	2.16	0.45
1:A:714:VAL:HG23	1:A:733:LEU:HD21	1.97	0.45
1:A:860:GLY:HA3	1:A:3136:THR:HB	1.98	0.45
1:A:1015:ASP:OD1	1:A:1016:GLY:N	2.45	0.45
1:A:2344:LEU:HD23	1:A:2347:LYS:HZ1	1.80	0.45
1:A:3139:GLN:HA	1:A:3142:ILE:HG12	1.98	0.45
1:A:3588:TRP:NE1	1:A:3613:MET:HB2	2.32	0.45
3:L:30:PRO:HB3	3:L:166:PRO:HB3	1.98	0.45
1:S:460:ALA:O	1:S:464:VAL:HG13	2.16	0.45
1:S:489:ARG:O	1:S:492:SER:OG	2.32	0.45
1:S:786:GLN:HA	1:S:789:TYR:CD2	2.51	0.45
1:S:1013:ILE:O	1:S:1017:ILE:HB	2.17	0.45
1:S:1663:THR:O	1:S:1665:HIS:ND1	2.49	0.45
1:S:1867:ILE:O	1:S:1871:MET:HG2	2.16	0.45
1:S:2155:GLU:H	1:S:2155:GLU:CD	2.16	0.45
1:S:2354:ASN:HA	1:S:2357:GLU:HG2	1.98	0.45
1:S:3964:THR:H	1:S:3967:PHE:HD2	1.65	0.45
1:S:3971:MET:SD	1:S:3974:MET:HB2	2.56	0.45
1:A:130:LEU:HD23	1:A:134:LEU:HD23	1.97	0.45
1:A:326:MET:SD	1:A:327:VAL:HG23	2.57	0.45
1:A:628:GLU:HA	1:A:631:ARG:HG2	1.98	0.45
1:A:649:PHE:O	1:A:652:GLU:HG3	2.17	0.45
1:A:1862:THR:N	1:A:1864:ASP:OD1	2.49	0.45
1:A:2147:ALA:HA	1:A:2150:VAL:HG12	1.99	0.45
1:A:2216:LEU:HD23	1:A:2219:LEU:HD21	1.97	0.45
1:A:2311:ARG:NH1	1:A:2312:TYR:HB2	2.32	0.45
1:A:2464:HIS:O	1:A:2470:ARG:NE	2.49	0.45
1:A:2833:THR:HG21	1:A:2867:ALA:HB1	1.99	0.45
1:A:3129:LEU:HA	1:A:3132:VAL:HG22	1.97	0.45
1:A:3264:LYS:O	1:A:3267:LYS:NZ	2.40	0.45
1:A:3809:THR:OG1	1:A:3929:MET:HB3	2.16	0.45
3:C:56:LEU:HD23	3:C:80:HIS:CD2	2.52	0.45
3:C:59:PHE:HB2	3:C:77:ILE:HG12	1.98	0.45
3:C:531:SER:HA	3:C:534:LYS:HG2	1.98	0.45
5:G:176:LEU:O	5:G:179:ARG:HG2	2.17	0.45
3:L:343:LEU:HD11	3:L:394:ARG:HB2	1.98	0.45
3:L:463:LEU:HG	2:T:349:GLY:HA3	1.98	0.45
1:S:645:TRP:HB3	1:S:649:PHE:HB2	1.98	0.45
1:S:655:LEU:O	1:S:659:ARG:HG2	2.16	0.45
1:S:893:SER:H	1:S:944:LYS:HZ2	1.64	0.45
1:S:947:GLN:HB2	1:S:2577:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2184:TYR:CE2	1:S:2734:ARG:HD2	2.51	0.45
1:S:2219:LEU:HD12	1:S:2220:MET:N	2.31	0.45
1:A:26:GLY:HA2	1:A:77:GLU:OE2	2.17	0.45
1:A:202:GLY:O	1:A:205:LYS:HG3	2.16	0.45
1:A:1565:GLU:HA	1:A:1568:ASN:HD22	1.81	0.45
1:A:2376:ASP:HB3	1:A:2404:ARG:HH22	1.81	0.45
1:A:2548:PRO:HB3	1:A:2847:THR:HA	1.98	0.45
1:A:3619:ASP:OD1	1:A:3619:ASP:N	2.49	0.45
2:B:191:GLY:HA2	2:B:194:ARG:HE	1.82	0.45
2:B:269:ILE:HA	2:B:375:VAL:HG11	1.99	0.45
3:C:30:PRO:HB3	3:C:166:PRO:HB3	1.99	0.45
3:C:89:ASP:O	3:C:92:GLU:HG2	2.16	0.45
6:I:659:PHE:CZ	6:I:729:CYS:HB3	2.51	0.45
1:S:153:PHE:CE1	1:S:189:MET:HG3	2.51	0.45
1:S:858:MET:O	1:S:862:LEU:HG	2.17	0.45
1:S:894:PHE:O	1:S:905:ILE:N	2.38	0.45
1:S:986:PRO:HB3	1:S:2777:HIS:HD2	1.81	0.45
1:S:2751:GLN:O	1:S:2755:LYS:HG2	2.16	0.45
1:S:3304:VAL:O	1:S:3305:SER:C	2.54	0.45
1:A:242:PRO:HB2	1:A:246:ARG:HH22	1.82	0.45
1:A:623:PHE:O	1:A:626:LEU:HG	2.17	0.45
1:A:985:GLU:HA	1:A:988:VAL:HG22	1.98	0.45
1:A:1574:ASN:ND2	1:A:1578:ALA:H	2.15	0.45
1:A:2896:ALA:HA	1:A:2899:ARG:HG2	1.99	0.45
1:A:3120:LEU:HA	1:A:3122:HIS:CE1	2.51	0.45
1:A:3140:GLU:O	1:A:3143:SER:OG	2.34	0.45
1:A:3259:LEU:HD12	1:A:3262:LEU:HD12	1.99	0.45
1:A:3274:VAL:O	1:A:3278:GLN:OE1	2.35	0.45
1:A:3416:LEU:HD21	1:A:3446:VAL:HG12	1.97	0.45
2:B:71:TYR:CE1	2:B:83:LEU:HD13	2.52	0.45
6:I:739:GLN:HG2	6:I:741:ARG:HD2	1.99	0.45
3:L:435:PHE:CD2	2:T:429:PRO:HB3	2.52	0.45
5:Q:87:ASN:HB2	5:Q:97:PHE:HA	1.98	0.45
1:S:583:LEU:HD21	1:S:662:LEU:HD11	1.98	0.45
1:S:1045:THR:OG1	1:S:1048:GLN:HG2	2.17	0.45
1:S:2817:LEU:HD13	1:S:2865:HIS:CE1	2.51	0.45
2:T:94:LYS:HE3	2:T:103:TYR:CE1	2.52	0.45
1:A:236:LYS:HE3	1:A:246:ARG:NH2	2.32	0.45
1:A:947:GLN:HB2	1:A:2577:PHE:CE1	2.49	0.45
1:A:1330:TYR:CE2	1:A:1334:LYS:HE2	2.52	0.45
1:A:1418:HIS:O	1:A:1422:LYS:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1580:LEU:O	1:A:1584:GLN:HG2	2.17	0.45
1:A:2167:PRO:O	1:A:2170:GLN:HG3	2.17	0.45
1:A:2264:ASP:HB3	1:A:2309:PHE:CE2	2.51	0.45
1:A:2748:VAL:O	1:A:2752:LYS:HG2	2.15	0.45
1:A:2782:ASP:OD1	1:A:2782:ASP:N	2.48	0.45
1:A:3184:THR:HA	1:A:3187:CYS:SG	2.57	0.45
1:A:3269:ARG:HG3	1:A:3272:TRP:HB3	1.99	0.45
1:A:3303:THR:HB	1:A:3307:LEU:HG	1.98	0.45
3:C:496:HIS:CD2	3:C:506:PRO:HD3	2.52	0.45
3:C:613:SER:O	3:C:616:LEU:HG	2.17	0.45
3:L:357:MET:HA	2:T:364:PRO:HG3	1.99	0.45
4:M:84:ALA:HB1	4:M:99:SER:HB2	1.98	0.45
5:Q:101:LEU:HD23	5:Q:101:LEU:H	1.82	0.45
6:R:659:PHE:HZ	6:R:729:CYS:HB3	1.81	0.45
1:S:296:VAL:HG22	1:S:300:TRP:CD1	2.52	0.45
1:S:475:LEU:O	1:S:479:ILE:HG12	2.17	0.45
1:S:1221:ILE:HD12	1:S:1225:GLU:HA	1.98	0.45
1:S:1479:VAL:O	1:S:1483:LEU:HG	2.16	0.45
1:S:3126:LEU:O	1:S:3130:GLN:HG2	2.17	0.45
1:S:3277:VAL:HG22	1:S:3306:LEU:HD23	1.98	0.45
1:S:4008:GLU:HG3	1:S:4011:PHE:HB2	1.98	0.45
2:T:48:MET:HG2	2:T:60:PHE:HB2	1.97	0.45
2:T:173:ASP:HB3	2:T:217:TYR:CE2	2.52	0.45
2:T:230:ARG:NH1	2:T:233:PHE:H	2.14	0.45
1:A:134:LEU:HD11	1:A:177:LEU:HD11	1.99	0.45
1:A:718:MET:HA	1:A:721:TYR:CD2	2.52	0.45
1:A:1131:ILE:HA	1:A:1134:LEU:HD12	1.99	0.45
1:A:1637:SER:HB2	1:A:1641:THR:OG1	2.16	0.45
1:A:1800:SER:O	1:A:1803:GLU:HG3	2.17	0.45
1:A:2253:TYR:CE1	1:A:2288:TYR:HA	2.52	0.45
1:A:2332:GLU:HB2	1:A:2334:LYS:NZ	2.32	0.45
1:A:2354:ASN:HA	1:A:2357:GLU:OE2	2.17	0.45
1:A:3075:LYS:O	1:A:3078:LEU:HB2	2.17	0.45
2:B:458:GLN:HB3	2:B:525:PHE:HE1	1.81	0.45
3:C:44:ARG:HG3	3:C:237:PHE:CZ	2.52	0.45
3:C:326:VAL:O	3:C:329:GLU:HG3	2.16	0.45
3:L:187:GLY:HA3	3:L:514:ASN:HB3	1.98	0.45
1:S:195:ASN:OD1	1:S:198:ARG:NH2	2.43	0.45
1:S:584:GLU:N	1:S:613:HIS:O	2.38	0.45
1:S:1864:ASP:N	1:S:1864:ASP:OD1	2.47	0.45
1:S:2321:GLU:HA	1:S:2366:LYS:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2438:ILE:O	1:S:2441:LYS:HG2	2.15	0.45
1:S:3633:ILE:HG13	1:S:3634:GLN:N	2.30	0.45
2:T:35:ARG:O	2:T:162:SER:N	2.38	0.45
1:A:529:ASP:O	1:A:532:ARG:HG2	2.16	0.45
1:A:653:LEU:HD22	1:A:669:LEU:HD13	1.99	0.45
1:A:1153:LEU:HD22	1:A:1160:SER:HB2	1.98	0.45
1:A:1205:ASN:OD1	1:A:1205:ASN:N	2.49	0.45
1:A:1271:ILE:O	1:A:1274:ARG:HD2	2.17	0.45
1:A:1431:LEU:HB3	1:A:1447:ARG:CZ	2.47	0.45
1:A:1576:ASP:OD1	1:A:1576:ASP:N	2.50	0.45
1:A:1649:LEU:HA	1:A:1652:ILE:HG12	1.97	0.45
1:A:2771:LEU:HD23	1:A:2771:LEU:H	1.81	0.45
1:A:4120:THR:HG21	1:A:4126:PRO:HB3	1.99	0.45
3:C:39:THR:HA	3:C:42:VAL:HG12	1.98	0.45
3:C:127:PHE:O	3:C:130:ARG:NH1	2.50	0.45
3:C:461:MET:HE1	3:C:526:SER:HB3	1.98	0.45
3:C:598:PHE:HA	3:C:601:LEU:HB3	1.99	0.45
5:H:70:LEU:HD13	5:H:108:LEU:HD11	1.99	0.45
6:I:739:GLN:HA	6:I:758:TYR:CE2	2.52	0.45
6:I:741:ARG:HH11	6:I:742:PHE:HB3	1.81	0.45
3:L:65:ASP:N	3:L:77:ILE:O	2.40	0.45
3:L:162:GLN:NE2	3:L:235:CYS:O	2.43	0.45
3:L:466:LYS:NZ	3:L:471:ASP:O	2.47	0.45
3:L:722:GLY:O	3:L:726:ASP:N	2.39	0.45
5:P:6:SER:HB2	5:P:76:SER:HB2	1.98	0.45
1:S:1368:LEU:HA	1:S:1371:VAL:HG22	1.99	0.45
1:S:1538:LEU:HD13	1:S:1553:PHE:CZ	2.52	0.45
1:S:1756:PRO:HA	1:S:1759:LEU:HD12	1.99	0.45
1:S:2312:TYR:HD2	1:S:2314:GLU:HG3	1.81	0.45
1:S:2440:TYR:HD1	1:S:2476:ILE:HD13	1.81	0.45
1:S:3015:SER:HA	1:S:3044:MET:HG3	1.98	0.45
2:T:60:PHE:O	2:T:64:ILE:HG12	2.16	0.45
2:T:526:LYS:O	2:T:530:TYR:N	2.50	0.45
1:A:245:SER:OG	1:A:246:ARG:N	2.50	0.45
1:A:710:PHE:O	1:A:713:GLU:HG3	2.17	0.45
1:A:865:GLN:HB2	1:A:3168:TYR:CD2	2.51	0.45
1:A:1506:SER:HA	1:A:1509:GLN:NE2	2.32	0.45
1:A:3150:ASN:ND2	1:A:3158:LYS:HE2	2.32	0.45
2:B:364:PRO:HD3	3:C:358:GLY:O	2.16	0.45
3:C:6:ASN:OD1	3:C:126:LYS:NZ	2.36	0.45
3:C:600:VAL:O	3:C:604:GLN:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:720:VAL:N	6:R:743:MET:HE1	2.32	0.45
1:S:32:HIS:O	1:S:36:ARG:HG2	2.17	0.45
1:S:200:PHE:CE2	1:S:227:LEU:HD22	2.51	0.45
1:S:447:PRO:HD3	1:S:527:TYR:CE1	2.52	0.45
1:S:910:PHE:O	1:S:914:VAL:HG12	2.16	0.45
1:S:985:GLU:HA	1:S:988:VAL:HG22	1.99	0.45
1:S:1672:PHE:O	1:S:1675:TYR:HB3	2.16	0.45
1:S:2215:LEU:HA	1:S:2218:PHE:CD2	2.52	0.45
1:S:2365:ASN:HD22	1:S:2396:LEU:HG	1.82	0.45
1:S:2936:TYR:CE1	1:S:2957:LEU:HB3	2.52	0.45
1:S:2962:ARG:HH11	1:S:3252:PHE:HD2	1.65	0.45
1:A:384:MET:O	1:A:387:GLU:HG3	2.17	0.44
1:A:1801:VAL:HA	1:A:1804:MET:HG3	1.99	0.44
1:A:3075:LYS:HA	1:A:3078:LEU:HD12	1.99	0.44
1:A:3275:SER:HA	1:A:3278:GLN:OE1	2.16	0.44
3:C:326:VAL:O	3:C:330:GLN:HG3	2.17	0.44
5:G:166:VAL:O	5:G:169:LYS:NZ	2.48	0.44
3:L:353:ARG:HA	3:L:356:PHE:HD2	1.82	0.44
6:R:665:CYS:O	6:R:701:ILE:N	2.41	0.44
1:S:229:SER:HA	1:S:278:HIS:HE1	1.82	0.44
1:S:244:THR:O	1:S:247:GLU:HB3	2.17	0.44
1:S:1167:ASP:HA	1:S:1170:LYS:NZ	2.33	0.44
1:S:1536:ALA:O	1:S:1555:HIS:ND1	2.48	0.44
1:S:1568:ASN:HA	1:S:1600:MET:HE2	1.97	0.44
1:S:2866:ALA:HA	1:S:2869:LEU:HG	2.00	0.44
1:S:3114:TYR:CD1	1:S:3128:LYS:HG2	2.51	0.44
1:S:3578:LEU:HD11	1:S:3681:LYS:HD2	1.99	0.44
2:T:392:LYS:O	2:T:393:GLU:HG3	2.17	0.44
1:A:241:ASP:N	1:A:242:PRO:HD2	2.33	0.44
1:A:655:LEU:O	1:A:658:THR:OG1	2.28	0.44
1:A:997:ASN:HA	1:A:1043:GLN:HE21	1.82	0.44
1:A:1401:ASN:HA	1:A:1404:LYS:HE2	2.00	0.44
1:A:2225:HIS:CD2	1:A:2230:VAL:HG23	2.52	0.44
1:A:3171:ALA:HA	1:A:3179:TRP:CZ2	2.45	0.44
1:A:3493:TRP:HZ3	1:A:3521:ILE:HG12	1.82	0.44
1:A:3812:LEU:HB2	1:A:3925:LEU:HD21	1.99	0.44
2:B:61:ASP:O	2:B:64:ILE:HG22	2.17	0.44
3:C:74:TYR:HD1	3:C:109:ASP:HB3	1.81	0.44
4:D:44:ALA:HB1	4:M:122:ARG:HB2	1.99	0.44
3:L:33:GLN:HA	3:L:36:LYS:HD2	1.99	0.44
3:L:135:PHE:HE1	3:L:164:PHE:CD1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:547:ASP:OD1	1:S:547:ASP:N	2.47	0.44
1:S:793:LEU:HD12	1:S:870:LEU:HB2	1.99	0.44
1:S:934:LEU:HD23	1:S:937:MET:SD	2.57	0.44
1:S:1528:LEU:O	1:S:1532:LEU:HD23	2.17	0.44
1:S:2287:PRO:HB3	1:S:2326:ILE:CD1	2.47	0.44
1:S:2402:LEU:HD11	1:S:2437:ASP:HB2	1.99	0.44
1:S:2472:GLN:O	1:S:2476:ILE:HG12	2.17	0.44
2:T:125:GLN:HA	2:T:128:GLN:HG2	2.00	0.44
1:A:294:PHE:CE2	1:A:298:LEU:HD11	2.53	0.44
1:A:486:GLY:O	1:A:490:ILE:HG12	2.17	0.44
1:A:1092:GLU:HG3	1:A:1095:LEU:HG	1.99	0.44
1:A:1428:ILE:HA	1:A:1431:LEU:HB2	1.99	0.44
1:A:1687:HIS:O	1:A:1745:LYS:NZ	2.50	0.44
1:A:2166:SER:OG	1:A:2167:PRO:HD3	2.17	0.44
1:A:3472:ILE:HA	1:A:3479:THR:HG21	1.98	0.44
2:B:350:PHE:N	3:C:461:MET:O	2.35	0.44
3:C:7:LYS:H	3:C:128:GLU:HB2	1.83	0.44
3:C:468:GLU:C	3:C:470:THR:H	2.20	0.44
3:C:496:HIS:CD2	3:C:505:LEU:HA	2.52	0.44
3:L:428:GLU:OE2	2:T:484:GLN:NE2	2.50	0.44
1:S:220:LEU:O	1:S:224:LEU:HG	2.17	0.44
1:S:314:SER:O	1:S:317:GLU:HG3	2.17	0.44
1:S:364:ARG:HG3	1:S:415:GLN:NE2	2.31	0.44
1:S:395:MET:HG3	1:S:413:PHE:HE2	1.82	0.44
1:S:1255:CYS:HA	1:S:1258:ASP:OD2	2.17	0.44
1:S:1576:ASP:O	1:S:1580:LEU:N	2.36	0.44
1:S:1772:HIS:CE1	1:S:1773:VAL:HG23	2.52	0.44
1:S:3493:TRP:CD1	1:S:3521:ILE:HA	2.53	0.44
1:S:3771:MET:HA	1:S:3774:ILE:HD12	2.00	0.44
1:S:3974:MET:HG2	1:S:3976:GLU:H	1.81	0.44
2:T:527:GLU:OE1	2:T:532:PRO:HG3	2.18	0.44
1:A:19:LEU:HD22	1:A:34:LEU:HD23	1.99	0.44
1:A:89:LEU:O	1:A:133:LYS:NZ	2.48	0.44
1:A:100:ILE:H	1:A:100:ILE:HD12	1.83	0.44
1:A:225:LYS:HZ1	1:A:273:ARG:HE	1.66	0.44
1:A:1336:THR:HA	1:A:1339:VAL:HG12	1.99	0.44
1:A:1710:LEU:H	1:A:1710:LEU:HD12	1.83	0.44
1:A:1762:MET:HA	1:A:1765:VAL:HG22	1.99	0.44
1:A:2891:ARG:O	1:A:2894:GLU:HG3	2.17	0.44
2:B:256:LEU:HB2	2:B:273:ILE:HB	1.99	0.44
2:B:261:LEU:O	2:B:268:VAL:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:ASP:OD2	3:C:394:ARG:NH1	2.35	0.44
3:C:200:GLN:O	3:C:203:GLU:HG2	2.17	0.44
5:G:3:ARG:NH2	5:G:126:LEU:HD22	2.33	0.44
3:L:256:ASN:ND2	2:T:522:VAL:HG21	2.32	0.44
3:L:458:ILE:HA	2:T:350:PHE:CE2	2.52	0.44
5:Q:115:LYS:HA	5:Q:115:LYS:HD2	1.74	0.44
1:S:63:PHE:HA	1:S:66:LEU:CB	2.48	0.44
1:S:451:PRO:O	1:S:455:LEU:HG	2.17	0.44
1:S:682:TYR:O	1:S:700:LYS:NZ	2.50	0.44
1:S:932:GLU:O	1:S:2773:ARG:NH2	2.51	0.44
1:S:1279:LEU:HA	1:S:1282:LEU:HB2	2.00	0.44
1:S:2246:LYS:HZ3	1:S:2284:ASP:H	1.66	0.44
1:S:2486:ASP:N	1:S:2486:ASP:OD1	2.47	0.44
1:S:3602:ASN:HA	1:S:3606:ILE:HG13	1.98	0.44
2:T:193:LEU:HD12	2:T:198:ILE:HG13	1.98	0.44
2:T:485:GLN:O	2:T:489:ASN:ND2	2.50	0.44
1:A:669:LEU:HA	1:A:672:ILE:HG22	1.99	0.44
1:A:2306:ASN:HA	1:A:2309:PHE:HB2	2.00	0.44
2:B:317:LYS:HD2	3:C:281:ALA:HA	2.00	0.44
3:C:646:ALA:HA	3:C:651:GLU:HG3	2.00	0.44
3:L:237:PHE:HD1	3:L:240:ILE:HD11	1.82	0.44
5:Q:172:LEU:O	5:Q:176:LEU:HG	2.18	0.44
6:R:706:ASN:O	6:R:710:LYS:HG2	2.17	0.44
1:S:460:ALA:HA	1:S:463:LYS:HD2	1.99	0.44
1:S:1384:PHE:HB3	1:S:1386:ILE:HG12	2.00	0.44
1:S:1960:LYS:HD2	1:S:1960:LYS:O	2.18	0.44
1:S:3735:PRO:HB2	1:S:3751:LEU:HD23	1.99	0.44
1:S:3958:LEU:HD12	1:S:3958:LEU:O	2.17	0.44
1:S:3979:LEU:O	1:S:3983:ILE:HG12	2.18	0.44
2:T:468:LYS:HD2	2:T:468:LYS:HA	1.82	0.44
1:A:668:LYS:O	1:A:671:SER:OG	2.29	0.44
1:A:741:ILE:HA	1:A:748:TYR:CE2	2.53	0.44
1:A:890:LYS:HD3	1:A:890:LYS:HA	1.76	0.44
1:A:921:ALA:N	1:A:927:LYS:HZ1	2.16	0.44
1:A:1922:ALA:HB1	1:A:1940:TYR:CE1	2.52	0.44
1:A:3078:LEU:HA	1:A:3082:TYR:HD2	1.82	0.44
1:A:3577:GLN:OE1	1:A:3629:ARG:HB3	2.18	0.44
1:A:3729:MET:HB2	1:A:3735:PRO:HG2	2.00	0.44
2:B:103:TYR:CD2	2:B:135:MET:HE1	2.53	0.44
2:B:463:LYS:HG2	3:C:387:LEU:HD21	1.99	0.44
3:C:8:ALA:HA	3:C:129:LYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:41:VAL:HG21	4:D:96:LEU:HD13	2.00	0.44
6:I:710:LYS:O	6:I:714:LEU:HG	2.18	0.44
6:I:757:GLU:HG3	6:I:758:TYR:CD2	2.53	0.44
6:R:746:MET:HB2	6:R:750:THR:HB	1.99	0.44
6:R:772:ASN:O	6:R:776:GLU:HG2	2.18	0.44
1:S:153:PHE:CZ	1:S:189:MET:HG3	2.53	0.44
1:S:710:PHE:O	1:S:713:GLU:HG3	2.17	0.44
1:S:2305:ASN:O	1:S:2308:SER:OG	2.26	0.44
1:S:2761:LEU:HA	1:S:2764:LYS:HE2	1.99	0.44
1:S:3581:PRO:HG3	1:S:3632:PHE:HD2	1.81	0.44
1:S:3588:TRP:HB2	1:S:3613:MET:SD	2.58	0.44
1:S:3622:ALA:HB2	1:S:3633:ILE:HD13	1.99	0.44
1:S:3750:PHE:HE1	1:S:3804:GLU:HG3	1.83	0.44
1:S:4006:VAL:HG21	1:S:4009:PRO:HB3	2.00	0.44
2:T:131:PHE:CE1	2:T:135:MET:HG2	2.53	0.44
2:T:348:MET:HE1	2:T:399:ARG:HE	1.83	0.44
1:A:705:ALA:O	1:A:709:LYS:HD3	2.18	0.44
1:A:1356:TRP:O	1:A:1359:LEU:HB2	2.18	0.44
1:A:1611:GLN:HB2	1:A:1613:HIS:HD1	1.83	0.44
1:A:2173:ALA:HA	1:A:2215:LEU:HD21	1.99	0.44
1:A:2335:ASN:OD1	1:A:2336:ILE:N	2.50	0.44
1:A:3809:THR:HA	1:A:3931:ALA:HA	2.00	0.44
2:B:143:LEU:O	2:B:146:VAL:HG22	2.18	0.44
5:G:194:LEU:O	5:G:197:LYS:HG3	2.18	0.44
5:P:176:LEU:HA	6:R:805:TRP:HH2	1.83	0.44
1:S:1023:SER:CA	1:S:1026:ARG:HE	2.24	0.44
1:S:1916:ILE:H	1:S:1916:ILE:HG13	1.64	0.44
1:S:3130:GLN:HB3	1:S:3178:ILE:HG21	2.00	0.44
1:A:23:ASP:OD1	1:A:23:ASP:N	2.50	0.44
1:A:66:LEU:O	1:A:67:VAL:C	2.56	0.44
1:A:203:GLU:O	1:A:207:GLN:HG2	2.18	0.44
1:A:409:GLN:N	1:A:409:GLN:OE1	2.51	0.44
1:A:446:PHE:CG	1:A:530:LEU:HD22	2.53	0.44
1:A:478:CYS:SG	1:A:479:ILE:N	2.91	0.44
1:A:1189:GLU:HB3	1:A:1193:LYS:NZ	2.32	0.44
1:A:1354:GLU:HA	1:A:1357:LYS:HB3	2.00	0.44
1:A:1769:GLU:HB3	1:A:1772:HIS:HB3	1.99	0.44
1:A:2830:ASN:O	1:A:2834:GLN:HG2	2.18	0.44
1:A:2955:SER:O	1:A:2958:LEU:HG	2.18	0.44
1:A:3137:GLU:HG2	1:A:3189:PHE:HE2	1.83	0.44
1:A:3493:TRP:O	1:A:3709:GLY:N	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3980:MET:SD	1:A:3981:TYR:N	2.91	0.44
3:C:528:ILE:HB	3:C:529:PRO:HD3	1.99	0.44
6:I:682:ILE:HA	6:I:730:PHE:HZ	1.83	0.44
6:I:743:MET:CE	6:I:746:MET:HB3	2.48	0.44
1:S:764:PRO:O	1:S:768:VAL:HG22	2.17	0.44
1:S:1949:ILE:HG23	1:S:2100:LEU:HD22	1.99	0.44
1:S:2892:LEU:HD13	1:S:2895:GLU:OE2	2.17	0.44
1:S:3509:ASP:N	1:S:3509:ASP:OD1	2.50	0.44
1:S:3915:HIS:HE1	1:S:3961:PHE:HA	1.83	0.44
1:A:581:LEU:HA	1:A:620:PHE:CE1	2.52	0.44
1:A:1169:VAL:O	1:A:1173:LEU:HG	2.17	0.44
1:A:2132:LYS:O	1:A:2135:ASN:ND2	2.51	0.44
1:A:3289:ARG:HG3	1:A:3290:SER:N	2.33	0.44
1:A:3410:ILE:O	1:A:3414:MET:HG2	2.18	0.44
1:A:3834:ALA:HB3	1:A:3835:PRO:HD3	1.99	0.44
2:B:89:GLY:O	2:B:139:SER:N	2.51	0.44
2:B:465:ILE:HG23	2:B:518:LEU:HD22	2.00	0.44
2:B:513:ALA:O	2:B:516:LYS:HG3	2.18	0.44
3:C:130:ARG:HB3	3:C:159:ILE:HG12	2.00	0.44
1:S:42:CYS:HA	1:S:88:PHE:CZ	2.53	0.44
1:S:1527:ARG:O	1:S:1530:SER:OG	2.28	0.44
1:S:1605:PHE:O	1:S:1608:ARG:NH2	2.50	0.44
1:S:2271:SER:O	1:S:2274:ILE:HB	2.18	0.44
1:S:3410:ILE:O	1:S:3414:MET:HG2	2.18	0.44
1:S:3588:TRP:CE2	1:S:3640:PHE:HZ	2.35	0.44
1:A:575:ILE:HG13	1:A:576:VAL:N	2.33	0.43
1:A:2196:TRP:NE1	1:A:2200:ALA:HB3	2.33	0.43
1:A:2362:VAL:HG12	1:A:2366:LYS:NZ	2.31	0.43
1:A:2363:CYS:O	1:A:2367:VAL:HG22	2.18	0.43
1:A:2831:ASN:O	1:A:2835:LYS:HG3	2.18	0.43
1:A:3127:THR:HA	1:A:3130:GLN:HG2	1.99	0.43
1:A:3289:ARG:HG3	1:A:3290:SER:H	1.83	0.43
1:A:3588:TRP:CZ3	1:A:3640:PHE:HZ	2.35	0.43
1:A:3657:SER:OG	1:A:3658:ASP:N	2.49	0.43
1:A:3733:ARG:NH2	1:A:3755:GLY:H	2.16	0.43
1:S:348:ILE:HG13	1:S:362:ALA:HB2	2.00	0.43
1:S:651:TYR:O	1:S:655:LEU:HG	2.18	0.43
1:S:935:HIS:HD2	1:S:987:LEU:HD11	1.83	0.43
1:S:1261:LEU:HD21	1:S:1337:VAL:HA	2.00	0.43
1:S:2164:TRP:O	1:S:2167:PRO:HD2	2.18	0.43
1:S:2406:GLU:H	1:S:2406:GLU:HG2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3413:TYR:HD2	1:S:3453:ALA:HB2	1.82	0.43
1:S:3476:PRO:O	1:S:3480:LEU:HB2	2.17	0.43
2:T:369:TYR:CG	2:T:370:PRO:HD2	2.52	0.43
1:A:746:ARG:O	1:A:750:PRO:HD3	2.18	0.43
1:A:2175:GLU:OE1	1:A:2182:ILE:HG23	2.18	0.43
1:A:2241:LEU:HA	1:A:2244:CYS:SG	2.58	0.43
1:A:2855:VAL:HG23	1:A:2885:GLN:HG3	2.00	0.43
1:A:3354:ASP:N	1:A:3354:ASP:OD1	2.52	0.43
1:A:3676:PRO:HG2	1:A:3726:VAL:HG21	1.99	0.43
2:B:190:ALA:O	2:B:193:LEU:HG	2.19	0.43
3:C:496:HIS:CE1	3:C:503:GLU:HB2	2.53	0.43
3:L:329:GLU:O	3:L:334:LYS:NZ	2.50	0.43
5:P:188:LYS:HA	5:P:191:ILE:HB	2.00	0.43
1:S:1131:ILE:HA	1:S:1134:LEU:HD12	2.00	0.43
1:S:2279:ILE:H	1:S:2279:ILE:HD12	1.83	0.43
1:S:2421:VAL:O	1:S:2425:ARG:HB2	2.18	0.43
1:S:3047:SER:O	1:S:3051:LEU:HG	2.18	0.43
1:S:3177:ASN:OD1	1:S:3178:ILE:N	2.47	0.43
1:S:4010:SER:H	1:S:4038:TRP:HE1	1.65	0.43
2:T:158:GLN:OE1	2:T:158:GLN:N	2.49	0.43
2:T:318:ARG:CB	2:T:329:LEU:O	2.54	0.43
1:A:60:SER:O	1:A:64:GLY:N	2.51	0.43
1:A:935:HIS:CE1	1:A:2773:ARG:HH21	2.37	0.43
1:A:1021:VAL:O	1:A:1026:ARG:NH1	2.51	0.43
1:A:1428:ILE:HD12	1:A:1431:LEU:HD12	1.99	0.43
1:A:1771:GLN:HE22	1:A:1774:MET:HA	1.83	0.43
1:A:1819:PHE:O	1:A:1823:SER:OG	2.36	0.43
1:A:2388:LYS:NZ	2:B:157:VAL:O	2.48	0.43
1:A:3122:HIS:O	1:A:3126:LEU:HG	2.18	0.43
1:A:3319:ASN:OD1	1:A:3322:ALA:N	2.49	0.43
1:A:3519:GLU:HA	1:A:3522:THR:HG22	1.99	0.43
1:A:3588:TRP:HE1	1:A:3609:MET:C	2.18	0.43
1:A:3633:ILE:HG13	1:A:3634:GLN:N	2.33	0.43
2:B:230:ARG:HG3	2:B:232:HIS:N	2.27	0.43
3:C:595:ALA:HB1	3:C:599:ARG:NH2	2.33	0.43
5:H:28:LEU:HD13	5:H:71:ARG:HH12	1.84	0.43
5:P:179:ARG:HD3	6:R:805:TRP:CH2	2.53	0.43
1:S:714:VAL:HG12	1:S:717:LYS:NZ	2.33	0.43
1:S:758:LEU:O	1:S:761:SER:OG	2.29	0.43
1:S:1352:SER:HB3	1:S:1356:TRP:HB2	1.99	0.43
1:S:2522:ARG:HG3	1:S:2561:PHE:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3050:LYS:HA	1:S:3050:LYS:HD3	1.76	0.43
1:S:3964:THR:HG22	1:S:3967:PHE:CD2	2.54	0.43
2:T:368:VAL:HG21	2:T:413:LEU:HD11	2.00	0.43
2:T:392:LYS:O	2:T:394:VAL:HG13	2.17	0.43
1:A:275:PHE:HE2	1:A:319:PHE:HB2	1.84	0.43
1:A:575:ILE:O	1:A:579:LEU:HG	2.17	0.43
1:A:974:CYS:HB2	1:A:1024:THR:HG22	2.00	0.43
1:A:1736:PHE:O	1:A:1740:VAL:HG13	2.18	0.43
1:A:1872:GLY:O	1:A:1876:ILE:HG12	2.18	0.43
1:A:2581:LEU:HD23	1:A:2781:PRO:HD2	2.01	0.43
1:A:3244:ASP:OD1	1:A:3245:SER:N	2.51	0.43
1:A:3413:TYR:CB	1:A:3453:ALA:HB2	2.48	0.43
1:A:3503:VAL:HG13	1:A:3536:SER:HB3	2.00	0.43
1:A:3581:PRO:HG3	1:A:3629:ARG:HA	1.98	0.43
1:A:3772:ASN:HD21	1:A:3788:LEU:HB3	1.84	0.43
1:A:3829:LEU:HA	1:A:3833:ARG:HB2	2.00	0.43
2:B:338:LYS:HE2	3:C:486:ARG:HH22	1.82	0.43
2:B:445:LYS:HD3	2:B:445:LYS:HA	1.72	0.43
5:G:179:ARG:NH2	6:I:805:TRP:HB3	2.34	0.43
3:L:226:SER:N	3:L:229:GLU:OE2	2.50	0.43
1:S:727:ALA:HB1	1:S:765:LEU:HD11	1.99	0.43
1:S:784:VAL:HG13	1:S:785:MET:SD	2.58	0.43
1:S:1357:LYS:HG3	1:S:1361:LYS:HZ3	1.84	0.43
1:S:1780:SER:HB2	1:S:1784:ARG:NH1	2.32	0.43
1:S:2435:CYS:O	1:S:2439:ILE:HG12	2.18	0.43
1:S:2571:ASP:HA	1:S:2574:ASN:HB2	2.00	0.43
1:S:3122:HIS:O	1:S:3126:LEU:HG	2.19	0.43
1:A:32:HIS:O	1:A:35:ILE:HG22	2.19	0.43
1:A:473:PRO:HA	1:A:476:ARG:NE	2.34	0.43
1:A:925:GLN:HA	1:A:2769:VAL:HG13	1.99	0.43
1:A:1307:ILE:HG12	1:A:1311:LYS:HD2	2.00	0.43
1:A:1710:LEU:O	1:A:1714:LEU:HG	2.19	0.43
1:A:2255:LEU:HA	1:A:2258:GLU:OE2	2.18	0.43
1:A:2731:ARG:HD3	1:A:2731:ARG:HA	1.68	0.43
1:A:3718:ARG:H	1:A:3743:HIS:CB	2.31	0.43
3:C:342:VAL:HA	3:C:393:VAL:HG12	1.99	0.43
3:L:479:THR:HB	2:T:410:PHE:CD2	2.53	0.43
5:P:191:ILE:HG23	5:P:195:HIS:CE1	2.53	0.43
6:R:727:LEU:O	6:R:731:LYS:NZ	2.52	0.43
6:R:752:GLU:HG3	6:R:756:ARG:NH2	2.33	0.43
1:S:1400:VAL:HG11	1:S:1460:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2102:LYS:NZ	1:S:2155:GLU:OE2	2.44	0.43
1:S:2484:TYR:C	1:S:2485:ARG:HD2	2.39	0.43
1:S:3035:PHE:HA	1:S:3038:GLU:HB2	2.00	0.43
1:S:3263:HIS:HB2	1:S:3276:TRP:CZ2	2.54	0.43
1:S:3283:LEU:O	1:S:3287:ARG:HG3	2.19	0.43
2:T:485:GLN:HG3	2:T:489:ASN:HD21	1.83	0.43
1:A:1353:PRO:HD2	1:A:1356:TRP:CZ3	2.54	0.43
1:A:1603:GLN:O	1:A:1603:GLN:NE2	2.52	0.43
1:A:1727:ARG:HH12	1:A:1772:HIS:CB	2.30	0.43
1:A:2310:VAL:HG13	1:A:2316:TYR:CE1	2.53	0.43
1:A:2967:GLU:O	1:A:2971:GLN:HG2	2.18	0.43
1:A:3511:ALA:O	1:A:3514:VAL:HG12	2.19	0.43
1:A:3519:GLU:O	1:A:3523:ASP:HB2	2.18	0.43
2:B:214:SER:HA	2:B:218:ARG:HG3	2.00	0.43
3:L:292:GLU:OE2	2:T:301:ARG:NH1	2.48	0.43
3:L:413:LYS:HD2	3:L:413:LYS:HA	1.88	0.43
3:L:510:GLN:HA	3:L:513:TRP:HD1	1.82	0.43
1:S:382:ASP:N	1:S:382:ASP:OD1	2.49	0.43
1:S:637:LYS:HE2	1:S:641:PHE:HE2	1.83	0.43
1:S:1626:TRP:CE2	1:S:1671:VAL:HG12	2.52	0.43
1:S:1693:VAL:HG11	1:S:1746:PHE:CE1	2.53	0.43
1:S:2090:ARG:HH21	1:S:2092:GLU:HG3	1.84	0.43
1:S:2295:GLN:HE21	1:S:2299:TYR:HA	1.83	0.43
1:S:2526:SER:HA	1:S:2531:LEU:HD12	2.00	0.43
1:S:2936:TYR:OH	1:S:2940:ARG:HB3	2.19	0.43
1:A:709:LYS:HA	1:A:712:LYS:HZ3	1.83	0.43
1:A:785:MET:HA	1:A:788:TYR:OH	2.19	0.43
1:A:1361:LYS:HE3	1:A:1411:TYR:CZ	2.52	0.43
1:A:1386:ILE:HG13	1:A:1387:GLY:H	1.84	0.43
1:A:1802:TYR:O	1:A:1805:PHE:HB3	2.19	0.43
1:A:3326:GLN:O	1:A:3329:LEU:HG	2.19	0.43
5:G:121:GLU:HA	5:G:124:ARG:HG2	2.01	0.43
5:G:161:ARG:NH2	6:I:847:PHE:HB3	2.29	0.43
6:I:719:ASP:HA	6:I:746:MET:HA	2.01	0.43
3:L:76:ASN:ND2	3:L:104:GLN:O	2.50	0.43
6:R:721:VAL:HG13	6:R:742:PHE:CE1	2.54	0.43
1:S:384:MET:HA	1:S:387:GLU:HG3	2.01	0.43
1:S:767:GLU:HA	1:S:770:LEU:HD12	2.01	0.43
1:S:1379:PRO:HB3	1:S:1385:ASN:ND2	2.33	0.43
1:S:1936:ARG:HH11	1:S:1937:ARG:NH1	2.16	0.43
1:S:2223:VAL:HG22	1:S:2231:PHE:CE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3580:ASN:ND2	1:S:3582:GLU:HB2	2.33	0.43
1:S:3591:ASP:O	1:S:3595:GLU:HG2	2.18	0.43
1:S:3834:ALA:HB3	1:S:3835:PRO:HD3	1.99	0.43
1:A:181:LEU:HD13	1:A:234:PHE:HZ	1.84	0.43
1:A:366:TYR:HD2	1:A:384:MET:CE	2.32	0.43
1:A:529:ASP:OD1	1:A:529:ASP:N	2.52	0.43
1:A:1111:LEU:HD12	1:A:1127:CYS:HB2	2.00	0.43
1:A:2295:GLN:HE21	1:A:2299:TYR:N	2.16	0.43
1:A:3045:ILE:HG13	1:A:3046:ARG:NH1	2.33	0.43
1:A:3467:ARG:HD2	1:A:4000:ASN:ND2	2.33	0.43
2:B:90:THR:HG23	2:B:92:LYS:O	2.19	0.43
2:B:143:LEU:HG	2:B:176:HIS:CD2	2.53	0.43
2:B:410:PHE:HB3	2:B:437:LEU:HD12	2.00	0.43
2:B:421:ASP:OD1	2:B:425:ILE:N	2.34	0.43
2:B:466:VAL:O	2:B:470:ARG:HG3	2.18	0.43
3:C:234:LEU:HB3	3:C:237:PHE:HD2	1.84	0.43
3:C:604:GLN:HE21	3:C:605:LYS:HZ2	1.65	0.43
5:H:32:PHE:CD1	5:H:74:LEU:HD11	2.54	0.43
6:I:753:HIS:O	6:I:757:GLU:HG2	2.17	0.43
3:L:129:LYS:HA	3:L:129:LYS:HD2	1.87	0.43
1:S:62:ASP:O	1:S:66:LEU:CB	2.66	0.43
1:S:913:ARG:NH1	1:S:917:LEU:HD11	2.34	0.43
1:S:1339:VAL:O	1:S:1343:GLU:OE1	2.37	0.43
1:S:1697:PRO:HG3	1:S:1749:ALA:O	2.18	0.43
1:S:2196:TRP:CD1	1:S:2199:LEU:HB2	2.54	0.43
1:S:2506:LEU:HB3	1:S:2525:TRP:HZ2	1.84	0.43
1:S:2806:LYS:NZ	1:S:2853:PRO:HA	2.33	0.43
1:S:2892:LEU:HA	1:S:2895:GLU:OE2	2.19	0.43
1:S:2991:LYS:HA	1:S:2994:TRP:CE3	2.54	0.43
1:S:3182:ILE:O	1:S:3186:ARG:HG2	2.18	0.43
1:S:3424:LEU:HD21	1:S:3443:PRO:HG3	2.00	0.43
2:T:441:ASP:N	2:T:441:ASP:OD1	2.52	0.43
1:A:341:PHE:HB3	1:A:345:PHE:CE2	2.54	0.43
1:A:802:THR:HG1	1:A:852:ARG:NH2	2.17	0.43
1:A:3094:ASP:OD1	1:A:3192:LYS:NZ	2.36	0.43
1:A:3330:LEU:HD23	1:A:3384:HIS:CD2	2.54	0.43
1:A:3881:ASP:O	1:A:3885:ARG:HG3	2.18	0.43
1:A:4089:ILE:O	1:A:4091:ALA:N	2.52	0.43
2:B:94:LYS:HD3	2:B:103:TYR:CZ	2.53	0.43
2:B:142:SER:HB3	2:B:145:GLU:HG2	2.01	0.43
3:C:497:ARG:HH11	3:C:501:PRO:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:I:753:HIS:N	6:I:756:ARG:HH21	2.17	0.43
1:S:1596:VAL:O	1:S:1600:MET:HG2	2.19	0.43
1:S:1748:ASP:OD1	1:S:1749:ALA:N	2.52	0.43
1:S:1760:GLU:OE1	1:S:1804:MET:HG2	2.19	0.43
1:S:1851:LEU:O	1:S:1870:LYS:NZ	2.41	0.43
1:S:1876:ILE:HG13	1:S:1877:LEU:HD22	2.01	0.43
1:S:2121:ASP:HA	1:S:2127:LYS:HD3	2.01	0.43
1:S:2274:ILE:HD11	1:S:2306:ASN:ND2	2.34	0.43
1:S:2517:LEU:HA	1:S:2520:ILE:HG22	2.01	0.43
1:S:3037:GLN:O	1:S:3041:LEU:HG	2.18	0.43
2:T:176:HIS:CG	2:T:182:LYS:HE3	2.53	0.43
1:A:307:GLU:HG2	1:A:308:LEU:N	2.33	0.43
1:A:578:LYS:HZ3	1:A:2036:LEU:HA	1.84	0.43
1:A:888:ARG:NH2	1:A:3889:ARG:HH11	2.17	0.43
1:A:1016:GLY:HA3	1:A:1026:ARG:HA	2.01	0.43
1:A:1151:ARG:HH11	1:A:1163:LEU:HB2	1.84	0.43
1:A:1151:ARG:HB2	1:A:1163:LEU:HD12	2.01	0.43
1:A:2937:ASP:O	1:A:2940:ARG:HG2	2.19	0.43
1:A:3177:ASN:OD1	1:A:3177:ASN:N	2.52	0.43
1:A:3476:PRO:HA	1:A:3479:THR:OG1	2.19	0.43
1:A:3494:GLN:HB3	1:A:3709:GLY:N	2.34	0.43
1:A:3880:ALA:HB2	1:A:3965:ARG:NH2	2.34	0.43
2:B:118:GLU:O	2:B:121:GLN:HG2	2.17	0.43
4:D:183:GLU:OE2	4:D:189:GLY:N	2.52	0.43
6:I:654:LYS:HB2	6:I:684:GLU:O	2.19	0.43
6:I:743:MET:HE3	6:I:744:ILE:N	2.33	0.43
3:L:332:LYS:HZ1	3:L:334:LYS:HG3	1.84	0.43
3:L:457:LEU:HD13	3:L:529:PRO:HB2	2.00	0.43
5:P:162:PHE:HA	5:P:165:CYS:SG	2.59	0.43
1:S:125:ILE:N	1:S:126:PRO:HD2	2.34	0.43
1:S:851:ILE:O	1:S:855:VAL:HG23	2.18	0.43
1:S:972:LEU:HB3	1:S:984:TYR:CE2	2.54	0.43
1:S:1104:LEU:O	1:S:1108:MET:HG2	2.19	0.43
1:S:1267:TYR:CE1	1:S:1281:VAL:HG21	2.53	0.43
1:S:2273:GLY:O	1:S:2276:LEU:HB2	2.17	0.43
1:S:2405:VAL:HG22	1:S:2441:LYS:HE3	2.00	0.43
1:S:2451:LEU:HD23	1:S:2455:LEU:HD23	2.00	0.43
1:S:2452:ARG:HE	1:S:2497:GLU:CD	2.22	0.43
1:S:2923:TRP:CZ3	1:S:2942:ILE:HD12	2.54	0.43
1:A:529:ASP:HA	1:A:532:ARG:HG2	2.00	0.42
1:A:629:PHE:O	1:A:632:GLU:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:VAL:HA	1:A:1297:PHE:CD2	2.54	0.42
1:A:1389:VAL:HG13	1:A:1391:VAL:HG12	2.00	0.42
1:A:2139:PRO:HB2	1:A:2142:ILE:HG12	2.01	0.42
1:A:3718:ARG:O	1:A:3743:HIS:N	2.51	0.42
3:C:130:ARG:HB3	3:C:159:ILE:HG23	2.01	0.42
3:C:633:MET:HA	3:C:636:ILE:HG12	2.01	0.42
3:L:234:LEU:HD21	3:L:483:PRO:HB3	2.00	0.42
5:Q:180:PHE:HA	5:Q:183:VAL:HG12	2.01	0.42
1:S:110:THR:O	1:S:114:VAL:HG23	2.19	0.42
1:S:118:ASP:O	1:S:122:LYS:HG2	2.19	0.42
1:S:974:CYS:HB3	1:S:1028:PHE:CD2	2.49	0.42
1:S:976:VAL:O	1:S:976:VAL:HG13	2.19	0.42
1:S:1602:ASP:HB2	1:S:1606:ARG:HH21	1.83	0.42
1:S:1620:THR:O	1:S:1623:LEU:HB2	2.18	0.42
1:S:2438:ILE:O	1:S:2442:MET:HG3	2.19	0.42
1:S:3981:TYR:HE2	1:S:4105:LYS:HB3	1.84	0.42
1:A:309:LYS:O	1:A:313:LEU:HG	2.19	0.42
1:A:408:TYR:N	1:A:409:GLN:OE1	2.52	0.42
1:A:648:SER:O	1:A:651:TYR:HB3	2.19	0.42
1:A:1238:GLN:HB2	1:A:1239:PRO:HD3	2.01	0.42
1:A:1278:ALA:O	1:A:1282:LEU:N	2.52	0.42
1:A:1539:SER:HA	1:A:1552:HIS:ND1	2.34	0.42
1:A:2750:GLU:HG3	1:A:2753:ARG:HH11	1.83	0.42
1:A:3007:GLU:O	1:A:3011:LEU:N	2.43	0.42
1:A:3014:CYS:SG	1:A:3043:TYR:HB3	2.59	0.42
1:A:3148:GLN:HE22	1:A:3150:ASN:HB2	1.83	0.42
1:A:3992:ARG:HD2	1:A:3992:ARG:HA	1.85	0.42
1:A:3992:ARG:HH12	1:A:4053:GLY:N	2.16	0.42
2:B:497:LEU:O	6:I:707:ILE:HG13	2.19	0.42
3:C:40:MET:HG2	3:C:44:ARG:NH1	2.34	0.42
3:C:632:PHE:O	3:C:636:ILE:HG23	2.19	0.42
3:C:642:PHE:HD2	3:C:655:PHE:CE1	2.36	0.42
3:L:342:VAL:HA	3:L:393:VAL:HG12	2.01	0.42
3:L:655:PHE:HA	3:L:658:PHE:HB2	2.01	0.42
1:S:344:GLN:O	1:S:348:ILE:HG12	2.18	0.42
1:S:1184:ARG:HH22	1:S:1265:GLU:CB	2.29	0.42
1:S:1769:GLU:O	1:S:1772:HIS:ND1	2.52	0.42
1:S:2174:SER:O	1:S:2174:SER:OG	2.31	0.42
1:S:2281:MET:HE3	1:S:2329:TYR:HD2	1.84	0.42
1:S:2405:VAL:O	1:S:2408:MET:HG2	2.20	0.42
1:S:3547:THR:HG23	1:S:3550:LYS:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3981:TYR:CE2	1:S:4105:LYS:HB3	2.54	0.42
1:A:1013:ILE:O	1:A:1017:ILE:HB	2.19	0.42
1:A:1403:MET:HA	1:A:1406:LEU:HD12	2.01	0.42
1:A:3090:TYR:HE2	1:A:3102:TYR:CE2	2.37	0.42
1:A:3090:TYR:O	1:A:3095:ASP:N	2.46	0.42
1:A:3443:PRO:HA	1:A:3446:VAL:HG22	2.01	0.42
1:A:3571:PHE:CE2	1:A:3575:LEU:HD11	2.55	0.42
1:A:3966:GLN:HA	1:A:3969:ASN:HB2	2.00	0.42
2:B:35:ARG:HG2	2:B:36:ASP:H	1.83	0.42
2:B:479:GLU:OE1	2:B:484:GLN:HG2	2.19	0.42
2:B:523:ASP:HA	2:B:526:LYS:HB3	2.01	0.42
3:C:406:GLY:HA3	3:C:421:TYR:CE2	2.55	0.42
5:G:122:VAL:O	5:G:126:LEU:HG	2.19	0.42
6:I:876:LYS:HA	6:I:876:LYS:HD3	1.82	0.42
3:L:479:THR:HG21	2:T:397:LEU:HD21	2.01	0.42
3:L:600:VAL:O	3:L:604:GLN:HB3	2.19	0.42
1:S:117:LYS:O	1:S:120:ALA:N	2.39	0.42
1:S:229:SER:HA	1:S:278:HIS:CE1	2.54	0.42
1:S:914:VAL:HG13	1:S:934:LEU:HD21	2.00	0.42
1:S:1871:MET:HE1	1:S:1940:TYR:N	2.34	0.42
1:S:1911:LEU:H	1:S:1911:LEU:HD12	1.84	0.42
1:S:2158:ARG:HD2	1:S:2158:ARG:HA	1.87	0.42
1:S:2748:VAL:O	1:S:2752:LYS:HG2	2.20	0.42
2:T:205:LEU:HD12	2:T:205:LEU:HA	1.86	0.42
1:A:225:LYS:HD2	1:A:270:ALA:HB1	2.00	0.42
1:A:410:MET:N	1:A:411:PRO:HD2	2.34	0.42
1:A:480:SER:HA	1:A:567:GLU:OE2	2.19	0.42
1:A:637:LYS:HD2	1:A:637:LYS:HA	1.74	0.42
1:A:1168:LEU:HA	1:A:1171:TRP:HB3	2.02	0.42
1:A:1367:HIS:O	1:A:1370:ARG:HG2	2.18	0.42
1:A:1827:LEU:HD12	1:A:1828:LEU:N	2.35	0.42
1:A:2318:ALA:O	1:A:2321:GLU:HG2	2.19	0.42
1:A:3239:LYS:O	1:A:3242:MET:HB3	2.19	0.42
1:A:3911:ILE:O	1:A:3915:HIS:CD2	2.73	0.42
1:A:3995:PRO:HG3	1:A:4051:LEU:HB3	2.01	0.42
2:B:303:PHE:CE2	2:B:308:GLY:HA2	2.54	0.42
2:B:330:GLU:H	2:B:333:GLU:HB2	1.84	0.42
5:G:122:VAL:O	5:G:125:GLU:HG2	2.19	0.42
6:I:706:ASN:O	6:I:710:LYS:HG2	2.19	0.42
3:L:492:GLN:O	3:L:495:LEU:HG	2.19	0.42
6:R:816:HIS:H	6:R:850:ALA:C	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:23:ASP:HB3	1:S:34:LEU:HD11	2.01	0.42
1:S:53:LEU:O	1:S:57:LEU:HG	2.19	0.42
1:S:62:ASP:O	1:S:66:LEU:N	2.49	0.42
1:S:301:CYS:HA	1:S:309:LYS:HA	2.00	0.42
1:S:571:SER:O	1:S:575:ILE:HG12	2.19	0.42
1:S:913:ARG:HH11	1:S:917:LEU:HD11	1.84	0.42
1:S:1102:GLU:H	1:S:1102:GLU:CD	2.21	0.42
1:S:3487:ILE:HD11	1:S:3516:HIS:HB2	2.01	0.42
2:T:219:ASP:N	2:T:219:ASP:OD1	2.48	0.42
1:A:242:PRO:HB2	1:A:246:ARG:NH2	2.34	0.42
1:A:1418:HIS:HA	1:A:1421:GLU:HB3	2.00	0.42
1:A:1448:LEU:HD23	1:A:1448:LEU:HA	1.90	0.42
1:A:1611:GLN:HB2	1:A:1613:HIS:ND1	2.35	0.42
1:A:2090:ARG:HD2	1:A:2090:ARG:HA	1.79	0.42
1:A:2554:PHE:CD2	1:A:2854:PHE:HE1	2.36	0.42
1:A:2722:ARG:HD2	1:A:2722:ARG:N	2.35	0.42
1:A:3101:TYR:O	1:A:3104:GLN:NE2	2.53	0.42
2:B:94:LYS:N	2:B:103:TYR:HA	2.34	0.42
2:B:219:ASP:N	2:B:219:ASP:OD1	2.53	0.42
2:B:418:GLU:OE1	3:C:437:SER:HB2	2.19	0.42
3:L:37:VAL:O	3:L:40:MET:HG3	2.19	0.42
3:L:595:ALA:HA	3:L:598:PHE:CZ	2.53	0.42
1:S:385:TYR:O	1:S:388:LEU:HB2	2.19	0.42
1:S:1087:ARG:HD3	1:S:1090:ARG:HH21	1.85	0.42
1:S:1671:VAL:O	1:S:1675:TYR:N	2.38	0.42
1:S:2145:PHE:O	1:S:2149:LEU:HD23	2.20	0.42
1:S:2409:THR:OG1	1:S:2410:GLU:N	2.52	0.42
1:S:3059:GLN:HB3	1:S:3062:LEU:HD23	2.02	0.42
1:S:3078:LEU:HD23	1:S:3082:TYR:CD2	2.54	0.42
2:T:269:ILE:HG23	2:T:378:SER:HB3	2.00	0.42
1:A:338:LEU:HD12	1:A:339:GLN:HG3	2.01	0.42
1:A:397:LEU:O	1:A:399:GLN:NE2	2.53	0.42
1:A:455:LEU:HB3	1:A:459:ARG:HH21	1.84	0.42
1:A:525:LYS:O	1:A:528:VAL:HG22	2.19	0.42
1:A:736:LEU:HB3	1:A:740:ILE:CG2	2.49	0.42
1:A:1115:HIS:CE1	1:A:1180:GLN:HA	2.54	0.42
1:A:2142:ILE:HA	1:A:2145:PHE:CD2	2.54	0.42
1:A:2269:ASP:N	1:A:2269:ASP:OD1	2.51	0.42
1:A:2925:GLU:HA	1:A:2928:LYS:HG3	2.01	0.42
1:A:3589:SER:HA	1:A:3592:VAL:HG12	2.02	0.42
1:A:3603:LYS:HE3	1:A:3603:LYS:HB3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:153:SER:O	3:C:156:LYS:HG2	2.19	0.42
3:L:205:LEU:HG	3:L:209:LYS:HD2	2.01	0.42
6:R:825:VAL:HG23	6:R:878:PHE:HZ	1.85	0.42
1:S:374:LYS:NZ	1:S:425:ASP:OD1	2.47	0.42
1:S:628:GLU:HA	1:S:631:ARG:CD	2.49	0.42
1:S:1233:SER:HA	1:S:1236:LEU:HB2	2.01	0.42
1:S:2306:ASN:HA	1:S:2309:PHE:CD2	2.55	0.42
1:S:3053:LEU:HD23	1:S:3092:LEU:HD22	2.00	0.42
1:S:3909:ALA:HB2	1:S:3980:MET:SD	2.59	0.42
1:A:160:LEU:HD11	1:A:178:LEU:HD21	2.02	0.42
1:A:461:ILE:O	1:A:464:VAL:HG22	2.20	0.42
1:A:720:GLN:HE21	1:A:1122:GLY:H	1.68	0.42
1:A:913:ARG:HA	1:A:916:GLU:OE2	2.19	0.42
1:A:1086:TYR:HA	1:A:1089:PHE:HB3	2.02	0.42
1:A:1877:LEU:HB3	1:A:1881:TYR:HE2	1.84	0.42
1:A:2182:ILE:O	1:A:2186:VAL:HG23	2.20	0.42
1:A:2247:ASP:OD1	1:A:2247:ASP:N	2.51	0.42
1:A:2376:ASP:HB3	1:A:2404:ARG:NH2	2.34	0.42
1:A:2531:LEU:HD23	1:A:2531:LEU:HA	1.89	0.42
1:A:3493:TRP:CZ3	1:A:3521:ILE:HG12	2.55	0.42
1:A:3867:THR:HG23	1:A:4118:GLY:N	2.35	0.42
2:B:38:LEU:HD11	2:B:165:ARG:HH21	1.85	0.42
2:B:288:LEU:HA	2:B:295:PRO:HA	2.02	0.42
2:B:388:LYS:HE3	3:C:451:LEU:HB3	2.01	0.42
3:C:347:LYS:NZ	3:C:388:ASP:HB3	2.35	0.42
3:C:493:CYS:HB3	3:C:505:LEU:HD22	2.01	0.42
5:G:183:VAL:HG21	6:I:805:TRP:CZ2	2.55	0.42
3:L:408:ALA:HB1	3:L:419:LEU:HD21	2.02	0.42
3:L:643:ARG:HD2	3:L:655:PHE:CD2	2.53	0.42
1:S:303:HIS:O	1:S:309:LYS:NZ	2.31	0.42
1:S:389:ILE:O	1:S:393:LYS:HG2	2.20	0.42
1:S:980:THR:O	1:S:983:LEU:HG	2.19	0.42
1:S:1782:PHE:HD1	1:S:1785:ILE:HD11	1.84	0.42
1:S:1961:PHE:HB2	1:S:2125:TRP:CZ2	2.54	0.42
1:S:2227:LYS:HE2	1:S:2227:LYS:HB2	1.90	0.42
1:S:2825:THR:O	1:S:2829:LYS:HG3	2.19	0.42
1:S:3179:TRP:CE3	1:S:3242:MET:HG3	2.53	0.42
1:S:3235:LYS:HB3	1:S:3239:LYS:NZ	2.34	0.42
2:T:112:GLY:O	2:T:116:ILE:HG12	2.20	0.42
2:T:194:ARG:HA	2:T:198:ILE:O	2.19	0.42
2:T:332:GLU:HG2	2:T:333:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:OG1	1:A:305:ASN:N	2.52	0.42
1:A:571:SER:HA	1:A:574:LYS:HG2	2.02	0.42
1:A:629:PHE:O	1:A:633:ILE:HG12	2.20	0.42
1:A:1019:ASP:OD1	1:A:1019:ASP:N	2.52	0.42
1:A:1177:GLY:H	1:A:1184:ARG:HG3	1.85	0.42
1:A:1184:ARG:HH12	1:A:1265:GLU:HG3	1.84	0.42
1:A:2165:LEU:HD11	1:A:2200:ALA:HB1	2.00	0.42
1:A:2365:ASN:HD21	1:A:2399:GLU:CD	2.22	0.42
1:A:2587:GLN:O	1:A:2777:HIS:N	2.52	0.42
1:A:2840:PHE:HA	1:A:2843:PHE:CD2	2.55	0.42
1:A:3137:GLU:O	1:A:3140:GLU:HG2	2.20	0.42
1:A:3574:ALA:O	1:A:3578:LEU:HG	2.19	0.42
1:A:3980:MET:HE3	1:A:3980:MET:H	1.84	0.42
2:B:490:LEU:HG	3:C:316:TYR:CE2	2.54	0.42
5:G:150:ARG:O	5:G:153:ARG:HG2	2.19	0.42
3:L:66:ASN:OD1	3:L:69:SER:HB2	2.20	0.42
6:R:754:PHE:O	6:R:758:TYR:N	2.43	0.42
1:S:87:LYS:HE2	1:S:91:ILE:HD13	2.00	0.42
1:S:446:PHE:CG	1:S:530:LEU:HD22	2.55	0.42
1:S:801:LYS:NZ	1:S:3125:ARG:HH12	2.17	0.42
1:S:887:ASP:OD1	1:S:960:GLN:NE2	2.52	0.42
1:S:890:LYS:HD3	1:S:890:LYS:HA	1.81	0.42
1:S:1019:ASP:OD1	1:S:1026:ARG:HD2	2.19	0.42
1:S:1211:VAL:HG12	1:S:1219:PHE:HZ	1.84	0.42
1:S:1527:ARG:O	1:S:1531:LEU:HG	2.19	0.42
1:S:1750:LEU:HD13	1:S:1758:LEU:HB2	2.02	0.42
1:S:2120:ARG:HD3	1:S:2120:ARG:HA	1.79	0.42
1:S:2950:LYS:HB3	1:S:2952:ILE:HG22	2.01	0.42
1:S:3134:ALA:O	1:S:3138:ILE:HG22	2.20	0.42
1:S:3263:HIS:HB2	1:S:3276:TRP:CH2	2.54	0.42
2:T:60:PHE:O	2:T:63:SER:OG	2.31	0.42
2:T:174:ASN:O	2:T:177:GLY:N	2.53	0.42
2:T:264:ASN:OD1	2:T:265:LYS:N	2.48	0.42
1:A:893:SER:N	1:A:944:LYS:HZ2	2.17	0.42
1:A:1151:ARG:NH1	1:A:1163:LEU:O	2.48	0.42
1:A:1393:ALA:O	1:A:1396:PRO:HD2	2.19	0.42
1:A:1525:CYS:O	1:A:1528:LEU:HG	2.19	0.42
1:A:1835:ALA:HA	1:A:1838:GLU:OE2	2.20	0.42
1:A:1921:ASP:OD1	1:A:1921:ASP:N	2.50	0.42
1:A:2762:LYS:HA	1:A:2765:GLN:NE2	2.35	0.42
2:B:87:PHE:HE2	2:B:105:LEU:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:529:PRO:O	3:C:533:ILE:HG12	2.19	0.42
6:I:813:PHE:HA	6:I:850:ALA:H	1.85	0.42
3:L:98:ILE:O	3:L:99:GLN:NE2	2.53	0.42
6:R:797:ALA:HB1	6:R:801:TYR:CZ	2.54	0.42
1:S:90:CYS:SG	1:S:133:LYS:HB2	2.60	0.42
1:S:412:SER:O	1:S:415:GLN:HG3	2.20	0.42
1:S:526:ASP:N	1:S:526:ASP:OD1	2.52	0.42
1:S:1458:LEU:HD11	1:S:1466:ASN:HD21	1.85	0.42
1:S:2555:LEU:HD11	1:S:2854:PHE:HD1	1.85	0.42
1:S:3299:THR:HG23	1:S:3299:THR:O	2.20	0.42
2:T:100:LYS:HA	2:T:100:LYS:HD3	1.86	0.42
1:A:749:VAL:O	1:A:753:GLN:HG2	2.20	0.42
1:A:1444:ASP:N	1:A:1444:ASP:OD1	2.51	0.42
1:A:1506:SER:HA	1:A:1509:GLN:HE21	1.85	0.42
1:A:1742:CYS:HA	1:A:1745:LYS:HD2	2.02	0.42
1:A:2466:SER:N	1:A:2470:ARG:HH21	2.18	0.42
1:A:2517:LEU:HA	1:A:2520:ILE:HG22	2.02	0.42
1:A:2863:CYS:HB2	1:A:2895:GLU:OE2	2.20	0.42
1:A:3130:GLN:NE2	1:A:3174:ASP:OD1	2.41	0.42
1:A:3588:TRP:CD1	1:A:3613:MET:HB2	2.55	0.42
1:A:3620:PRO:HB3	1:A:3638:LYS:NZ	2.35	0.42
2:B:75:ILE:HG21	3:C:316:TYR:CE1	2.55	0.42
2:B:92:LYS:HE2	2:B:135:MET:SD	2.60	0.42
2:B:260:LYS:NZ	2:B:270:SER:HB3	2.35	0.42
3:C:639:ILE:HD13	3:C:639:ILE:HA	1.93	0.42
3:C:674:PHE:HD2	3:C:675:TRP:CD2	2.37	0.42
3:L:332:LYS:HZ2	3:L:334:LYS:HA	1.83	0.42
5:Q:3:ARG:NH1	5:Q:21:GLN:O	2.53	0.42
1:S:637:LYS:HD2	1:S:637:LYS:HA	1.86	0.42
1:S:669:LEU:HD12	1:S:670:LEU:N	2.35	0.42
1:S:1651:LYS:O	1:S:1654:GLN:HG3	2.20	0.42
1:S:2327:LEU:HG	1:S:2371:PHE:CG	2.55	0.42
1:S:2372:PRO:HB3	1:S:2403:CYS:O	2.20	0.42
1:S:2534:ASN:HB3	1:S:2537:ASP:HB2	2.02	0.42
1:S:3137:GLU:HA	1:S:3140:GLU:OE2	2.19	0.42
1:S:3413:TYR:CD1	1:S:3449:LYS:HB3	2.55	0.42
1:S:3956:PRO:HG2	1:S:4121:TRP:HB2	2.02	0.42
2:T:174:ASN:N	2:T:175:PRO:HD3	2.35	0.42
1:A:31:GLY:HA3	1:A:77:GLU:HB2	2.01	0.41
1:A:740:ILE:HG22	1:A:741:ILE:HD12	2.02	0.41
1:A:1479:VAL:HG21	1:A:1518:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1803:GLU:HA	1:A:1806:ARG:CZ	2.49	0.41
1:A:3150:ASN:ND2	1:A:3197:LEU:HD13	2.35	0.41
1:A:3568:ILE:H	1:A:3568:ILE:HD12	1.85	0.41
2:B:57:LEU:HB3	2:B:61:ASP:CB	2.50	0.41
2:B:211:PHE:N	2:B:231:VAL:O	2.53	0.41
5:G:20:LEU:HD13	5:G:34:ILE:HD13	2.02	0.41
5:H:21:GLN:HE21	5:H:126:LEU:HG	1.85	0.41
6:I:810:LEU:HB3	6:I:848:HIS:HB3	2.02	0.41
3:L:461:MET:HA	3:L:522:VAL:HG13	2.01	0.41
3:L:686:ILE:HD11	3:L:703:LYS:HA	2.02	0.41
1:S:116:THR:HG21	1:S:155:LYS:HZ3	1.84	0.41
1:S:286:LEU:HD13	1:S:319:PHE:CE1	2.55	0.41
1:S:1280:GLN:O	1:S:1284:THR:HB	2.20	0.41
1:S:1780:SER:CB	1:S:1784:ARG:HH12	2.33	0.41
1:S:2169:LEU:HD21	1:S:2211:LEU:HB2	2.02	0.41
1:S:2514:ASN:HB3	1:S:2517:LEU:HD12	2.01	0.41
1:S:3232:ARG:HA	1:S:3235:LYS:HE2	2.02	0.41
1:S:3300:VAL:HG13	1:S:3300:VAL:O	2.20	0.41
1:S:3575:LEU:HD12	1:S:3752:VAL:HG11	2.02	0.41
1:A:40:GLN:OE1	1:A:2427:ARG:NE	2.47	0.41
1:A:655:LEU:O	1:A:659:ARG:NH1	2.52	0.41
1:A:1438:GLY:O	1:A:1445:ARG:NH2	2.33	0.41
1:A:2168:LEU:HB3	1:A:2193:ILE:HD11	2.01	0.41
1:A:2237:ILE:HD13	1:A:2237:ILE:HA	1.90	0.41
1:A:2358:ASP:O	1:A:2362:VAL:HG23	2.20	0.41
1:A:2750:GLU:O	1:A:2753:ARG:HG2	2.21	0.41
1:A:3052:LEU:HD21	1:A:3058:ASP:OD1	2.21	0.41
1:A:3997:LEU:HA	1:A:4000:ASN:HD22	1.84	0.41
2:B:166:ILE:HD13	2:B:166:ILE:HA	1.92	0.41
2:B:288:LEU:N	3:C:311:ILE:O	2.44	0.41
2:B:341:ASP:OD1	2:B:341:ASP:N	2.52	0.41
2:B:355:LEU:HD11	3:C:473:LEU:HB3	2.01	0.41
3:C:336:GLU:H	3:C:336:GLU:CD	2.24	0.41
3:C:374:ALA:O	3:C:377:LEU:HG	2.20	0.41
4:D:7:PRO:HB3	4:D:77:ARG:HG3	2.02	0.41
5:H:181:ILE:HD13	5:H:181:ILE:HA	1.95	0.41
3:L:291:LYS:HE2	2:T:302:THR:HG22	2.02	0.41
3:L:446:PRO:HB3	2:T:384:ALA:HB2	2.03	0.41
3:L:457:LEU:HD11	3:L:530:LEU:HG	2.01	0.41
5:P:97:PHE:HZ	5:P:108:LEU:HD22	1.85	0.41
1:S:58:VAL:HG21	1:S:3098:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:89:LEU:C	1:S:133:LYS:HZ1	2.24	0.41
1:S:461:ILE:O	1:S:464:VAL:HG22	2.20	0.41
1:S:614:PRO:HB3	1:S:620:PHE:CE1	2.55	0.41
1:S:1133:HIS:O	1:S:1137:ILE:HG12	2.20	0.41
1:S:1298:LEU:HG	1:S:1367:HIS:CE1	2.55	0.41
1:S:1452:VAL:HA	1:S:1517:LEU:HD11	2.03	0.41
1:S:1611:GLN:HB2	1:S:1613:HIS:HD1	1.85	0.41
1:S:2246:LYS:NZ	1:S:2284:ASP:OD1	2.41	0.41
1:S:3277:VAL:HG22	1:S:3306:LEU:CD2	2.50	0.41
1:S:3300:VAL:HG13	1:S:3303:THR:HA	2.02	0.41
1:S:3988:LEU:HA	1:S:3991:PHE:CD2	2.55	0.41
2:T:202:LEU:HD11	2:T:211:PHE:HE1	1.85	0.41
1:A:168:ASP:OD2	1:A:170:VAL:HG22	2.20	0.41
1:A:1787:ARG:HE	1:A:1830:HIS:HE1	1.68	0.41
1:A:2570:PRO:O	1:A:2573:PRO:HD2	2.20	0.41
1:A:3088:LEU:HD23	1:A:3138:ILE:HD12	2.02	0.41
1:A:3090:TYR:O	1:A:3094:ASP:N	2.53	0.41
1:A:3100:LYS:HA	1:A:3103:ILE:HG22	2.02	0.41
1:A:3103:ILE:HD11	1:A:3135:LEU:HA	2.03	0.41
1:A:3183:ILE:HD12	1:A:3238:MET:HB3	2.01	0.41
1:A:3457:ASN:N	1:A:3457:ASN:OD1	2.53	0.41
1:A:3483:MET:SD	1:A:3511:ALA:HB1	2.60	0.41
1:A:3875:GLU:HB2	1:A:3965:ARG:HE	1.84	0.41
1:A:3998:LEU:HD21	1:A:4051:LEU:HG	2.02	0.41
2:B:154:PHE:O	2:B:157:VAL:HG12	2.19	0.41
2:B:403:ARG:HG2	2:B:406:ILE:HD12	2.01	0.41
3:C:94:ILE:HA	3:C:98:ILE:HD13	2.01	0.41
3:C:142:PHE:HZ	3:C:203:GLU:HG3	1.85	0.41
6:I:722:LYS:HD2	6:I:722:LYS:HA	1.86	0.41
6:I:810:LEU:HD13	6:I:847:PHE:CE2	2.55	0.41
3:L:169:LEU:HD22	3:L:224:ILE:O	2.19	0.41
1:S:697:ASP:HB2	1:S:700:LYS:HG3	2.03	0.41
1:S:893:SER:H	1:S:944:LYS:NZ	2.18	0.41
1:S:966:PHE:HB2	1:S:1011:GLU:OE1	2.21	0.41
1:S:1793:THR:O	1:S:1797:LEU:HD13	2.20	0.41
1:S:2121:ASP:OD1	1:S:2121:ASP:N	2.53	0.41
1:S:2138:VAL:HG13	1:S:2143:ARG:HG2	2.01	0.41
1:S:2206:PRO:HA	1:S:2209:GLU:OE2	2.20	0.41
1:S:2379:MET:HA	1:S:2382:VAL:HG12	2.02	0.41
1:S:2569:SER:HB3	1:S:2572:TYR:HB2	2.01	0.41
1:S:2760:GLU:HG2	1:S:2761:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2881:LEU:HA	1:S:2886:GLN:OE1	2.19	0.41
1:S:3530:VAL:HG12	1:S:3562:LEU:HD22	2.02	0.41
2:T:71:TYR:CD1	2:T:83:LEU:HD13	2.55	0.41
1:A:709:LYS:HA	1:A:712:LYS:NZ	2.36	0.41
1:A:737:PRO:O	1:A:740:ILE:HG22	2.21	0.41
1:A:860:GLY:HA3	1:A:3136:THR:CB	2.51	0.41
1:A:903:PRO:HG3	1:A:2816:ILE:HD13	2.02	0.41
1:A:1307:ILE:HD12	1:A:1307:ILE:HA	1.91	0.41
1:A:1728:GLU:HG3	1:A:1729:PHE:CD1	2.55	0.41
1:A:1759:LEU:HD12	1:A:1797:LEU:HD22	2.01	0.41
1:A:2304:VAL:O	1:A:2307:MET:HB2	2.19	0.41
1:A:2380:ASN:N	1:A:2380:ASN:OD1	2.52	0.41
1:A:3392:ALA:HB1	1:A:3409:VAL:HA	2.01	0.41
1:A:3508:LYS:O	1:A:3551:ASN:ND2	2.54	0.41
2:B:289:TYR:HD2	2:B:292:THR:H	1.68	0.41
2:B:463:LYS:HA	3:C:387:LEU:HD11	2.02	0.41
3:C:43:GLN:HE21	3:C:495:LEU:HB2	1.84	0.41
3:L:327:ASP:O	3:L:330:GLN:HG3	2.20	0.41
3:L:640:ARG:NH1	3:L:682:GLY:HA2	2.35	0.41
4:M:42:THR:HB	4:M:47:LEU:HD12	2.01	0.41
6:R:812:MET:O	6:R:850:ALA:HB3	2.20	0.41
1:S:386:VAL:HG13	1:S:431:TYR:OH	2.21	0.41
1:S:1069:HIS:CE1	1:S:3745:GLU:HG2	2.56	0.41
1:S:1172:LEU:HD11	1:S:1187:SER:HB2	2.02	0.41
1:S:1489:LYS:HD2	1:S:1492:ALA:HB3	2.02	0.41
1:S:1565:GLU:HG2	1:S:1566:THR:N	2.36	0.41
1:S:3811:THR:HA	1:S:3929:MET:HA	2.02	0.41
1:A:38:LEU:HD11	1:A:85:ILE:CG1	2.46	0.41
1:A:451:PRO:HA	1:A:454:GLN:NE2	2.36	0.41
1:A:584:GLU:C	1:A:613:HIS:HB3	2.40	0.41
1:A:1115:HIS:CD2	1:A:1182:GLU:H	2.38	0.41
1:A:1357:LYS:HG3	1:A:1411:TYR:OH	2.21	0.41
1:A:1761:LEU:O	1:A:1764:GLU:HG3	2.21	0.41
1:A:3620:PRO:HB3	1:A:3638:LYS:HZ2	1.85	0.41
2:B:109:ASP:OD1	2:B:110:ASN:N	2.53	0.41
2:B:318:ARG:HB3	3:C:276:TRP:CE3	2.55	0.41
2:B:525:PHE:HA	2:B:528:LEU:HD12	2.03	0.41
3:C:297:LEU:HB3	3:C:299:ASP:OD1	2.19	0.41
3:C:365:PHE:CE2	3:C:418:CYS:HB3	2.55	0.41
3:C:443:LYS:HE3	3:C:443:LYS:HB2	1.90	0.41
4:D:194:LYS:HD3	4:D:195:PRO:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:183:VAL:HG21	6:I:805:TRP:HZ2	1.86	0.41
6:I:668:SER:O	6:I:703:GLY:N	2.53	0.41
6:I:841:LYS:HD3	6:I:867:GLU:H	1.84	0.41
5:P:61:MET:HB2	5:P:65:LYS:NZ	2.35	0.41
1:S:157:TYR:O	1:S:160:LEU:HG	2.21	0.41
1:S:682:TYR:CZ	1:S:700:LYS:HG2	2.55	0.41
1:S:709:LYS:HB2	1:S:709:LYS:HE3	1.89	0.41
1:S:1184:ARG:HH21	1:S:1262:ALA:HA	1.84	0.41
1:S:1278:ALA:HB3	1:S:1356:TRP:CD1	2.55	0.41
1:S:1466:ASN:OD1	1:S:1466:ASN:N	2.53	0.41
1:S:1761:LEU:O	1:S:1764:GLU:HG3	2.20	0.41
1:S:1844:VAL:O	1:S:1848:ILE:HG13	2.21	0.41
1:S:2168:LEU:O	1:S:2172:ALA:N	2.39	0.41
1:S:2505:VAL:O	1:S:2509:GLY:N	2.49	0.41
1:S:3137:GLU:HA	1:S:3140:GLU:CD	2.40	0.41
1:S:3838:GLU:O	1:S:3842:TRP:HB2	2.20	0.41
1:A:327:VAL:HG13	1:A:333:MET:HB2	2.02	0.41
1:A:741:ILE:HG23	1:A:748:TYR:CD2	2.47	0.41
1:A:924:ARG:NH2	1:A:2766:ASP:O	2.53	0.41
1:A:1133:HIS:O	1:A:1137:ILE:HG12	2.20	0.41
1:A:1816:ARG:NE	3:C:625:ASP:OD1	2.51	0.41
1:A:2233:HIS:CE1	1:A:2728:LEU:HA	2.56	0.41
1:A:2339:GLU:HA	1:A:2342:CYS:SG	2.60	0.41
1:A:2750:GLU:HA	1:A:2753:ARG:HG2	2.02	0.41
1:A:2981:TRP:CD1	1:A:2984:GLY:HA2	2.54	0.41
1:A:3592:VAL:N	1:A:3609:MET:HE1	2.36	0.41
1:A:4083:GLY:HA3	1:A:4088:ASN:HB3	2.02	0.41
1:A:4125:GLU:HG3	1:A:4128:MET:HB2	2.03	0.41
3:C:45:GLN:HA	3:C:50:ASN:ND2	2.35	0.41
3:C:477:PHE:CE1	3:C:518:PRO:HA	2.56	0.41
3:C:633:MET:O	3:C:636:ILE:HG12	2.20	0.41
5:G:159:GLN:OE1	5:H:158:VAL:HG21	2.21	0.41
6:I:878:PHE:O	6:I:881:THR:OG1	2.26	0.41
3:L:523:THR:HG22	3:L:527:GLN:NE2	2.35	0.41
1:S:112:THR:OG1	1:S:155:LYS:NZ	2.53	0.41
1:S:907:LEU:HA	1:S:910:PHE:HD2	1.85	0.41
1:S:1106:ILE:O	1:S:1109:GLU:HG3	2.21	0.41
1:S:1253:THR:O	1:S:1257:LEU:HG	2.20	0.41
1:S:1601:LEU:HD13	1:S:1651:LYS:HB3	2.02	0.41
1:S:2106:ARG:HA	1:S:2106:ARG:CZ	2.50	0.41
1:S:2427:ARG:HH21	1:S:2464:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3078:LEU:HD23	1:S:3082:TYR:HD2	1.85	0.41
1:S:3104:GLN:NE2	1:S:3105:ASN:OD1	2.53	0.41
1:S:3118:ASP:OD1	1:S:3119:VAL:N	2.54	0.41
1:S:3380:ARG:O	1:S:3384:HIS:ND1	2.54	0.41
1:S:3744:ASP:N	1:S:3744:ASP:OD1	2.49	0.41
2:T:165:ARG:HA	2:T:199:PHE:O	2.20	0.41
1:A:801:LYS:HZ2	1:A:3115:SER:HA	1.86	0.41
1:A:984:TYR:O	1:A:988:VAL:HG13	2.21	0.41
1:A:996:THR:HG23	1:A:1043:GLN:NE2	2.36	0.41
1:A:1166:LEU:O	1:A:1170:LYS:HG2	2.21	0.41
1:A:1827:LEU:O	1:A:1831:CYS:N	2.53	0.41
1:A:1839:PHE:CE2	1:A:1843:ILE:HD13	2.56	0.41
1:A:2332:GLU:HB2	1:A:2334:LYS:HZ1	1.86	0.41
1:A:2377:ARG:HB2	1:A:2378:PHE:CE2	2.55	0.41
1:A:2930:TYR:HB2	1:A:2939:LEU:HD21	2.02	0.41
1:A:3151:LEU:H	1:A:3151:LEU:HD23	1.86	0.41
1:A:3234:CYS:O	1:A:3238:MET:HG2	2.21	0.41
1:A:3321:LEU:HA	1:A:3324:ARG:HE	1.84	0.41
1:A:3390:GLN:O	1:A:3394:GLU:HG2	2.20	0.41
1:A:3552:LYS:HA	1:A:3552:LYS:HD3	1.88	0.41
1:A:3959:MET:CE	1:A:4124:TRP:HE1	2.33	0.41
2:B:203:MET:SD	2:B:239:LEU:HG	2.61	0.41
2:B:234:GLU:HG2	2:B:236:SER:H	1.85	0.41
2:B:303:PHE:HB2	2:B:309:GLY:O	2.20	0.41
5:G:70:LEU:HD12	5:G:70:LEU:HA	1.88	0.41
3:L:333:TYR:OH	2:T:505:ASP:OD2	2.35	0.41
1:S:104:SER:O	1:S:108:LYS:N	2.38	0.41
1:S:1582:LEU:HD12	1:S:1593:VAL:HG12	2.02	0.41
1:S:2168:LEU:HB3	1:S:2193:ILE:HD11	2.02	0.41
1:S:2927:ALA:O	1:S:2931:ARG:HG2	2.21	0.41
2:T:468:LYS:HE2	2:T:517:ARG:HB3	2.02	0.41
2:T:469:LEU:HG	2:T:514:MET:SD	2.61	0.41
1:A:586:GLN:HB2	1:A:613:HIS:ND1	2.36	0.41
1:A:990:GLN:HB3	1:A:2781:PRO:CD	2.47	0.41
1:A:1537:VAL:HA	1:A:1554:SER:HA	2.01	0.41
1:A:1565:GLU:HG2	1:A:1566:THR:N	2.35	0.41
1:A:1638:PRO:O	1:A:1641:THR:OG1	2.30	0.41
1:A:1711:ARG:O	1:A:1714:LEU:HB2	2.20	0.41
1:A:1770:GLN:NE2	1:A:1775:GLU:OE2	2.53	0.41
1:A:2185:MET:O	1:A:2189:ILE:HG12	2.20	0.41
1:A:3603:LYS:NZ	1:A:3647:GLY:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3763:ARG:NH1	1:A:4007:LYS:HA	2.36	0.41
2:B:131:PHE:O	2:B:135:MET:N	2.52	0.41
3:C:282:LYS:HB2	3:C:282:LYS:HE2	1.88	0.41
6:I:729:CYS:SG	6:I:736:VAL:N	2.87	0.41
3:L:207:ILE:O	3:L:211:VAL:HG23	2.21	0.41
3:L:332:LYS:HG2	2:T:486:HIS:HE1	1.85	0.41
3:L:343:LEU:N	3:L:392:ILE:O	2.43	0.41
6:R:731:LYS:HA	6:R:731:LYS:HD3	1.93	0.41
1:S:146:GLU:CD	1:S:146:GLU:H	2.24	0.41
1:S:297:LEU:HB3	1:S:316:LEU:HD12	2.02	0.41
1:S:384:MET:O	1:S:387:GLU:HG3	2.21	0.41
1:S:452:LYS:HG3	1:S:453:MET:HE3	2.02	0.41
1:S:853:ILE:HG13	1:S:854:ARG:N	2.36	0.41
1:S:1081:ALA:O	1:S:1085:ILE:HG23	2.20	0.41
1:S:1121:LEU:HG	1:S:1123:THR:H	1.86	0.41
1:S:1374:GLN:HA	1:S:1377:CYS:SG	2.61	0.41
1:S:1665:HIS:H	1:S:1668:PHE:HB3	1.85	0.41
1:S:2185:MET:O	1:S:2189:ILE:HG12	2.20	0.41
1:S:2349:LEU:HB3	1:S:2360:PHE:CE2	2.56	0.41
1:S:2548:PRO:HB2	1:S:2848:PHE:HD1	1.86	0.41
1:S:2572:TYR:CE1	1:S:2791:ILE:HD11	2.53	0.41
1:S:2576:MET:HB2	1:S:2783:ILE:HG22	2.03	0.41
1:S:2928:LYS:HG2	1:S:2931:ARG:NH2	2.36	0.41
1:S:2940:ARG:O	1:S:2944:THR:HG23	2.20	0.41
1:S:3101:TYR:O	1:S:3104:GLN:HG3	2.21	0.41
1:S:3167:ARG:N	1:S:3167:ARG:HD2	2.35	0.41
1:S:3472:ILE:HA	1:S:3479:THR:HG21	2.02	0.41
2:T:230:ARG:HH22	2:T:233:PHE:HD2	1.69	0.41
1:A:377:ASN:HB3	1:A:380:ASP:HB2	2.02	0.41
1:A:717:LYS:HD2	1:A:717:LYS:HA	1.79	0.41
1:A:770:LEU:O	1:A:773:LEU:HG	2.20	0.41
1:A:840:LEU:H	1:A:840:LEU:HD23	1.85	0.41
1:A:910:PHE:O	1:A:914:VAL:HG12	2.20	0.41
1:A:1049:GLN:O	1:A:1055:ASN:HB3	2.20	0.41
1:A:1086:TYR:CD1	1:A:1133:HIS:HB3	2.56	0.41
1:A:1118:GLU:HG2	1:A:1120:SER:H	1.86	0.41
1:A:1256:TRP:CZ2	1:A:1260:LEU:HD11	2.55	0.41
1:A:1913:LYS:HB3	3:L:730:ASP:HA	2.02	0.41
1:A:1948:ALA:O	1:A:1952:ILE:HG12	2.20	0.41
1:A:2105:HIS:ND1	1:A:2156:VAL:HG23	2.36	0.41
1:A:2167:PRO:O	1:A:2171:LEU:HG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2174:SER:O	1:A:2174:SER:OG	2.34	0.41
1:A:2303:LEU:HD13	1:A:2323:LEU:HD21	2.03	0.41
1:A:2920:VAL:O	1:A:2923:TRP:HB2	2.21	0.41
1:A:2969:ALA:HB2	1:A:3001:CYS:SG	2.60	0.41
1:A:3762:GLN:NE2	1:A:3795:PRO:HD2	2.35	0.41
1:A:3789:ARG:HH12	1:A:3931:ALA:HB3	1.86	0.41
1:A:3820:MET:SD	1:A:3824:GLU:HB3	2.61	0.41
2:B:250:GLU:CG	4:D:187:ASN:HD21	2.33	0.41
2:B:353:LEU:HB2	2:B:393:GLU:OE2	2.21	0.41
3:C:497:ARG:NH2	3:C:503:GLU:O	2.49	0.41
5:H:135:ALA:O	5:H:138:GLN:HG3	2.20	0.41
6:I:682:ILE:HA	6:I:730:PHE:CZ	2.56	0.41
6:I:721:VAL:HG13	6:I:742:PHE:CD2	2.55	0.41
6:I:816:HIS:HA	6:I:851:LYS:HB2	2.02	0.41
6:I:902:GLU:HB3	6:I:904:GLN:HE21	1.86	0.41
3:L:327:ASP:HB3	3:L:331:MET:HE3	2.03	0.41
3:L:458:ILE:HA	2:T:350:PHE:HE2	1.85	0.41
3:L:653:GLN:HA	3:L:656:ASN:HB2	2.02	0.41
3:L:724:ASP:O	3:L:728:LEU:N	2.52	0.41
5:P:135:ALA:HA	5:P:138:GLN:HG2	2.02	0.41
6:R:748:PRO:HA	6:R:751:LYS:HB2	2.03	0.41
1:S:184:VAL:HG23	1:S:186:PRO:HD3	2.02	0.41
1:S:294:PHE:CE2	1:S:298:LEU:HD11	2.55	0.41
1:S:703:CYS:HB3	1:S:707:PHE:CE2	2.55	0.41
1:S:802:THR:HG21	1:S:922:SER:H	1.86	0.41
1:S:881:LYS:HZ3	1:S:881:LYS:HG3	1.63	0.41
1:S:883:TYR:CE1	1:S:3120:LEU:HD22	2.56	0.41
1:S:1062:ARG:HH12	1:S:3745:GLU:HG3	1.86	0.41
1:S:1513:GLY:O	1:S:1517:LEU:HG	2.21	0.41
1:S:1884:LEU:HD22	1:S:1885:PRO:HD2	2.02	0.41
1:S:1921:ASP:OD1	1:S:1921:ASP:N	2.54	0.41
1:S:2137:ILE:O	1:S:2137:ILE:HG23	2.21	0.41
1:S:2276:LEU:O	1:S:2280:VAL:HG23	2.21	0.41
1:S:2328:ARG:HB2	1:S:2370:SER:O	2.21	0.41
1:S:2757:ILE:HA	1:S:2760:GLU:OE1	2.21	0.41
1:S:3005:LEU:HD13	1:S:3253:SER:HB3	2.03	0.41
1:S:3061:LEU:O	1:S:3065:ILE:HG12	2.21	0.41
1:S:3106:GLY:O	1:S:3110:PHE:HD2	2.03	0.41
1:S:3291:GLN:O	1:S:3291:GLN:HG3	2.21	0.41
1:S:3347:CYS:O	1:S:3351:ILE:HG13	2.21	0.41
1:S:3442:TYR:O	1:S:3446:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3480:LEU:HA	1:S:3483:MET:HB2	2.03	0.41
1:S:3893:SER:H	1:S:3896:ALA:HB3	1.86	0.41
1:S:3962:ARG:NH2	1:S:4125:GLU:OE1	2.53	0.41
2:T:109:ASP:O	2:T:115:ARG:NH1	2.54	0.41
2:T:230:ARG:HD3	2:T:232:HIS:N	2.35	0.41
2:T:420:LEU:HB3	2:T:424:LYS:HA	2.02	0.41
1:A:81:CYS:O	1:A:85:ILE:HG13	2.20	0.41
1:A:153:PHE:HZ	1:A:192:ASN:HB2	1.85	0.41
1:A:207:GLN:HG3	1:A:217:LEU:HB3	2.03	0.41
1:A:296:VAL:HA	1:A:299:LYS:HG2	2.02	0.41
1:A:745:VAL:O	1:A:749:VAL:HG23	2.21	0.41
1:A:1454:ALA:HA	1:A:1457:GLN:OE1	2.20	0.41
1:A:1723:PRO:HG3	3:C:594:PRO:HD3	2.02	0.41
1:A:2481:HIS:ND1	1:A:2499:PHE:HE1	2.18	0.41
1:A:2525:TRP:CZ3	1:A:2545:LEU:HD21	2.56	0.41
1:A:3742:GLY:N	1:A:3746:ARG:O	2.53	0.41
1:A:3837:CYS:SG	1:A:3873:LYS:HG2	2.61	0.41
2:B:182:LYS:HA	2:B:185:ARG:HG2	2.03	0.41
2:B:326:GLN:HE21	2:B:328:ILE:HD11	1.86	0.41
4:D:122:ARG:HE	4:M:45:ALA:HB2	1.86	0.41
5:H:3:ARG:NH1	5:H:21:GLN:OE1	2.54	0.41
3:L:371:GLU:HG3	2:T:452:ILE:HD13	2.02	0.41
3:L:395:TYR:HB3	3:L:404:GLN:HG2	2.01	0.41
5:Q:128:CYS:O	5:Q:131:LEU:HG	2.21	0.41
6:R:707:ILE:HA	6:R:710:LYS:HG2	2.02	0.41
1:S:217:LEU:O	1:S:217:LEU:HD12	2.21	0.41
1:S:247:GLU:HG2	1:S:251:PHE:CE2	2.56	0.41
1:S:573:LEU:HD11	1:S:645:TRP:CD1	2.56	0.41
1:S:851:ILE:O	1:S:854:ARG:HG2	2.21	0.41
1:S:1741:ASP:O	1:S:1744:LYS:HG2	2.21	0.41
1:S:2102:LYS:HZ2	1:S:2153:THR:HG22	1.86	0.41
1:S:2365:ASN:O	1:S:2368:THR:HG22	2.21	0.41
1:S:2746:LYS:O	1:S:2749:ALA:HB3	2.21	0.41
1:S:3169:PRO:O	1:S:3170:ASP:HB2	2.21	0.41
1:S:3455:LYS:HA	1:S:3490:VAL:HG23	2.02	0.41
1:S:3898:LEU:HG	1:S:3901:ARG:NH2	2.35	0.41
1:S:4038:TRP:CH2	1:S:4040:PRO:HG3	2.56	0.41
1:A:1100:VAL:HG23	1:A:1101:PHE:N	2.36	0.40
1:A:1183:CYS:O	1:A:1186:LYS:HG2	2.21	0.40
1:A:1528:LEU:O	1:A:1532:LEU:HG	2.21	0.40
1:A:1851:LEU:HB3	1:A:1852:LYS:NZ	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2145:PHE:O	1:A:2149:LEU:HD23	2.21	0.40
1:A:3369:ASP:HB3	1:A:3372:LYS:HG2	2.04	0.40
1:A:3535:ILE:HD12	1:A:3535:ILE:HA	1.91	0.40
2:B:70:VAL:HG13	4:D:186:ILE:HD11	2.04	0.40
3:C:267:ILE:HB	3:C:361:VAL:HB	2.03	0.40
5:G:73:ALA:HB1	5:G:86:PHE:HZ	1.86	0.40
6:I:663:GLU:HA	6:I:688:TYR:HB2	2.02	0.40
6:I:863:VAL:HG11	6:I:886:PHE:HA	2.02	0.40
3:L:9:ALA:HB2	3:L:127:PHE:CG	2.57	0.40
6:R:697:THR:HB	6:R:718:HIS:HE2	1.86	0.40
1:S:627:VAL:HG11	1:S:665:GLY:HA2	2.03	0.40
1:S:887:ASP:HB2	1:S:961:LEU:HD21	2.03	0.40
1:S:985:GLU:HG2	1:S:986:PRO:CD	2.51	0.40
1:S:1017:ILE:HD12	1:S:1017:ILE:H	1.85	0.40
1:S:1881:TYR:CE1	1:S:1951:VAL:HA	2.55	0.40
1:S:2175:GLU:OE1	1:S:2182:ILE:HG23	2.21	0.40
1:S:2510:LEU:HA	1:S:2521:ILE:HD13	2.03	0.40
1:S:2835:LYS:HA	1:S:2835:LYS:HD3	1.90	0.40
1:S:2965:TYR:CD2	1:S:3253:SER:HB2	2.54	0.40
1:S:3097:ASP:O	1:S:3100:LYS:HG3	2.21	0.40
1:S:3120:LEU:HD12	1:S:3895:GLU:HB2	2.04	0.40
1:A:528:VAL:HG11	1:A:632:GLU:OE2	2.20	0.40
1:A:528:VAL:HG23	1:A:529:ASP:N	2.36	0.40
1:A:914:VAL:HA	1:A:917:LEU:HB2	2.03	0.40
1:A:994:TRP:CZ3	1:A:2582:SER:HB2	2.56	0.40
1:A:1071:ASN:HD22	1:A:1074:LYS:NZ	2.19	0.40
1:A:1081:ALA:O	1:A:1085:ILE:HG23	2.21	0.40
1:A:1787:ARG:NE	1:A:1830:HIS:HE1	2.19	0.40
1:A:2485:ARG:HH22	1:A:2530:ARG:HA	1.87	0.40
1:A:2940:ARG:O	1:A:2944:THR:HG23	2.21	0.40
1:A:3154:GLN:OE1	1:A:3227:ILE:HG13	2.21	0.40
1:A:3263:HIS:HB2	1:A:3276:TRP:CZ2	2.57	0.40
1:A:3292:GLY:O	1:A:3296:GLN:HB2	2.21	0.40
1:A:3293:CYS:SG	1:A:3340:ALA:HB1	2.62	0.40
1:A:3981:TYR:O	1:A:3985:VAL:HG23	2.21	0.40
1:A:4055:ASN:ND2	1:A:4091:ALA:O	2.53	0.40
3:C:20:MET:O	3:C:30:PRO:HD2	2.21	0.40
3:C:35:LYS:HA	3:C:38:ILE:HG12	2.03	0.40
3:C:138:LEU:HB3	3:C:201:GLN:HA	2.03	0.40
3:C:352:GLN:HB2	3:C:355:PHE:CE2	2.57	0.40
3:C:598:PHE:CE2	3:C:616:LEU:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:663:GLN:HG3	3:C:667:GLU:OE1	2.21	0.40
6:I:657:ASN:HA	6:I:660:GLU:HG3	2.03	0.40
3:L:34:ALA:HB1	3:L:135:PHE:HD2	1.86	0.40
3:L:420:VAL:HG21	2:T:359:HIS:HB3	2.02	0.40
3:L:497:ARG:HH21	3:L:505:LEU:HD23	1.86	0.40
6:R:712:ILE:HD13	6:R:712:ILE:HA	1.98	0.40
1:S:197:PHE:O	1:S:201:LEU:HG	2.22	0.40
1:S:237:SER:HA	1:S:281:GLN:HG3	2.03	0.40
1:S:670:LEU:HB2	1:S:732:PHE:CZ	2.55	0.40
1:S:1417:THR:O	1:S:1421:GLU:N	2.45	0.40
1:S:1641:THR:O	1:S:1645:VAL:HG13	2.21	0.40
1:S:1881:TYR:OH	1:S:1954:CYS:HB3	2.21	0.40
1:S:2921:LEU:O	1:S:2924:VAL:HG12	2.22	0.40
1:S:3234:CYS:O	1:S:3238:MET:HG2	2.21	0.40
1:S:4009:PRO:HA	1:S:4038:TRP:HZ2	1.86	0.40
1:S:4101:GLU:HG2	1:S:4102:THR:N	2.36	0.40
1:A:49:ALA:O	1:A:53:LEU:HG	2.21	0.40
1:A:163:LYS:HE2	2:B:302:THR:H	1.87	0.40
1:A:1149:LYS:HB2	1:A:1151:ARG:NH2	2.37	0.40
1:A:1261:LEU:HD21	1:A:1337:VAL:HA	2.03	0.40
1:A:1784:ARG:HA	1:A:1787:ARG:NE	2.36	0.40
1:A:2817:LEU:HD23	1:A:2865:HIS:NE2	2.36	0.40
1:A:3416:LEU:HD22	1:A:3449:LYS:HD2	2.02	0.40
1:A:3912:CYS:HA	1:A:3915:HIS:CD2	2.56	0.40
1:A:4055:ASN:O	1:A:4059:ILE:HG12	2.21	0.40
2:B:69:SER:OG	2:B:243:LEU:HA	2.22	0.40
2:B:79:ASP:N	2:B:79:ASP:OD1	2.54	0.40
2:B:196:THR:OG1	2:B:198:ILE:HG12	2.21	0.40
2:B:214:SER:HA	2:B:218:ARG:CG	2.52	0.40
2:B:270:SER:O	2:B:371:GLU:HG2	2.21	0.40
2:B:490:LEU:O	2:B:493:LEU:HG	2.20	0.40
3:C:285:LYS:HB3	3:C:287:GLU:OE1	2.22	0.40
5:G:176:LEU:HD23	5:G:179:ARG:HD3	2.03	0.40
5:H:43:TRP:NE1	5:H:119:PRO:HB3	2.36	0.40
5:P:28:LEU:HD23	5:P:70:LEU:HB3	2.03	0.40
5:Q:38:ASP:N	5:Q:38:ASP:OD1	2.53	0.40
6:R:759:ASP:CG	6:R:763:ASP:HB3	2.41	0.40
1:S:320:LEU:HA	1:S:323:VAL:HG22	2.03	0.40
1:S:493:LYS:HE3	1:S:522:PRO:O	2.21	0.40
1:S:737:PRO:HG2	1:S:740:ILE:HG12	2.02	0.40
1:S:1171:TRP:O	1:S:1175:HIS:ND1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1714:LEU:HD13	1:S:1758:LEU:HD21	2.02	0.40
1:S:2238:ILE:HA	1:S:2241:LEU:HG	2.02	0.40
1:S:2273:GLY:HA2	1:S:2276:LEU:HD12	2.02	0.40
1:S:2531:LEU:HD23	1:S:2531:LEU:HA	1.88	0.40
1:S:3389:VAL:O	1:S:3393:GLU:HG3	2.21	0.40
1:S:3772:ASN:OD1	1:S:3788:LEU:HB3	2.21	0.40
2:T:78:SER:HB2	2:T:250:GLU:OE2	2.22	0.40
2:T:102:ILE:HD12	2:T:146:VAL:HG12	2.02	0.40
2:T:176:HIS:O	2:T:183:ALA:HB2	2.22	0.40
1:A:207:GLN:O	1:A:215:PRO:HA	2.21	0.40
1:A:221:ALA:O	1:A:224:LEU:HG	2.20	0.40
1:A:232:CYS:SG	1:A:281:GLN:HG3	2.61	0.40
1:A:446:PHE:CZ	1:A:530:LEU:HB2	2.57	0.40
1:A:472:GLY:O	1:A:475:LEU:HB3	2.21	0.40
1:A:849:GLU:HG2	1:A:850:GLU:N	2.36	0.40
1:A:1000:LYS:HA	1:A:1000:LYS:HD3	1.95	0.40
1:A:1009:LEU:HD12	1:A:1010:LEU:N	2.37	0.40
1:A:1012:ALA:HA	1:A:1015:ASP:OD2	2.21	0.40
1:A:2493:ASN:OD1	1:A:2494:ASP:N	2.54	0.40
1:A:3604:LYS:HG3	1:A:3605:ASN:H	1.85	0.40
1:A:3988:LEU:HD23	1:A:4100:GLU:HA	2.03	0.40
2:B:381:LEU:HD11	3:C:537:PHE:HB3	2.03	0.40
3:L:380:LEU:O	3:L:384:LEU:HD23	2.21	0.40
3:L:540:ILE:HD11	2:T:376:ILE:HD13	2.03	0.40
4:M:187:ASN:HB3	4:M:190:PHE:CD1	2.57	0.40
5:Q:66:TYR:HE1	5:Q:108:LEU:HA	1.86	0.40
1:S:860:GLY:HA3	1:S:3136:THR:OG1	2.22	0.40
1:S:983:LEU:O	1:S:986:PRO:HD2	2.21	0.40
1:S:990:GLN:HG2	1:S:2781:PRO:HD3	2.03	0.40
1:S:1685:ASP:HB3	1:S:1688:LEU:HG	2.02	0.40
1:S:1713:VAL:HA	1:S:1716:GLN:HG2	2.04	0.40
1:S:1715:GLU:O	1:S:1719:VAL:HG23	2.21	0.40
1:S:2044:ASP:O	1:S:2048:GLY:N	2.55	0.40
1:S:2427:ARG:HE	1:S:2464:HIS:HE2	1.68	0.40
1:S:2471:GLU:HB3	1:S:2517:LEU:HD21	2.01	0.40
1:S:2892:LEU:O	1:S:2895:GLU:HG2	2.21	0.40
1:S:3302:LYS:C	1:S:3304:VAL:H	2.24	0.40
1:S:3419:PHE:O	1:S:3423:GLN:HG2	2.22	0.40
1:A:106:GLU:O	1:A:110:THR:HG23	2.22	0.40
1:A:313:LEU:HD23	1:A:316:LEU:HD12	2.04	0.40
1:A:487:LEU:HD13	1:A:575:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:733:LEU:O	1:A:736:LEU:HD23	2.22	0.40
1:A:851:ILE:O	1:A:855:VAL:HG23	2.21	0.40
1:A:1420:ARG:HG2	1:A:1467:ILE:HD12	2.02	0.40
1:A:2318:ALA:HA	1:A:2321:GLU:HG2	2.04	0.40
1:A:2739:LEU:HD12	1:A:2740:SER:N	2.37	0.40
1:A:2950:LYS:HB3	1:A:2952:ILE:HG22	2.03	0.40
1:A:3513:ALA:HA	1:A:3516:HIS:ND1	2.36	0.40
2:B:357:LYS:HB2	2:B:360:HIS:CD2	2.57	0.40
5:G:72:LYS:HZ1	5:G:99:LYS:HE2	1.86	0.40
3:L:247:TRP:HB3	3:L:263:ALA:HB3	2.03	0.40
3:L:444:TYR:CD1	2:T:379:SER:HB3	2.56	0.40
1:S:217:LEU:HD13	1:S:221:ALA:HB3	2.03	0.40
1:S:243:GLN:HA	1:S:246:ARG:HH11	1.86	0.40
1:S:300:TRP:HE3	1:S:308:LEU:HD21	1.87	0.40
1:S:738:HIS:HB2	1:S:780:ILE:HD11	2.04	0.40
1:S:781:ASP:HB2	1:S:783:HIS:ND1	2.37	0.40
1:S:913:ARG:O	1:S:916:GLU:HG3	2.22	0.40
1:S:1038:LYS:HB3	1:S:1038:LYS:HE2	1.73	0.40
1:S:1627:LYS:NZ	1:S:1670:GLU:HB2	2.36	0.40
1:S:1881:TYR:OH	1:S:1955:VAL:HG23	2.21	0.40
1:S:2216:LEU:O	1:S:2219:LEU:HG	2.22	0.40
1:S:2801:ASP:OD2	1:S:2804:ILE:HG12	2.21	0.40
1:S:3119:VAL:HA	1:S:3125:ARG:NE	2.32	0.40
1:S:3131:SER:O	1:S:3135:LEU:HG	2.22	0.40
1:S:3781:CYS:O	1:S:3785:ALA:N	2.55	0.40
2:T:372:GLU:OE1	2:T:378:SER:N	2.55	0.40
2:T:525:PHE:HA	2:T:528:LEU:HD12	2.04	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	3476/4128 (84%)	3213 (92%)	259 (8%)	4 (0%)	51 85
1	S	3464/4128 (84%)	3210 (93%)	252 (7%)	2 (0%)	51 85
2	B	505/609 (83%)	471 (93%)	34 (7%)	0	100 100
2	T	498/609 (82%)	470 (94%)	28 (6%)	0	100 100
3	C	660/732 (90%)	619 (94%)	41 (6%)	0	100 100
3	L	644/732 (88%)	615 (96%)	29 (4%)	0	100 100
4	D	139/204 (68%)	137 (99%)	2 (1%)	0	100 100
4	M	160/204 (78%)	160 (100%)	0	0	100 100
5	G	199/336 (59%)	195 (98%)	4 (2%)	0	100 100
5	H	190/336 (56%)	188 (99%)	2 (1%)	0	100 100
5	P	199/336 (59%)	196 (98%)	3 (2%)	0	100 100
5	Q	190/336 (56%)	188 (99%)	2 (1%)	0	100 100
6	I	242/911 (27%)	219 (90%)	23 (10%)	0	100 100
6	R	242/911 (27%)	216 (89%)	26 (11%)	0	100 100
All	All	10808/14512 (74%)	10097 (93%)	705 (6%)	6 (0%)	54 85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	S	3304	VAL
1	A	68	PHE
1	A	1231	GLN
1	A	66	LEU
1	S	956	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	2999/3671 (82%)	2984 (100%)	15 (0%)	88 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	S	3045/3671 (83%)	3030 (100%)	15 (0%)	88 93
2	B	443/548 (81%)	441 (100%)	2 (0%)	88 93
2	T	446/548 (81%)	441 (99%)	5 (1%)	73 85
3	C	581/649 (90%)	579 (100%)	2 (0%)	92 95
3	L	570/649 (88%)	566 (99%)	4 (1%)	84 90
4	D	110/160 (69%)	109 (99%)	1 (1%)	78 87
4	M	120/160 (75%)	118 (98%)	2 (2%)	60 78
5	G	180/303 (59%)	177 (98%)	3 (2%)	60 78
5	H	177/303 (58%)	174 (98%)	3 (2%)	60 78
5	P	180/303 (59%)	180 (100%)	0	100 100
5	Q	177/303 (58%)	176 (99%)	1 (1%)	86 92
6	I	218/808 (27%)	217 (100%)	1 (0%)	88 93
6	R	217/808 (27%)	214 (99%)	3 (1%)	67 81
All	All	9463/12884 (73%)	9406 (99%)	57 (1%)	86 92

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	67	VAL
1	A	205	LYS
1	A	899	ARG
1	A	1178	ARG
1	A	1727	ARG
1	A	2120	ARG
1	A	2207	LYS
1	A	2311	ARG
1	A	2931	ARG
1	A	3113	ASN
1	A	3725	ARG
1	A	4014	LYS
1	A	4075	ARG
1	A	4090	ARG
2	B	258	ARG
2	B	516	LYS
3	C	130	ARG
3	C	502	ARG

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Mol	Chain	Res	Type
4	D	193	LYS
5	G	4	LYS
5	G	161	ARG
5	G	197	LYS
5	H	146	LYS
5	H	188	LYS
5	H	197	LYS
6	I	741	ARG
3	L	130	ARG
3	L	469	LYS
3	L	502	ARG
3	L	634	LYS
4	M	138	ARG
4	M	194	LYS
5	Q	102	LYS
6	R	741	ARG
6	R	782	LYS
6	R	885	LYS
1	S	24	ARG
1	S	631	ARG
1	S	675	ARG
1	S	1026	ARG
1	S	1031	ARG
1	S	1155	ARG
1	S	1329	ARG
1	S	1447	ARG
1	S	1727	ARG
1	S	2207	LYS
1	S	2416	LYS
1	S	3100	LYS
1	S	3621	LYS
1	S	4090	ARG
1	S	4105	LYS
2	T	114	LYS
2	T	152	ASN
2	T	230	ARG
2	T	297	LYS
2	T	299	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	330	ASN
1	A	454	GLN
1	A	978	GLN
1	A	1069	HIS
1	A	1598	ASN
1	A	1611	GLN
1	A	1665	HIS
1	A	1725	GLN
1	A	1771	GLN
1	A	2291	GLN
1	A	2295	GLN
1	A	2306	ASN
1	A	2365	ASN
1	A	3105	ASN
1	A	3112	GLN
1	A	3139	GLN
1	A	3515	GLN
1	A	3915	HIS
1	A	3924	HIS
1	A	4000	ASN
2	B	176	HIS
2	B	489	ASN
3	C	330	GLN
3	C	604	GLN
4	D	187	ASN
5	G	148	ASN
6	I	848	HIS
6	I	904	GLN
3	L	188	HIS
5	P	21	GLN
6	R	718	HIS
1	S	33	GLN
1	S	136	GLN
1	S	415	GLN
1	S	561	ASN
1	S	753	GLN
1	S	865	GLN
1	S	990	GLN
1	S	1426	GLN
1	S	1654	GLN
1	S	1754	GLN
1	S	2234	ASN

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Mol	Chain	Res	Type
1	S	3113	ASN
1	S	3166	ASN
1	S	3915	HIS
1	S	4000	ASN
2	T	95	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

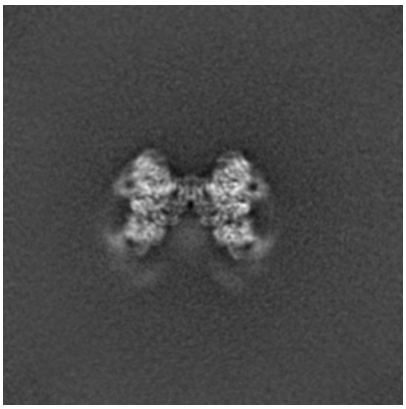
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16044. These allow visual inspection of the internal detail of the map and identification of artifacts.

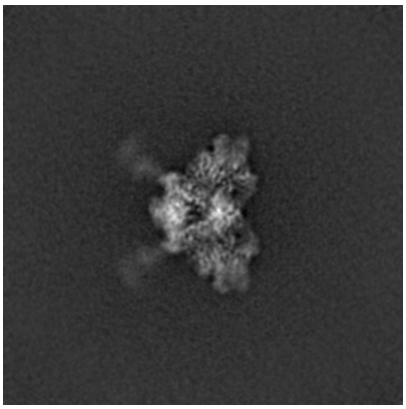
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

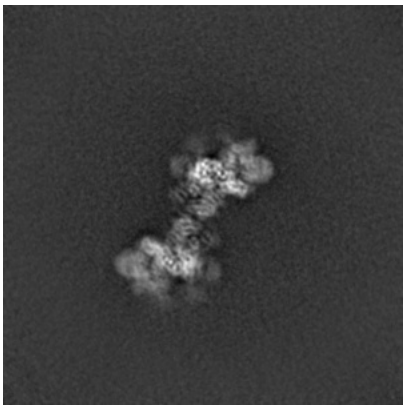
6.1.1 Primary map



X

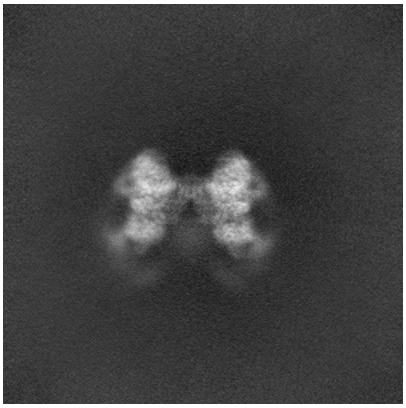


Y

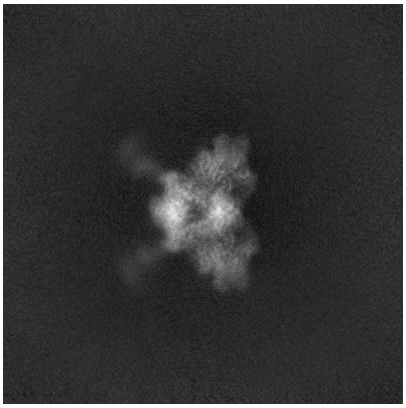


Z

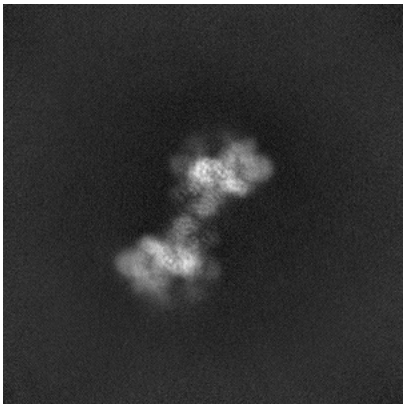
6.1.2 Raw map



X



Y

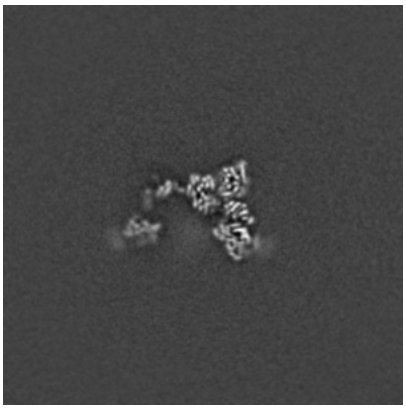


Z

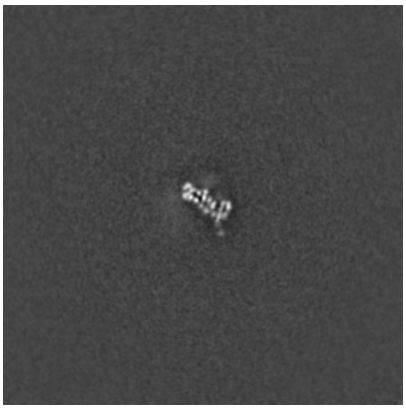
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

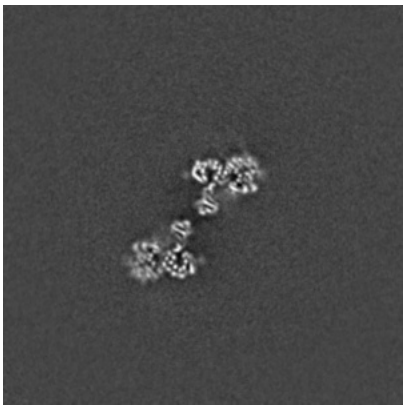
6.2.1 Primary map



X Index: 270

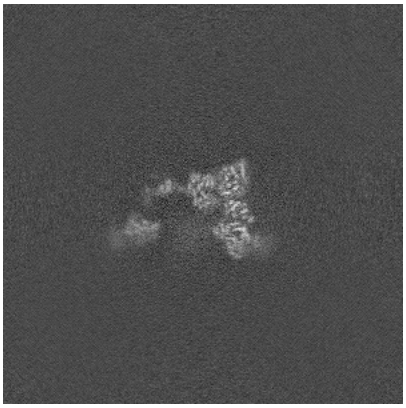


Y Index: 270

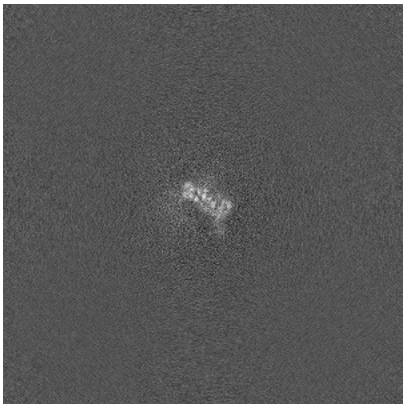


Z Index: 270

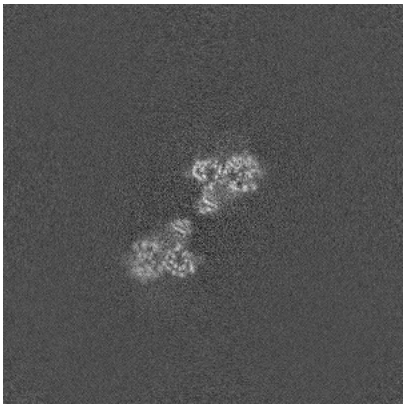
6.2.2 Raw map



X Index: 270



Y Index: 270

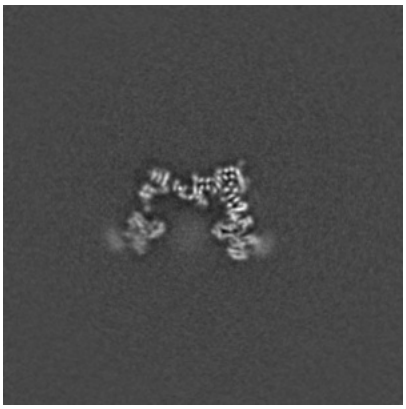


Z Index: 270

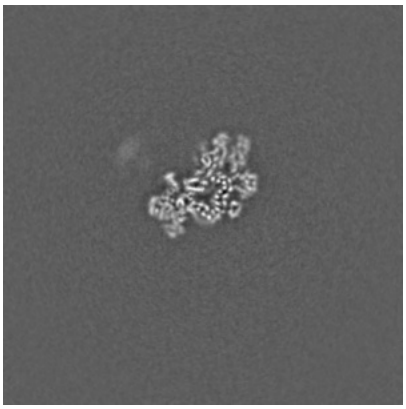
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

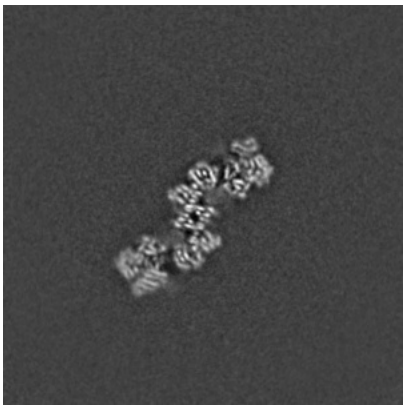
6.3.1 Primary map



X Index: 263

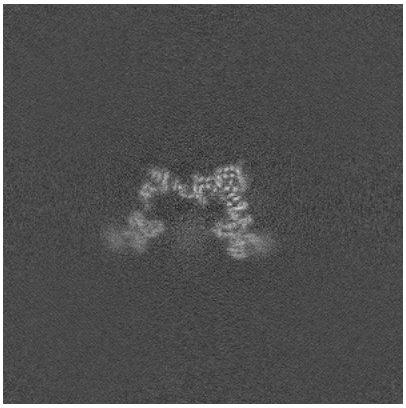


Y Index: 312

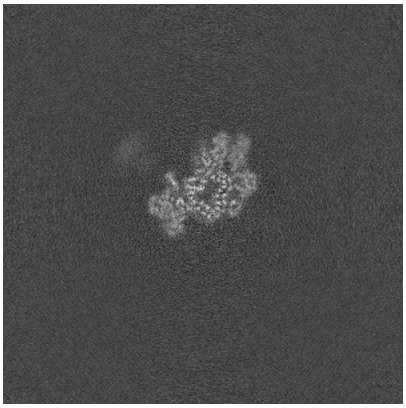


Z Index: 289

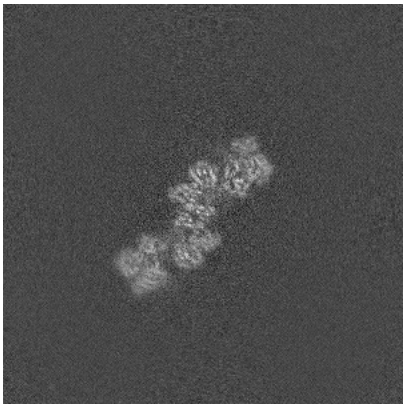
6.3.2 Raw map



X Index: 263



Y Index: 313

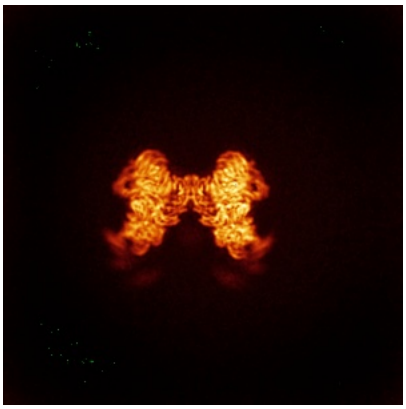


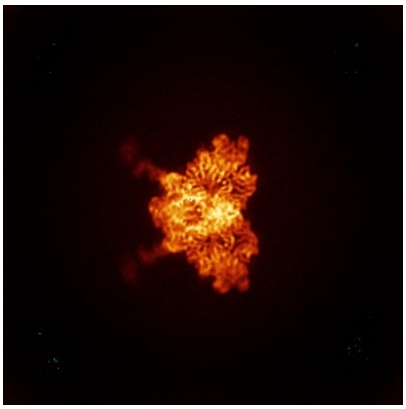
Z Index: 289

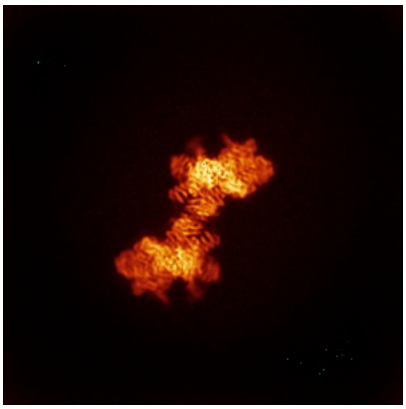
The images above show the largest variance slices of the map in three orthogonal directions.

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

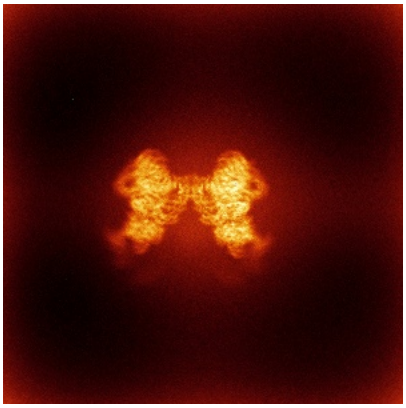
6.4.1 Primary map

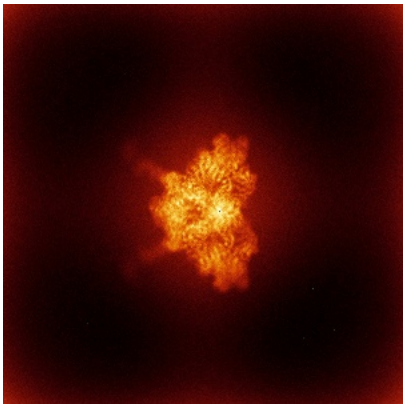

X

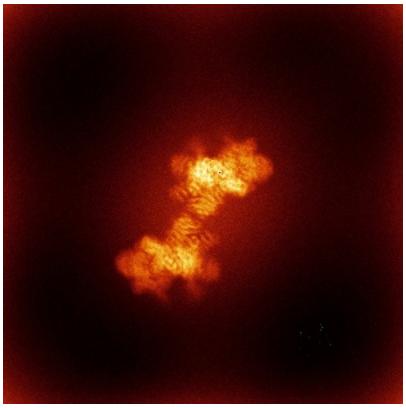

Y


Z

6.4.2 Raw map


X

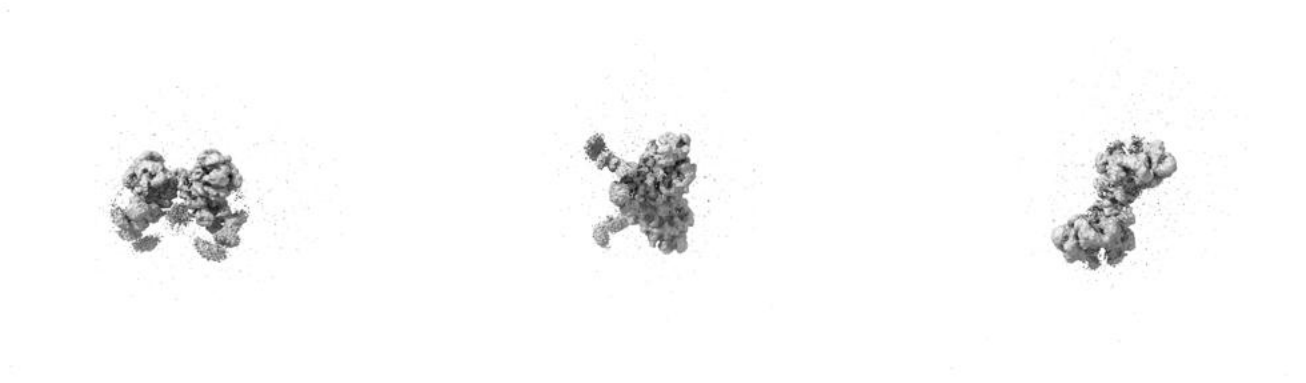

Y


Z

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

6.5 Orthogonal surface views (i)

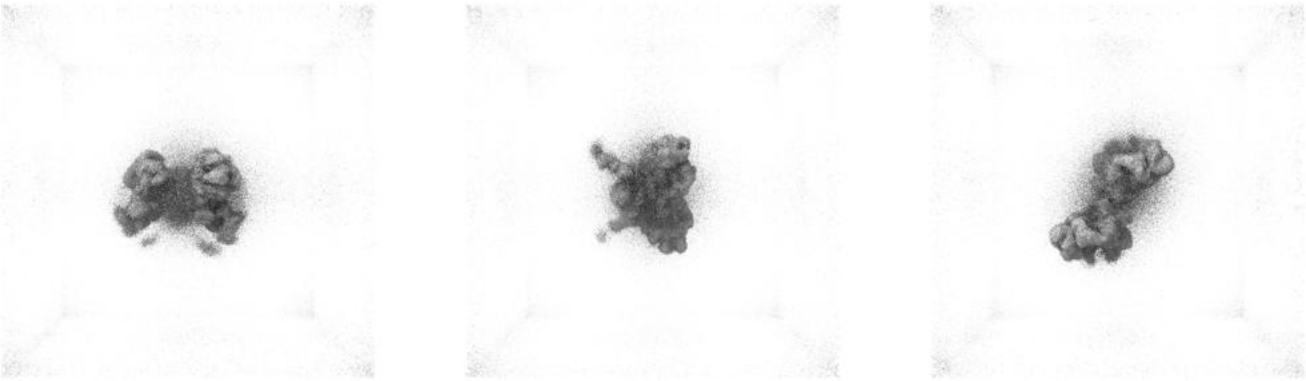
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.061. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

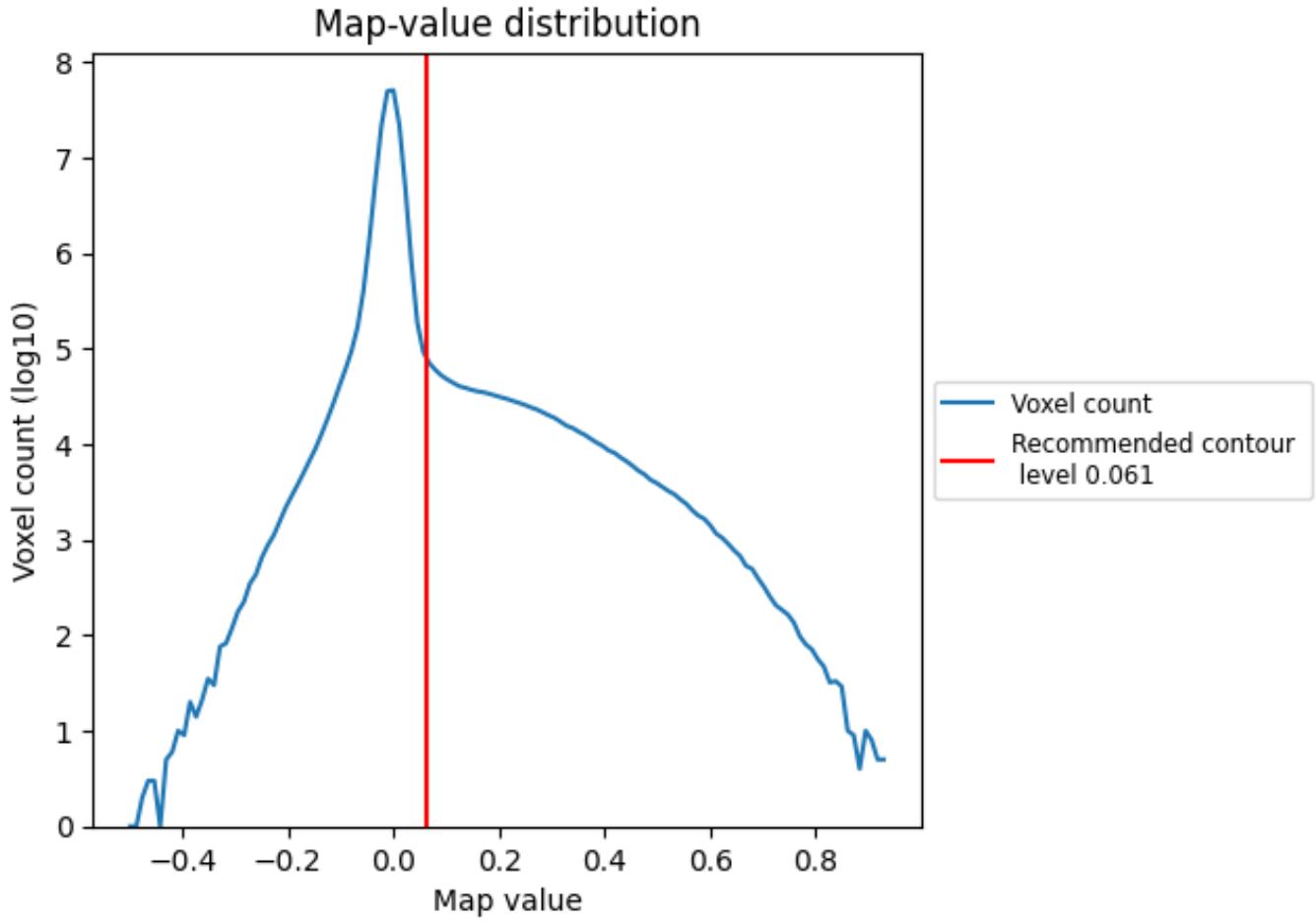
6.6 Mask visualisation (i)

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

7 Map analysis

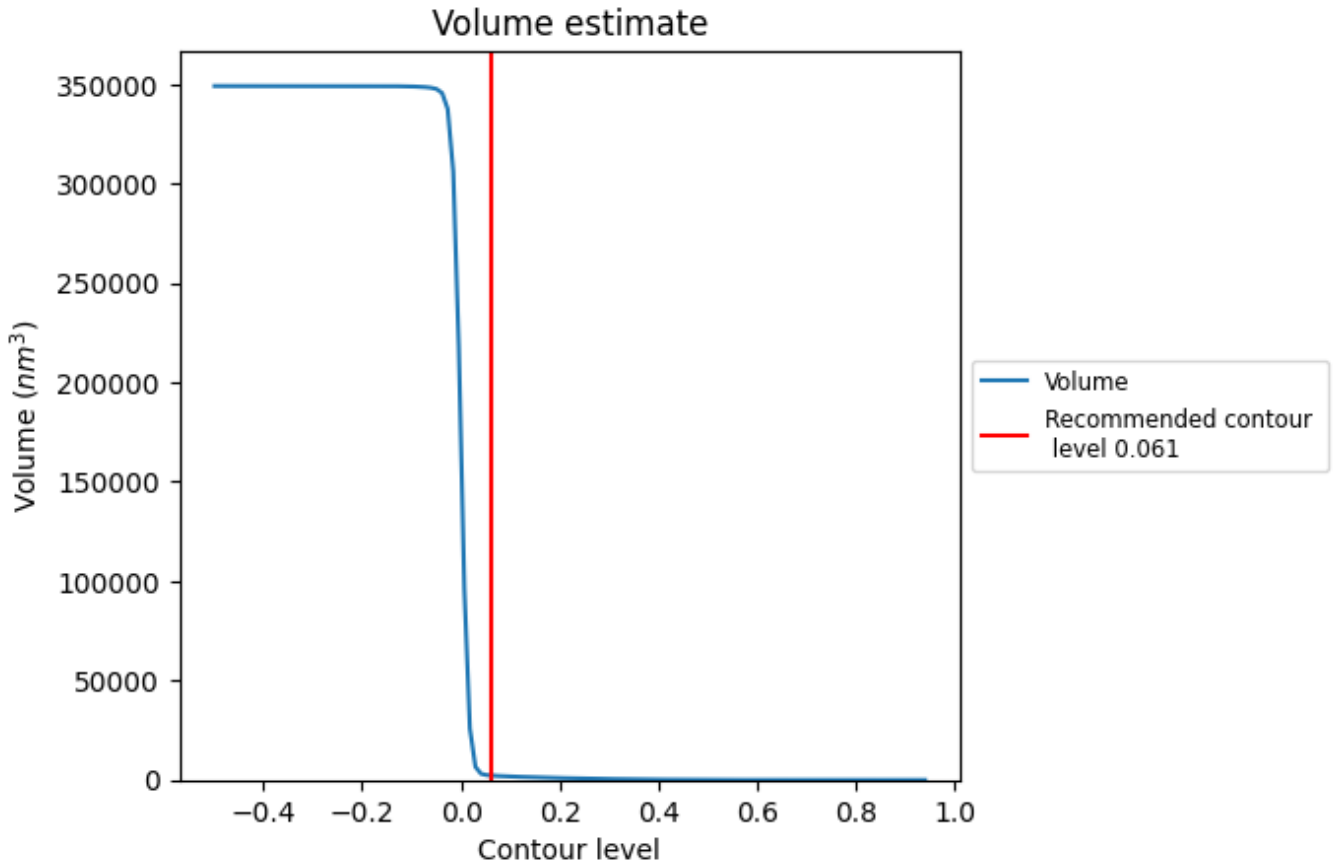
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

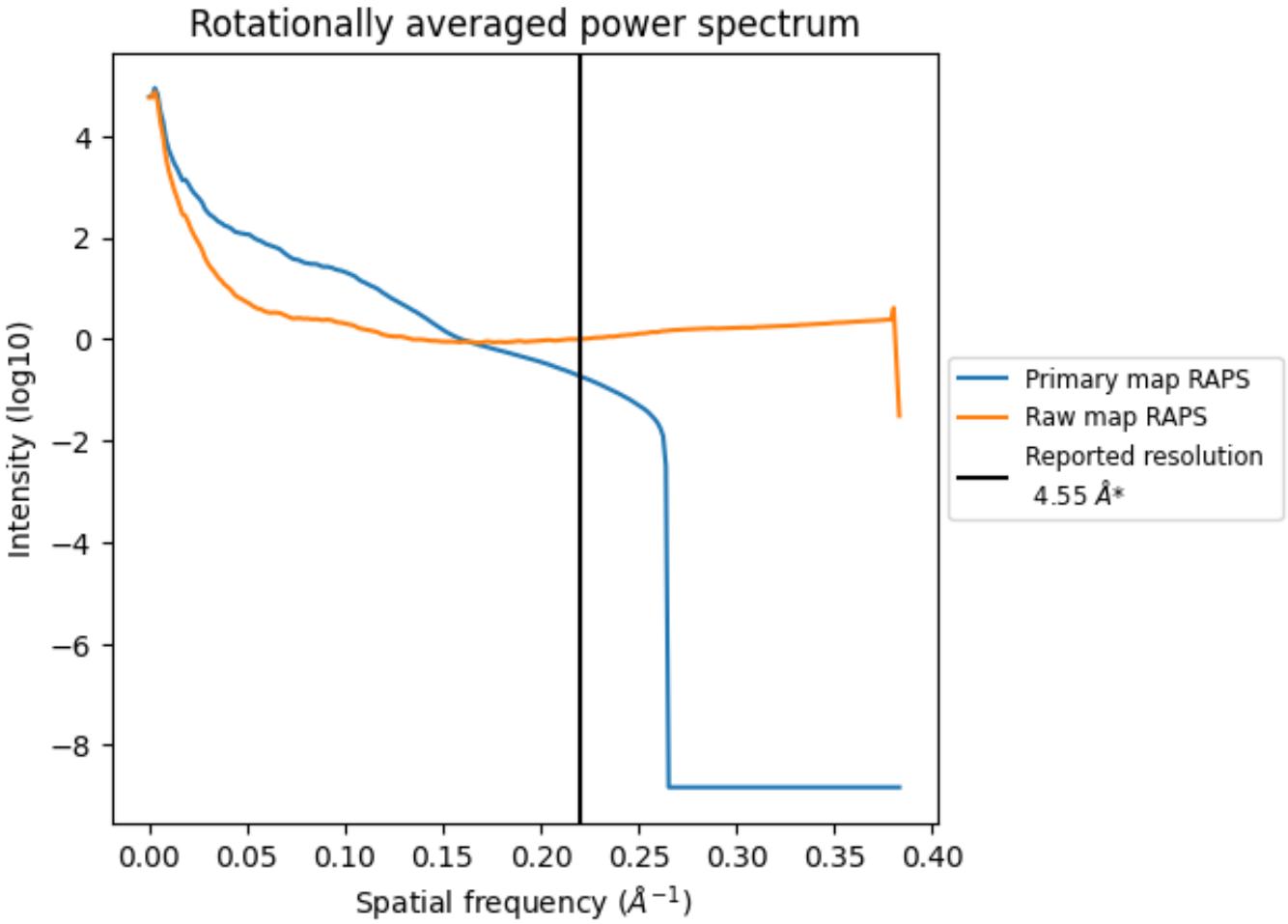
7.2 Volume estimate



The volume at the recommended contour level is 2251 nm^3; this corresponds to an approximate mass of 2033 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)

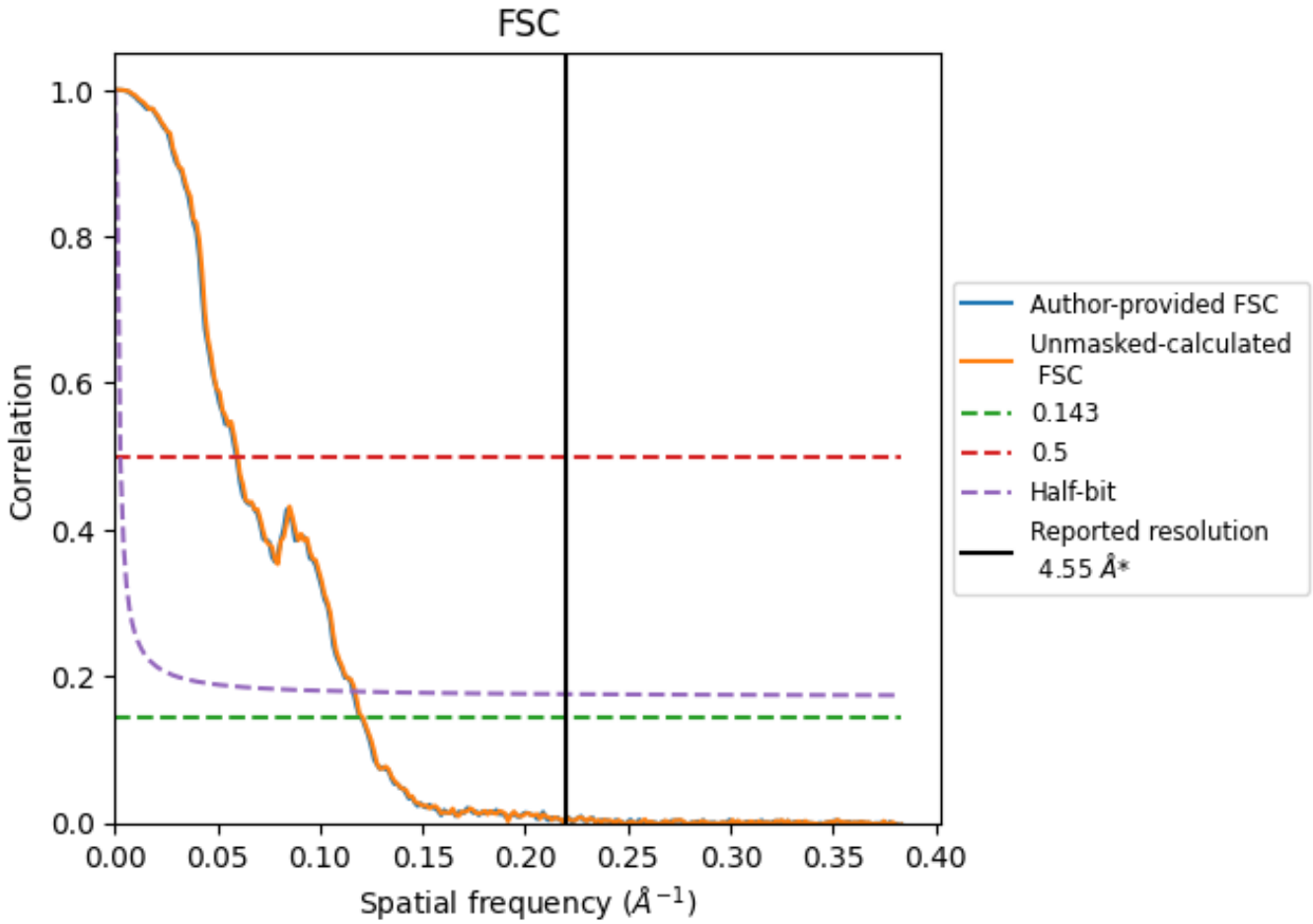


*Reported resolution corresponds to spatial frequency of 0.220 Å^{-1}

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 0.220 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.55	-	-
Author-provided FSC curve	8.33	16.86	8.61
Unmasked-calculated*	8.27	16.69	8.54

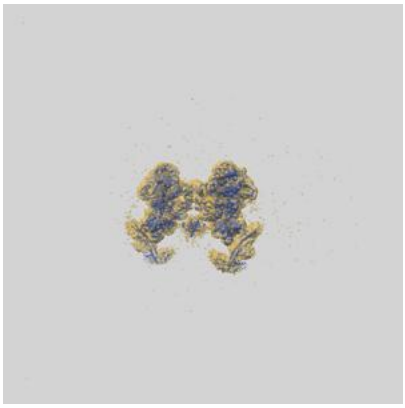
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.33 differs from the reported value 4.55 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.27 differs from the reported value 4.55 by more than 10 %

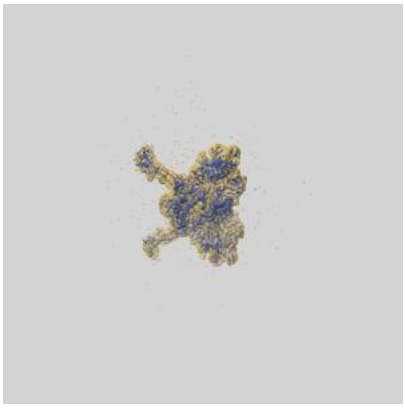
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16044 and PDB model 8BH3. Per-residue inclusion information can be found in section 3 on page 6.

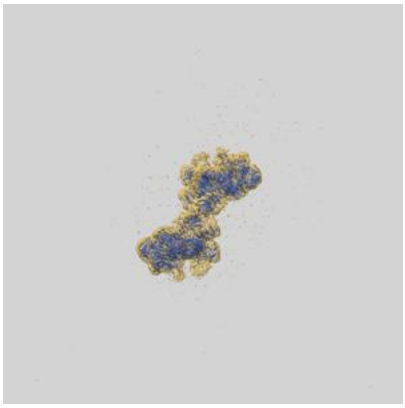
9.1 Map-model overlay



X



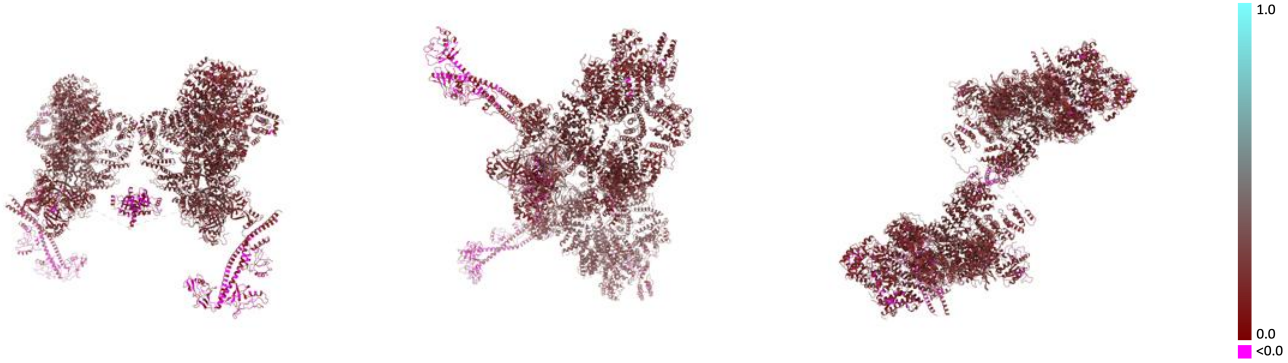
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.061 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.

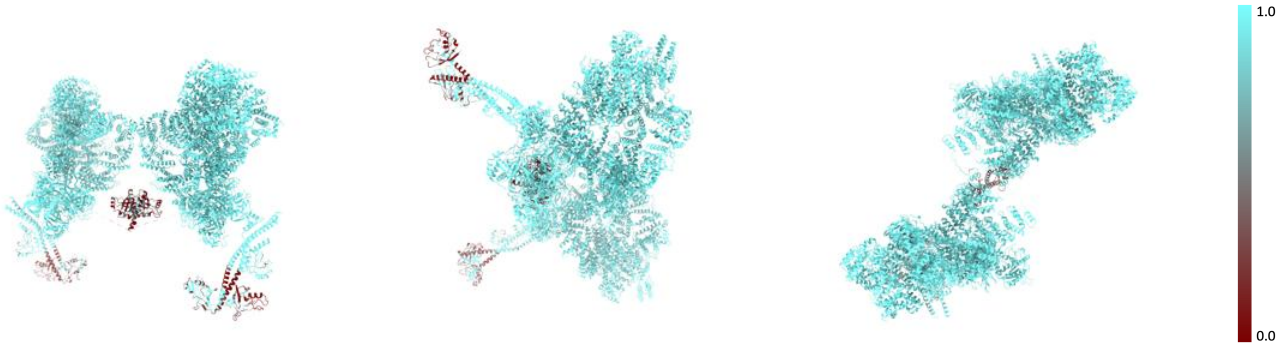
9.2 Q-score mapped to coordinate model (i)



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.

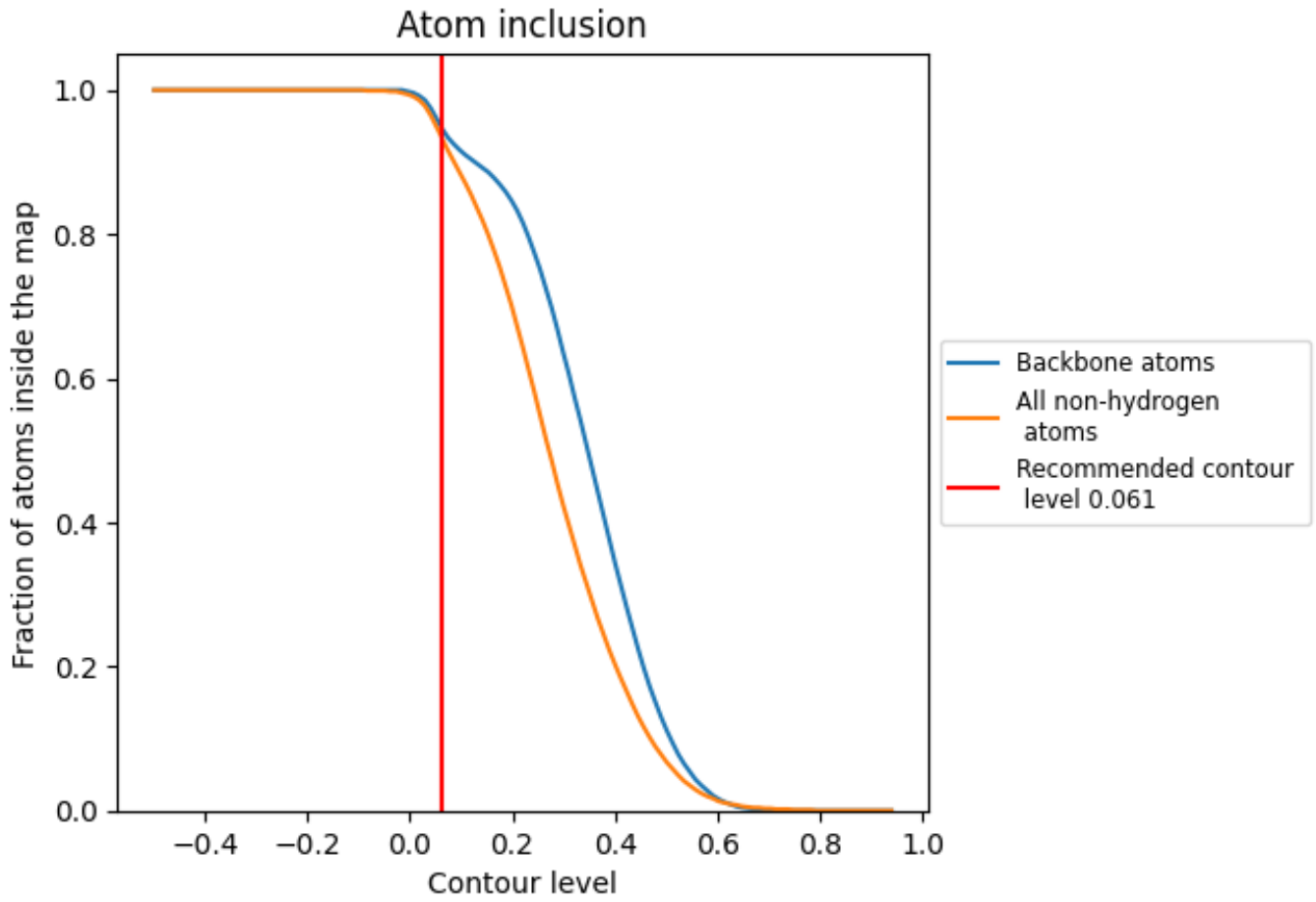
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.061).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.061) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9360	0.1850
A	0.9770	0.2080
B	0.9830	0.2240
C	0.9910	0.2020
D	0.3570	0.0660
G	0.6710	0.0690
H	0.5320	0.0630
I	0.9650	0.1450
L	0.9950	0.1760
M	0.3810	0.0790
P	0.5560	0.0560
Q	0.5170	0.0730
R	0.9550	0.1280
S	0.9800	0.1910
T	0.9870	0.1920
d	0.9920	0.2600
e	0.9970	0.2720
i	1.0000	0.2550
j	0.9900	0.2460