Full wwPDB EM Validation Report

Jul 14, 2024 – 09:24 am BST

PDB ID	:	8BWY
EMDB ID	:	EMD-16304
Title	:	In situ outer dynein arm from Chlamydomonas reinhardtii in a pre-power stroke state
Authors	:	Zimmermann, N.E.L.; Noga, A.; Obbineni, J.M.; Ishikawa, T.
Deposited on	:	2022-12-07
Resolution	:	38.00 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:

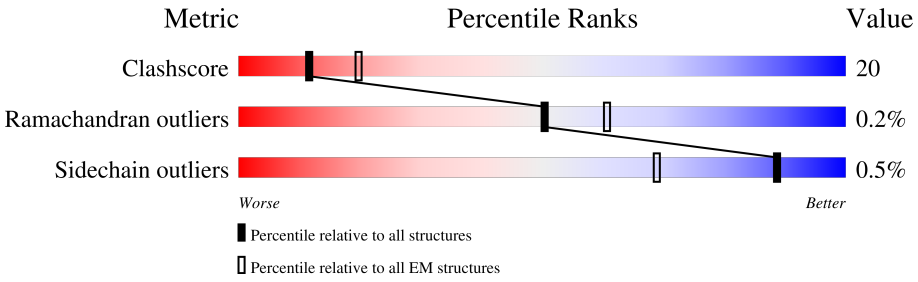
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 38.00 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	4168	27% 74% 9% 17%
2	B	4595	33% 74% 18% · 6%
3	C	4620	28% 76% 16% 8%
4	d	667	5% 69% 31%
5	e	670	20% 80% · 19%
6	F	133	10% 36% 37% · 26%
7	G	159	9% 25% 35% 40%
8	H	92	8% 36% 55% · 8%

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Mol	Chain	Length	Quality of chain
9	I	110	13% 35% 45% 19%
10	J	93	65% 26% 10%
11	K	111	22% 48% 38% 14%
12	L	111	20% 45% 42% 13%
13	M	87	59% 40%
14	N	132	5% 48% 35% 17%
15	O	117	14% 50% 44% 5%
16	P	110	18% 46% 29% 6%
17	T	309	12% 28% 15% 58%
18	V	130	16% 73% 25%
18	x	130	24% 78% 22%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 87003 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 Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	3455	18127	10919	3573	3623	12	0	0

- Molecule 2 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	4299	25545	15697	4785	5025	38	0	0

- Molecule 3 is a protein called Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	4264	25046	15335	4744	4923	44	0	0

- Molecule 4 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	459	3626	2316	609	680	21	0	0

- Molecule 5 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	545	3948	2473	697	759	19	0	0

- Molecule 6 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	98	781	493	137	149	2	0	0

- Molecule 7 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	N	O	S	0	0
			744	468	128	147	1		

- Molecule 8 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	85	Total	C	N	O	S	0	0
			702	453	115	130	4		

- Molecule 9 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	89	Total	C	N	O	S	0	0
			694	443	111	136	4		

- Molecule 10 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	84	Total	C	N	O	S	0	0
			702	459	114	125	4		

- Molecule 11 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			803	525	134	139	5		

- Molecule 12 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	97	Total	C	N	O	S	0	0
			773	506	131	133	3		

- Molecule 13 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	86	Total	C	N	O	S	0	0
			726	472	122	128	4		

- Molecule 14 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	109	Total 897	C 581	N 154	O 159	S 3	0	0

- Molecule 15 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	111	Total 878	C 558	N 143	O 174	S 3	0	0

- Molecule 16 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	103	Total 847	C 549	N 134	O 161	S 3	0	0

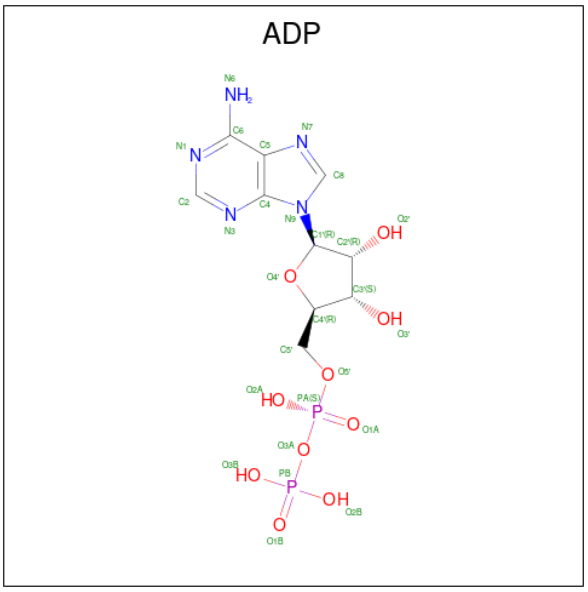
- Molecule 17 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	131	Total 1057	C 655	N 181	O 215	S 6	0	0

- Molecule 18 is a protein called Docking complex 1/2 protein.

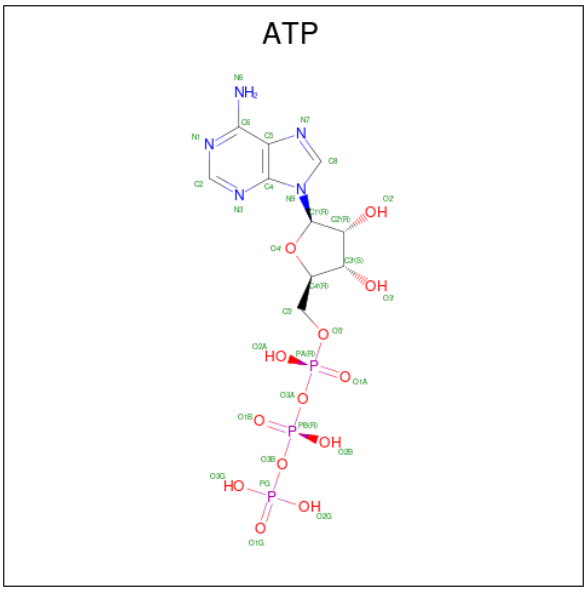
Mol	Chain	Residues	Atoms				AltConf	Trace
18	V	98	Total 490	C 294	N 98	O 98	0	0
18	x	101	Total 505	C 303	N 101	O 101	0	0

- Molecule 19 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
19	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 20 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



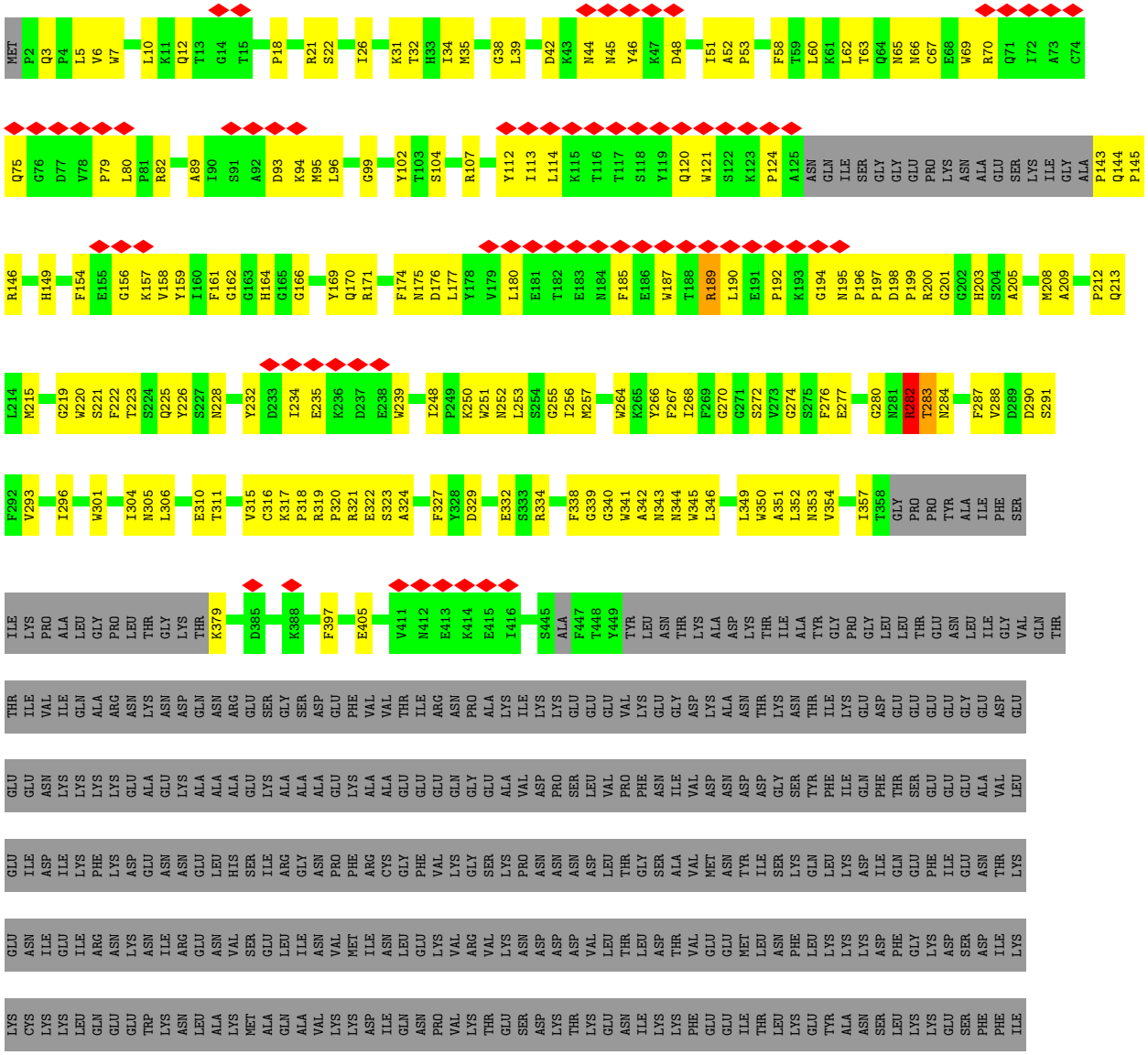
Mol	Chain	Residues	Atoms					AltConf
20	C	1	Total	C	N	O	P	0
			31	10	5	13	3	

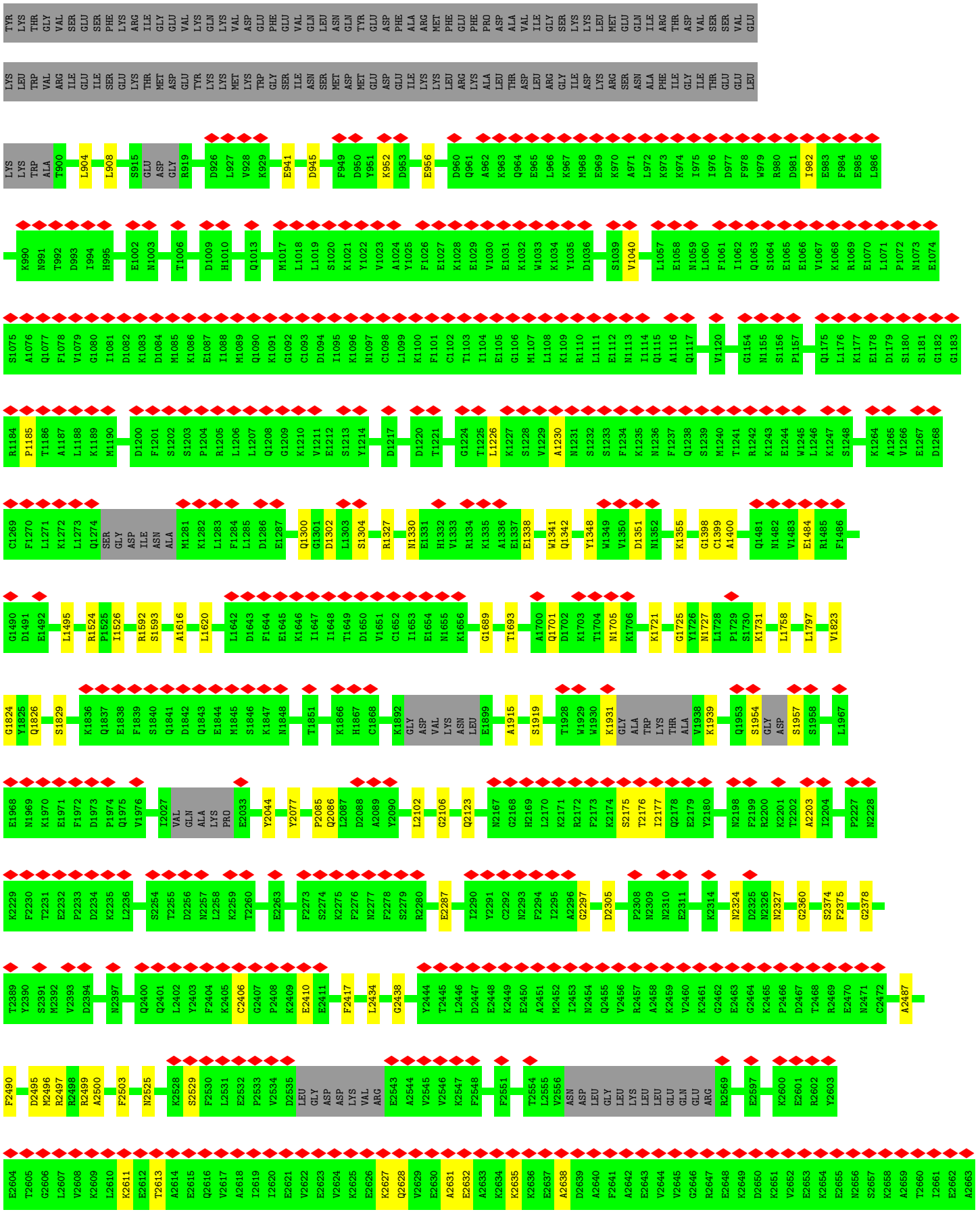
3 Residue-property plots (i)

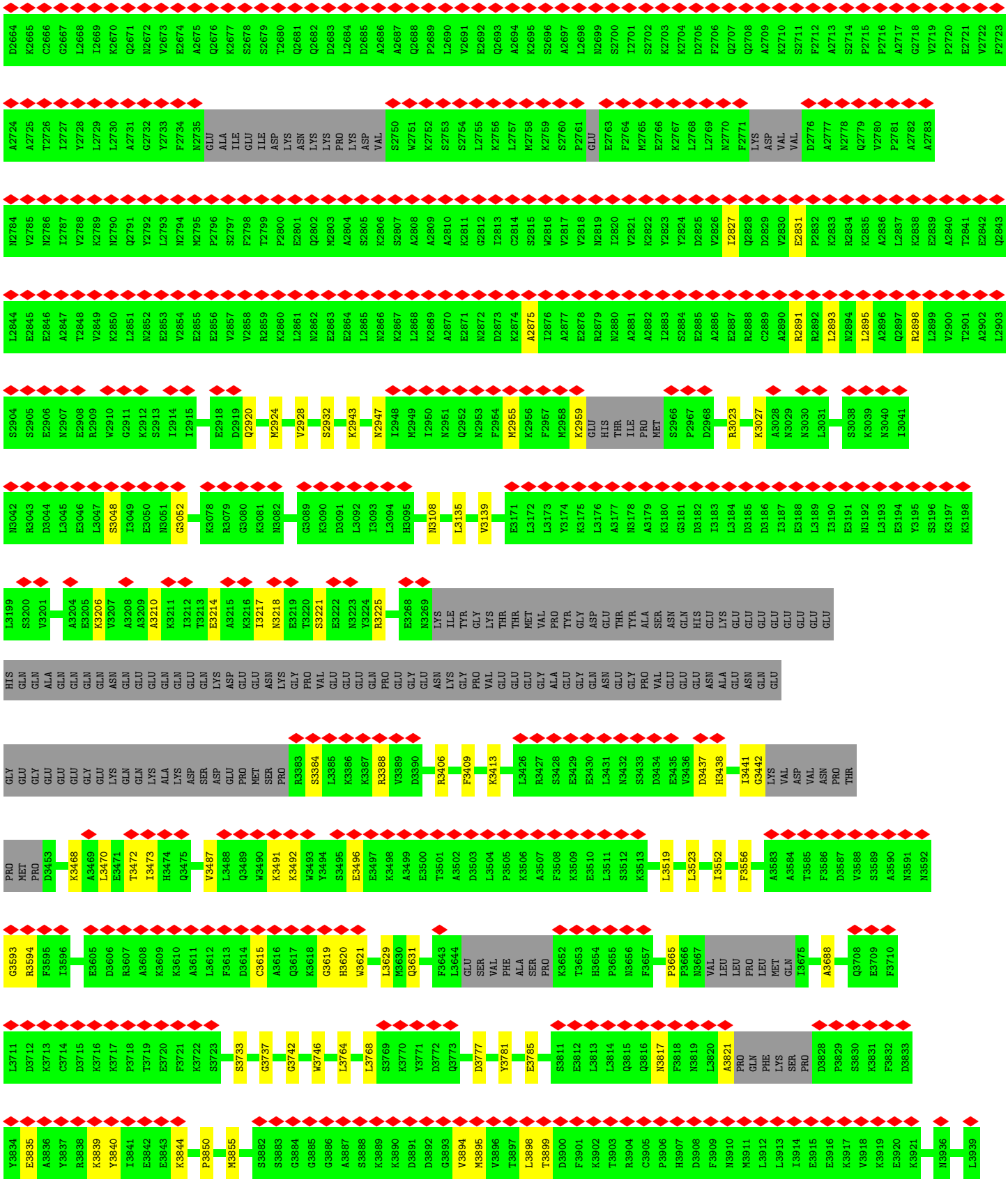
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Dynein-1-alpha heavy chain, flagellar inner arm I1 complex protein, putative

Chain A:




TYR LYS THR GLY VAL SER GLU SER PHE LYS ARG ILE GLY GLU VAL LYS GLN LYS VAL ASP GLU PHE GLU VAL GLN LEU ASN GLN TYR GLU ASP TYR GLU ASP PHE ALA ARG MET PHE GLU PRO ASP ALA VAL ILE GLY SER LYS LYS LEU MET GLU GLN ILE ARG THR ASP VAL SER SER VAL GLU
LYS LEU TRP VAL ARG ILE GLU ILE SER GLU LYS THR MET ASP GLU TYR LYS LYS MET LYS TRP GLY SER ILE ASN SER MET ASP MET GLU ASP GLU ILE LYS LYS LEU ARG LYS ALA LEU THR ASP LEU ARG GLY ILE ASP SER ASN ALA PHE ILE GLY ILE THR GLU GLU LEU
LYS LYS TRP ALA T900 L904 L908 S915 GLU ASP GLY R919 D926 L927 V928 K929 E941 D945 F949 D950 Y951 K952 D953 E956 D960 Q961 A962 K963 Q964 E965 L966 K967 M968 E969 K970 A971 L972 K973 K974 I975 I976 D977 F978 W979 R980 D981 I982 E983 F984 E985 L986
K990 N991 T992 D993 I994 H995 E1002 N1003 T1006 D1009 H1010 Q1013 M1017 L1018 L1019 S1020 K1021 Y1022 V1023 A1024 Y1025 F1026 E1027 K1028 E1029 V1030 E1031 K1032 W1033 K1034 Y1035 D1036 S1039 V1040 L1057 E1058 N1059 L1060 F1061 I1062 Q1063 S1064 E1065 E1066 V1067 K1068 R1069 E1070 L1071 P1072 N1073 E1074
S1075 A1076 Q1077 F1078 V1079 G1080 I1081 D1082 K1083 D1084 M1085 K1086 E1087 I1088 M1089 Q1090 K1091 G1092 C1093 D1094 I1095 K1096 N1097 C1098 L1099 K1100 F1101 C1102 T1103 I1104 E1105 G1106 M1107 L1108 K1109 R1110 L1111 E1112 N1113 I1114 Q1115 A1116 Q1117 V1120 G1154 N1155 S1156 P1157 Q1175 L1176 K1177 E1178 D1179 S1180 S1181 G1182 G1183
R1184 P1185 T1186 A1187 L1188 K1189 M1190 D1200 F1201 S1202 S1203 P1204 R1205 L1206 L1207 Q1208 G1209 K1210 V1211 E1212 S1213 Y1214 D1217 D1220 T1221 G1224 T1225 L1226 K1227 S1228 V1229 A1230 N1231 S1232 S1233 F1234 K1235 N1236 F1237 Q1238 S1239 M1240 T1241 R1242 K1243 E1244 W1245 L1246 K1247 S1248 K1264 A1265 V1266 E1267 D1268
C1269 F1270 L1271 K1272 L1273 Q1274 SER GLY ASP ILE ASN ALA M1281 K1282 L1283 F1284 L1285 D1286 E1287 Q1300 G1301 D1302 L1303 S1304 R1327 N1330 E1331 H1332 V1333 R1334 K1335 A1336 E1337 E1338 W1341 Q1342 Y1348 W1349 V1350 D1351 N1352 K1355 G1398 C1399 A1400 Q1481 N1482 V1483 E1484 R1485 F1486
G1490 D1491 E1492 L1495 R1524 P1525 I1526 R1592 S1593 A1616 L1620 L1642 D1643 F1644 E1645 K1646 I1647 I1648 T1649 D1650 V1651 C1652 I1653 E1654 N1655 K1656 G1689 T1693 A1700 Q1701 D1702 K1703 T1704 N1705 K1706 K1721 G1725 Y1726 N1727 L1728 P1729 S1730 K1731 L1758 L1797 V1823
G1824 Y1825 Q1826 S1829 K1836 Q1837 E1838 F1839 S1840 Q1841 D1842 Q1843 E1844 M1845 S1846 K1847 N1848 T1851 K1866 H1867 C1868 K1892 GLY ASP VAL LYS ASN LEU E1899 A1915 S1919 T1928 W1929 W1930 K1931 GLY ALA TRP LYS THR ALA V1938 K1939 Q1953 S1954 GLY ASP S1957 S1958 L1967
E1968 N1969 K1970 E1971 F1972 D1973 P1974 Q1975 V1976 I2027 VAL GLN ALA LYS PRO E2033 Y2044 Y2077 P2085 Q2086 L2087 D2088 A2089 Y2090 L2102 G2106 Q2123 N2167 G2168 H2169 L2170 K2171 R2172 F2173 K2174 S2175 T2176 I2177 Q2178 E2179 Y2180 N2198 F2199 R2200 K2201 T2202 A2203 I2204 P2227 N2228
K2229 F2230 T2231 E2232 P2233 D2234 K2235 L2236 S2254 T2255 D2256 N2257 L2258 K2259 T2260 E2263 F2273 S2274 K2275 F2276 N2277 F2278 S2279 R2280 E2287 I2290 Y2291 C2292 N2293 F2294 I2295 A2296 G2297 D2305 P2308 N2309 N2310 E2311 K2314 N2324 D2325 N2326 N2327 G2360 S2374 F2375 G2378
T2389 Y2390 S2391 M2392 V2393 D2394 N2397 Q2400 Q2401 L2402 Y2403 F2404 K2405 C2406 G2407 P2408 K2409 E2410 E2411 F2417 L2434 G2438 Y2444 T2445 L2446 D2447 E2448 K2449 E2450 A2451 M2452 I2453 N2454 Q2455 V2456 R2457 A2458 K2459 V2460 K2461 G2462 E2463 G2464 K2465 P2466 D2467 T2468 R2469 E2470 N2471 C2472 A2487
F2490 D2495 M2496 R2497 R2498 R2499 A2500 F2503 N2525 K2528 S2529 F2530 L2531 E2532 P2533 V2534 D2535 LEU GLY ASP ASP LYS VAL ARG E2543 A2544 V2545 V2546 K2547 F2548 F2551 T2554 L2555 V2556 ASN ASP LEU GLY LEU LYS LEU LEU GLU GLN GLU ARG R2569 E2597 K2600 E2601 R2602 Y2603
E2604 T2605 G2606 L2607 V2608 K2609 L2610 K2611 E2612 T2613 A2614 E2615 Q2616 V2617 A2618 I2619 I2620 E2621 V2622 E2623 V2624 K2625 E2626 K2627 Q2628 V2629 E2630 A2631 E2632 A2633 K2634 K2635 K2636 E2637 A2638 D2639 A2640 F2641 A2642 E2643 V2644 V2645 G2646 R2647 E2648 K2649 D2650 K2651 V2652 E2653 K2654 E2655 N2656 S2657 K2658 A2659 T2660 I2661 E2662 A2663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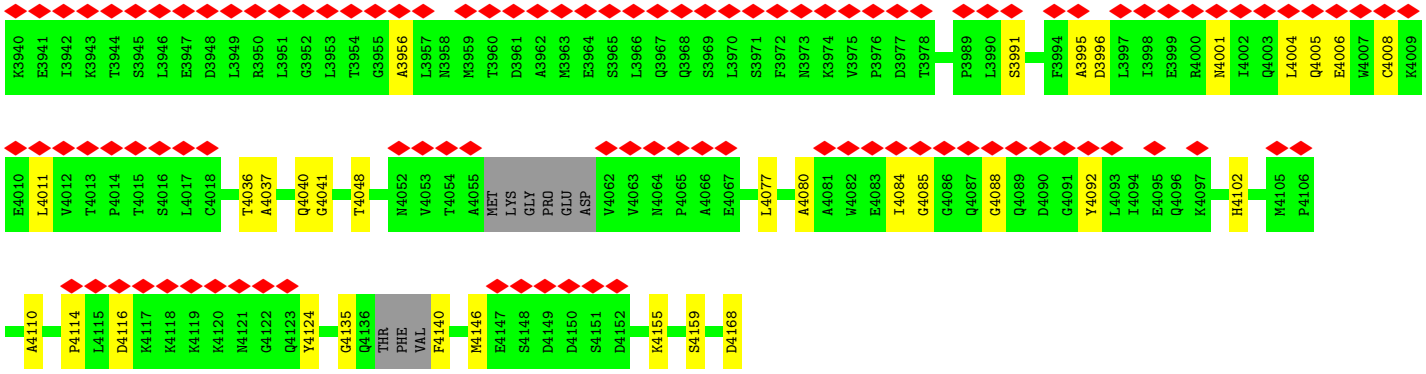
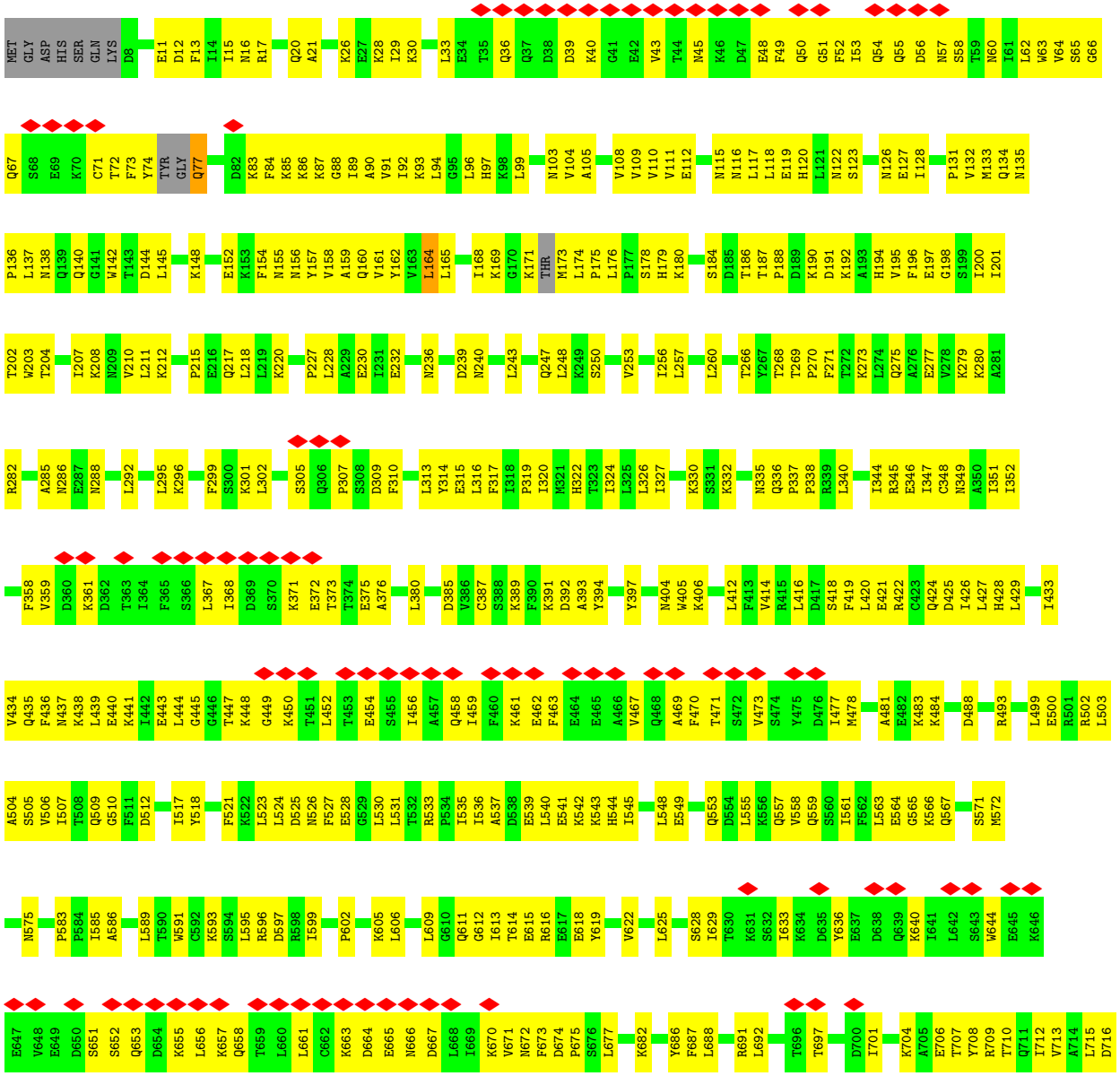
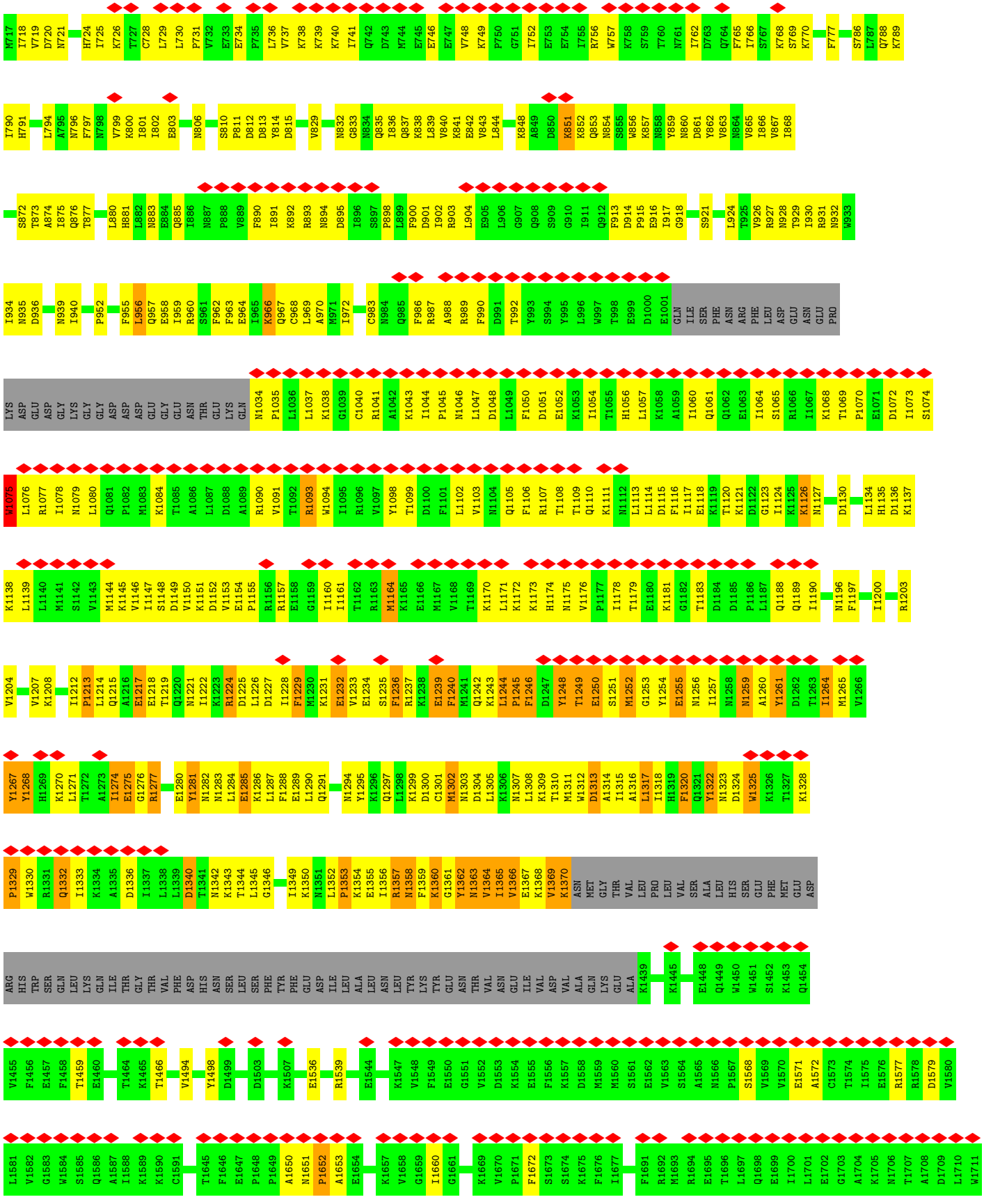
A2724 A2725 T2726 I2727 Y2728 L2729 L2730 A2731 G2732 Y2733 F2734 N2735 GLU ALA ILE GLU ILE ASP LYS ASN LYS LYS PRO LYS ASP VAL S2750 V2751 K2752 S2753 S2754 L2755 K2756 L2757 M2758 K2759 S2760 P2761 GLU E2763 F2764 M2765 E2766 K2767 L2768 L2769 N2770 F2771 LYS ASP VAL VAL D2776 A2777 N2778 Q2779 V2780 P2781 A2782 A2783
N2784 V2785 N2786 I2787 V2788 K2789 N2790 Q2791 Y2792 L2793 N2794 M2795 P2796 S2797 F2798 T2799 P2800 E2801 Q2802 M2803 A2804 S2805 K2806 S2807 A2808 A2809 A2810 K2811 G2812 I2813 C2814 S2815 W2816 V2817 V2818 N2819 I2820 V2821 K2822 Y2823 Y2824 D2825 V2826 I2827 Q2828 D2829 V2830 E2831 P2832 K2833 R2834 K2835 A2836 L2837 K2838 E2839 A2840 T2841 E2842 Q2843
L2844 E2845 E2846 A2847 T2848 V2849 K2850 L2851 N2852 E2853 V2854 E2855 E2856 V2857 V2858 R2859 K2860 L2861 N2862 E2863 E2864 L2865 N2866 K2867 L2868 K2869 A2870 E2871 N2872 D2873 K2874 A2875 I2876 A2877 E2878 R2879 N2880 A2881 A2882 I2883 S2884 E2885 A2886 E2887 R2888 C2889 A2890 R2891 R2892 L2893 N2894 L2895 A2896 Q2897 R2898 L2899 V2900 T2901 A2902 L2903
S2904 S2905 E2906 N2907 E2908 R2909 W2910 G2911 K2912 S2913 I2914 I2915 E2918 D2919 Q2920 M2924 V2928 S2932 K2943 N2947 I2948 M2949 I2950 N2951 Q2952 N2953 F2954 M2955 K2956 F2957 M2958 K2959 GLU HIS THR ILE PRO MET S2966 P2967 D2968 R3023 K3027 A3028 N3029 N3030 L3031 S3038 K3039 N3040 I3041
N3042 R3043 D3044 L3045 E3046 L3047 S3048 I3049 E3050 N3051 G3052 K3078 R3079 G3080 K3081 N3082 G3089 K3090 D3091 L3092 I3093 L3094 H3095 N3108 L3135 V3139 E3171 L3172 L3173 Y3174 K3175 L3176 A3177 N3178 A3179 K3180 G3181 D3182 I3183 L3184 D3185 D3186 I3187 E3188 L3189 I3190 E3191 N3192 L3193 E3194 Y3195 S3196 K3197 K3198
L3199 S3200 V3201 A3204 E3205 K3206 V3207 A3208 A3209 A3210 K3211 I3212 T3213 E3214 A3215 K3216 I3217 N3218 E3219 T3220 S3221 E3222 N3223 Y3224 R3225 E3268 N3269 LYS ILE TYR GLY LYS THR THR MET VAL PRO TYR GLY ASP GLU THR TYR ALA SER ASN GLN HIS GLU LYS GLU GLU GLU GLU GLU GLU GLU GLU
HIS GLN GLN ALA GLN GLN GLN GLN ASN GLN GLU GLU GLN GLN GLU GLN LYS ASP GLU GLU ASN LYS GLY GLU GLU GLN PRO GLU GLY GLU ASN LYS GLY PRO VAL GLU GLU GLU GLY ALA GLU GLY GLN ASN GLU GLY PRO VAL GLU GLU GLU GLU ASN ALA GLU ASN GLN GLU
GLY GLU GLY GLU GLU GLY GLU LYS GLN LYS ALA LYS ASP SER ASP GLU PRO MET SER PRO R3383 S3384 L3385 K3386 K3387 R3388 V3389 D3390 R3406 F3409 K3413 L3426 R3427 S3428 E3429 E3430 L3431 N3432 S3433 D3434 E3435 V3436 D3437 H3438 I3441 G3442 LYS VAL ASP VAL ASN PRO THR
PRO MET PRO D3453 K3468 A3469 L3470 E3471 T3472 I3473 H3474 Q3475 V3487 L3488 Q3489 W3490 K3491 K3492 W3493 Y3494 S3495 E3496 E3497 K3498 A3499 E3500 T3501 A3502 D3503 L3504 P3505 K3506 A3507 F3508 K3509 E3510 L3511 S3512 K3513 L3519 L3523 I3552 F3556 A3583 A3584 T3585 F3586 D3587 V3588 S3589 A3590 N3591 N3592
G3593 R3594 F3595 I3596 E3605 D3606 R3607 A3608 K3609 K3610 A3611 L3612 F3613 D3614 C3615 A3616 Q3617 K3618 G3619 H3620 W3621 L3629 M3630 Q3631 F3643 L3644 GLU SER VAL PHE ALA SER PRO K3652 T3653 H3654 P3655 N3656 F3657 P3665 P3666 N3667 VAL LEU LEU PRO LEU MET GLN I3675 A3688 Q3708 E3709 F3710
L3711 D3712 K3713 C3714 D3715 K3716 K3717 P3718 T3719 E3720 F3721 K3722 S3723 S3733 G3737 G3742 W3746 L3764 L3768 S3769 K3770 Y3771 D3772 Q3773 D3777 Y3781 E3785 S3811 E3812 L3813 L3814 Q3815 Q3816 N3817 F3818 N3819 L3820 A3821 PRO GLN PHE LYS SER PRO D3828 P3829 S3830 K3831 F3832 D3833
Y3834 E3835 A3836 Y3837 R3838 K3839 Y3840 I3841 E3842 E3843 K3844 P3850 M3855 S3882 S3883 G3884 G3885 G3886 A3887 S3888 K3889 K3890 D3891 D3892 G3893 V3894 M3895 V3896 T3897 L3898 T3899 D3900 F3901 K3902 T3903 R3904 C3905 P3906 H3907 D3908 F3909 N3910 M3911 L3912 L3913 I3914 E3915 E3916 K3917 V3918 K3919 E3920 K3921 N3936 L3939



• Molecule 2: Outer arm dynein beta heavy chain

Chain B:

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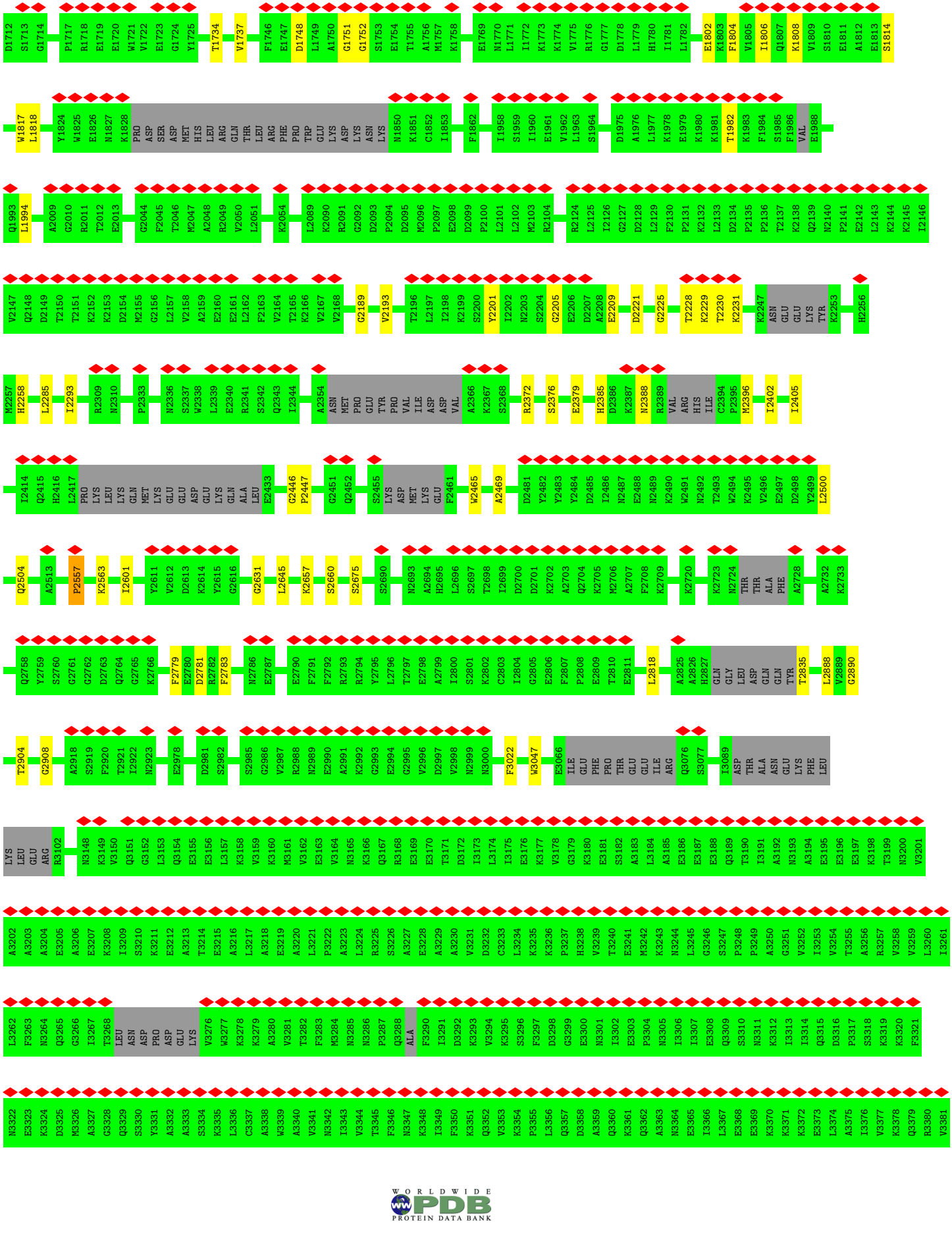
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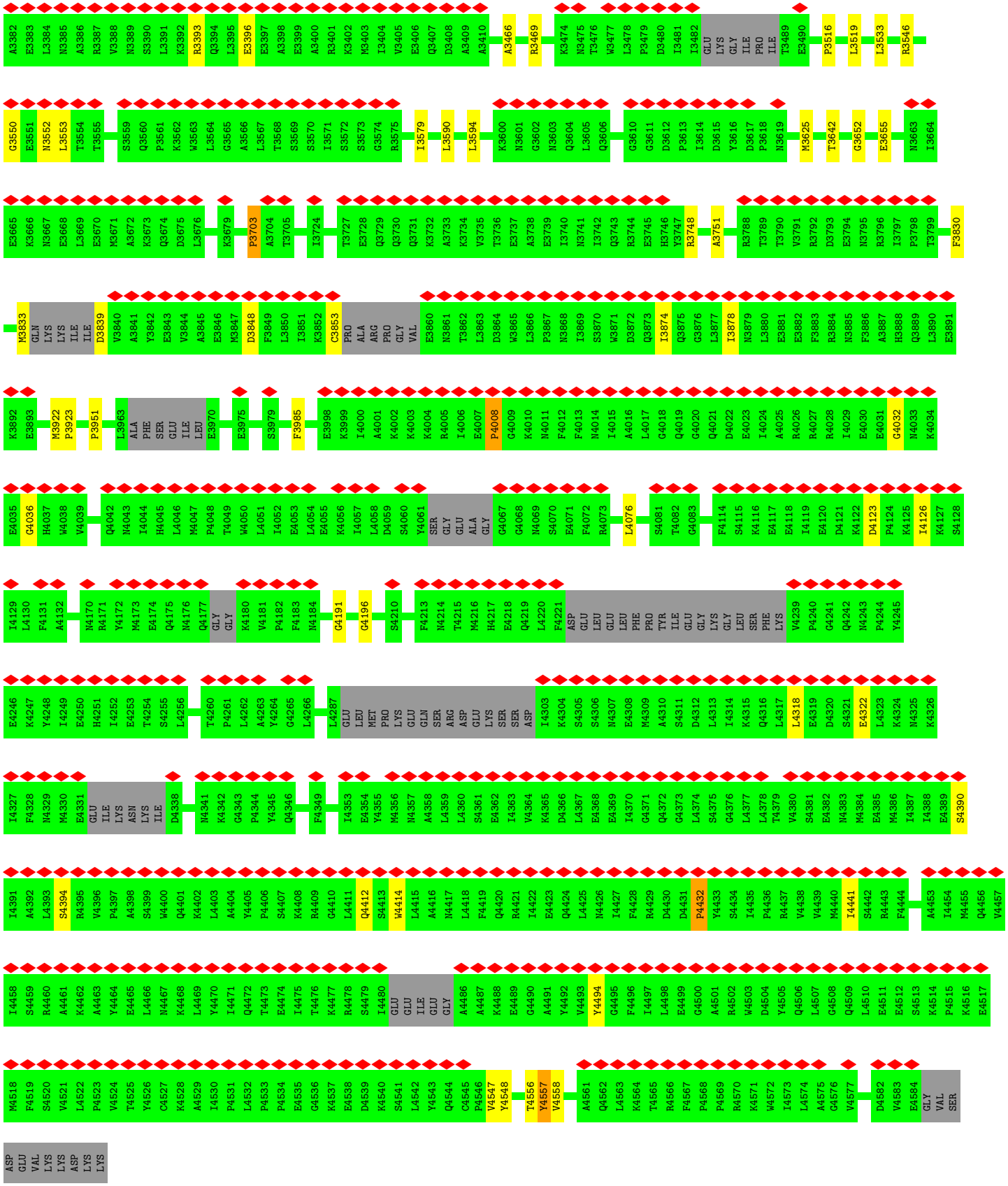
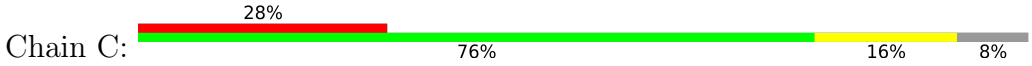
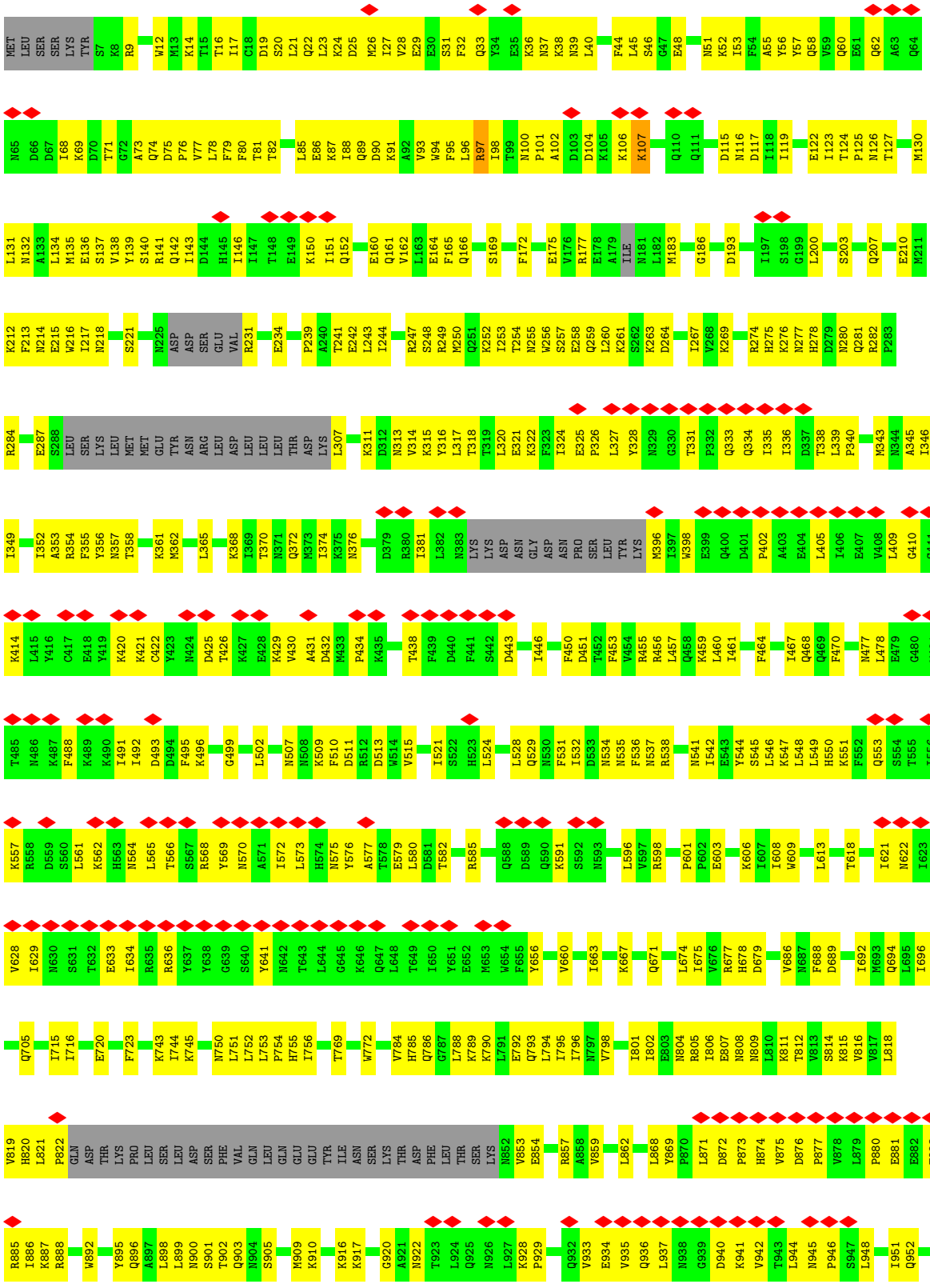
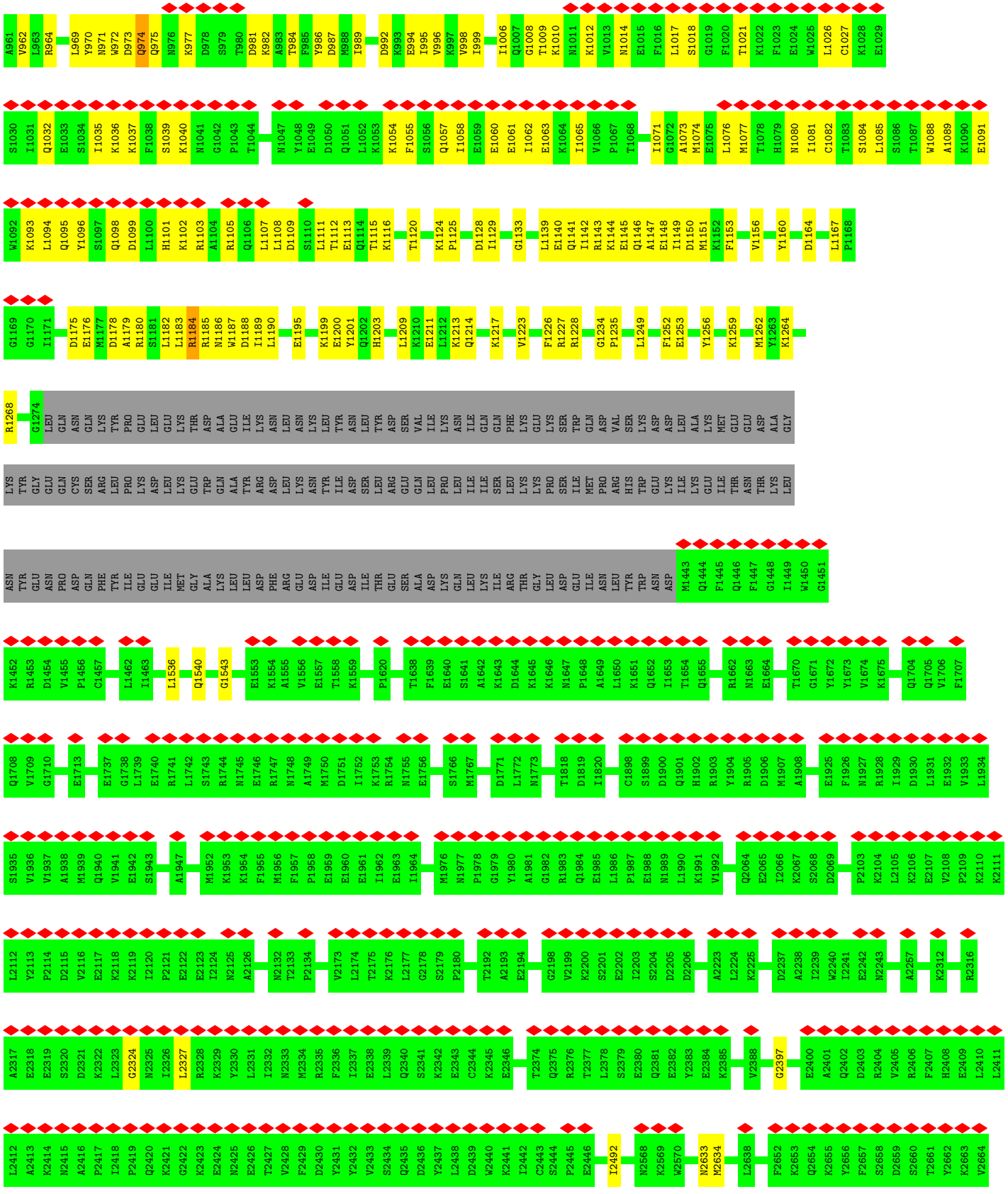


• Molecule 3: Dynein heavy chain, outer arm protein

Chain C:



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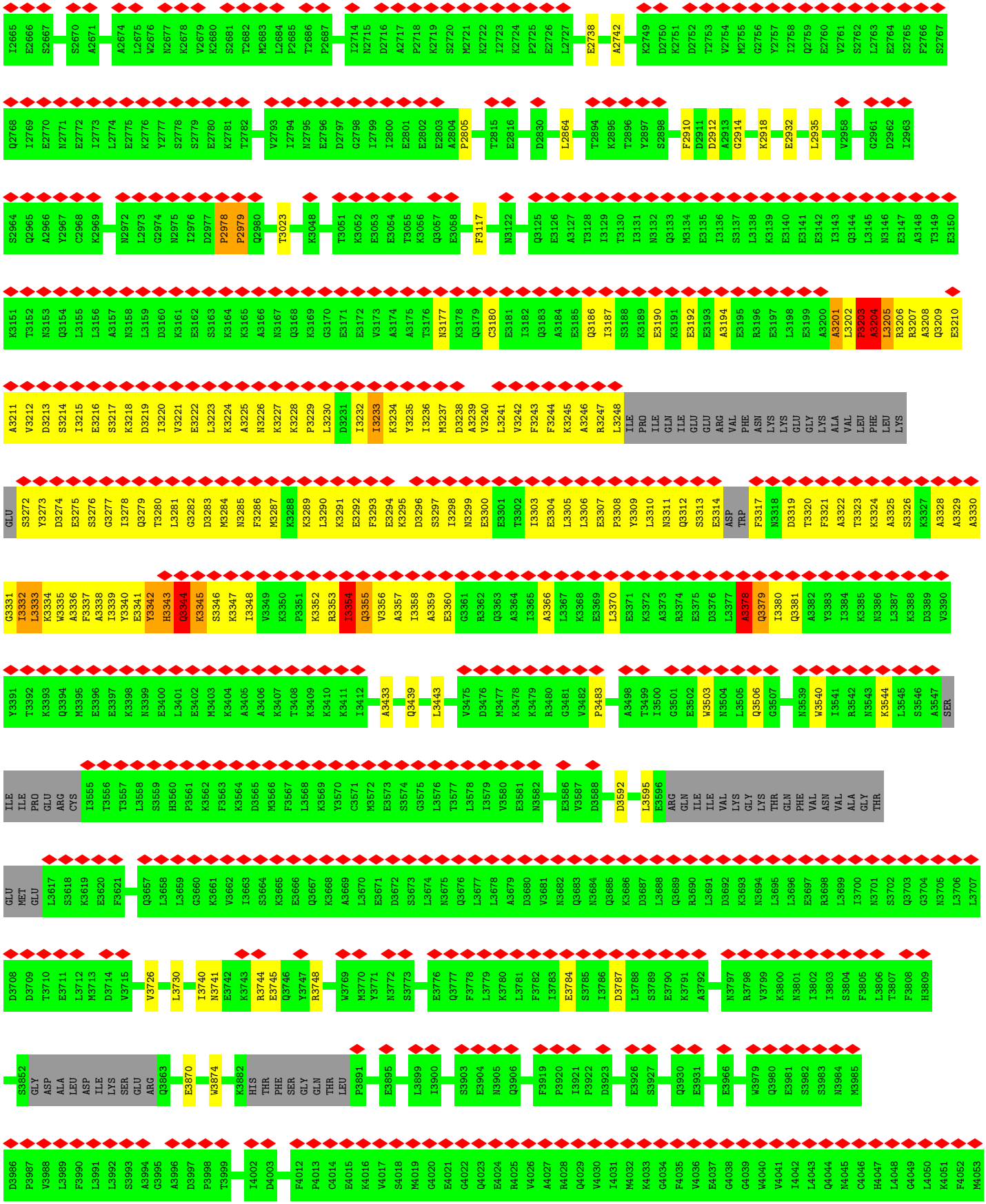
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GLU S3272 Y3273 D3274 E3275 S3276 G3277 I3278 Q3279 T3280 L3281 G3282 D3283 M3284 N3285 F3286 M3287 K3288 K3289 L3290 K3291 E3292 F3293 E3294 K3295 D3296 S3297 I3298 N3299 E3300 E3301 T3302 I3303 E3304 L3305 L3306 E3307 P3308 Y3309 L3310 N3311 Q3312 S3313 E3314 ASP TRP F3317 N3318 D3319 T3320 F3321 A3322 T3323 K3324 A3325 S3326 K3327 A3328 A3329 A3330
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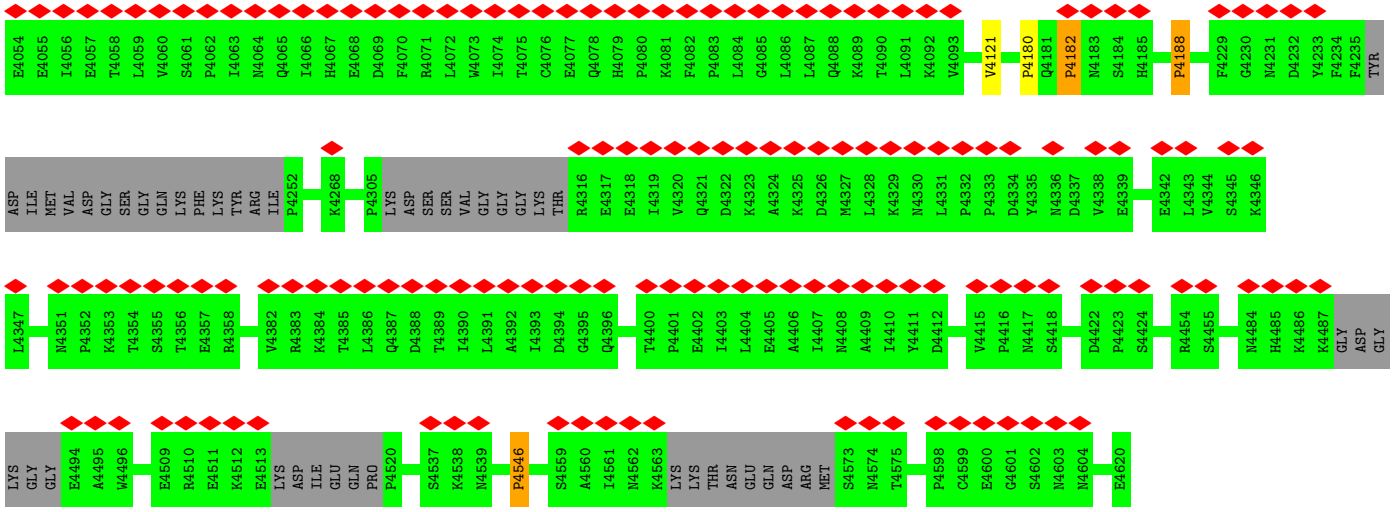
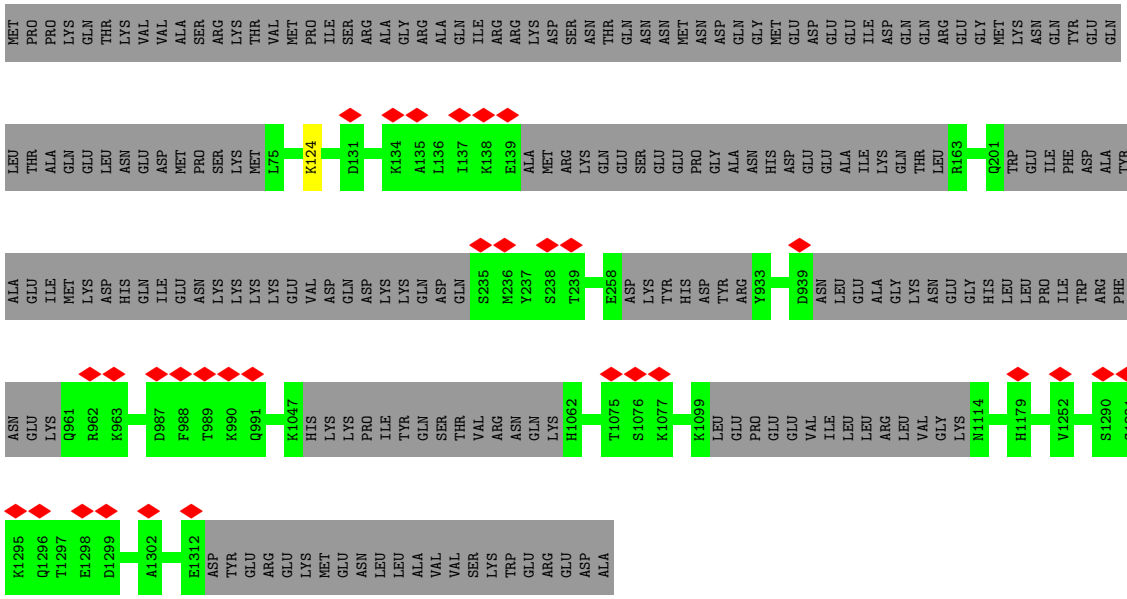
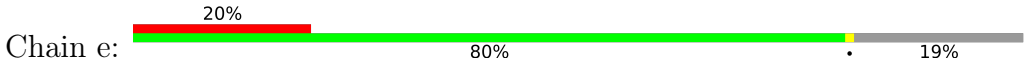
Y3391 T3392 K3393 Q3394 M3395 E3396 E3397 K3398 N3399 E3400 L3401 E3402 M3403 K3404 A3405 A3406 K3407 T3408 K3409 K3410 K3411 I3412 A3433 Q3439 L3443 V3475 D3476 H3477 K3478 K3479 R3480 G3481 V3482 P3483 A3498 T3499 I3500 G3501 E3502 W3503 N3504 L3505 Q3506 G3507 N3539 W3540 I3541 R3542 N3543 K3544 L3545 S3546 A3547 SER
ILE ILE PRO GLU ARG CYS I3555 T3556 T3557 L3558 S3559 H3560 P3561 K3562 F3563 K3564 D3565 M3566 F3567 L3568 K3569 Y3570 C3571 M3572 E3573 S3574 G3575 L3576 T3577 L3578 I3579 V3580 E3581 N3582 E3586 V3587 D3588 D3592 L3595 E3596 ARG GLN ILE ILE VAL LYS GLY LYS THR GLN PHE VAL ASN VAL ALA GLY THR
GLU MET GLU L3617 S3618 K3619 E3620 F3621 Q3657 L3658 L3659 G3660 K3661 V3662 I3663 S3664 K3665 E3666 Q3667 K3668 A3669 L3670 E3671 D3672 S3673 L3674 N3675 Q3676 L3677 L3678 A3679 D3680 V3681 N3682 Q3683 N3684 Q3685 K3686 D3687 L3688 Q3689 R3690 L3691 D3692 K3693 N3694 L3695 L3696 E3697 R3698 L3699 I3700 N3701 S3702 Q3703 G3704 N3705 L3706 L3707
D3708 D3709 T3710 E3711 L3712 M3713 D3714 V3715 V3726 L3730 I3740 N3741 E3742 K3743 R3744 E3745 Q3746 Y3747 R3748 W3769 M3770 Y3771 N3772 S3773 E3776 Q3777 F3778 L3779 K3780 L3781 F3782 I3783 E3784 S3785 I3786 D3787 L3788 S3789 E3790 K3791 A3792 N3797 R3798 V3799 K3800 N3801 I3802 I3803 S3804 F3805 L3806 T3807 F3808 H3809
S3852 GLY ASP ALA LEU ASP ILE LYS SER GLU ARG Q3863 E3870 W3874 K3882 HIS THR PHE SER GLY GLN THR LEU P3891 E3895 L3899 I3900 S3903 E3904 N3905 Q3906 F3919 P3920 I3921 P3922 D3923 E3926 S3927 Q3930 E3931 E3966 W3979 Q3980 E3981 S3982 S3983 N3984 M3985
D3986 P3987 V3988 L3989 F3990 L3991 L3992 S3993 A3994 G3995 A3996 D3997 P3998 T3999 I4002 D4003 F4012 P4013 C4014 E4015 K4016 V4017 S4018 M4019 G4020 E4021 G4022 Q4023 E4024 R4025 V4026 A4027 R4028 Q4029 V4030 I4031 M4032 K4033 G4034 F4035 V4036 E4037 G4038 G4039 W4040 V4041 I4042 L4043 Q4044 N4045 C4046 H4047 L4048 G4049 L4050 K4051 F4052 M4053

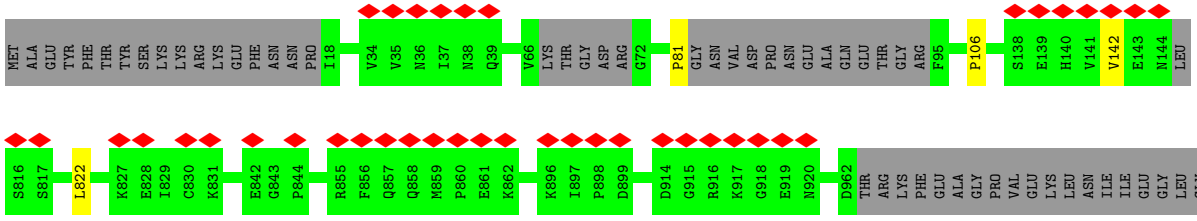


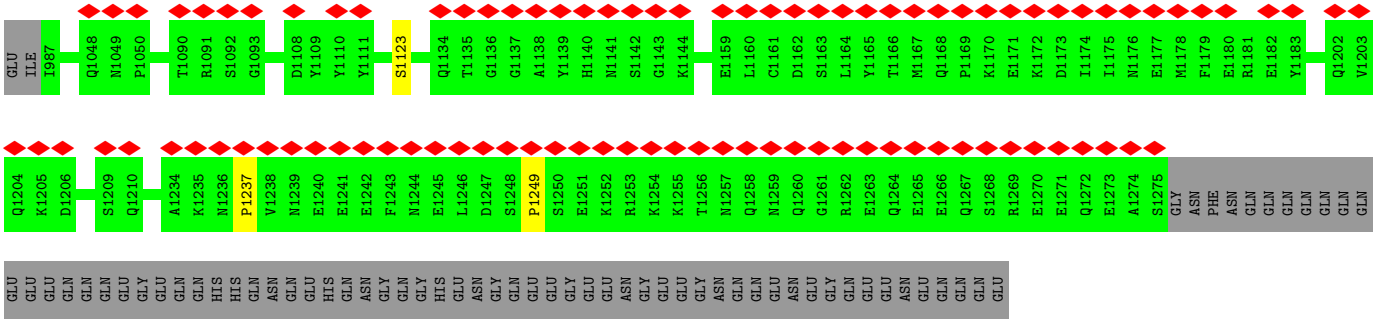
• Molecule 4: Dynein intermediate chain 2



• Molecule 5: Flagellar outer dynein arm intermediate protein, putative

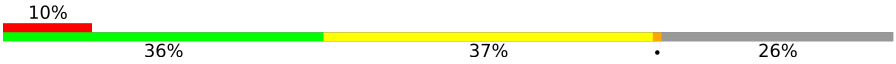


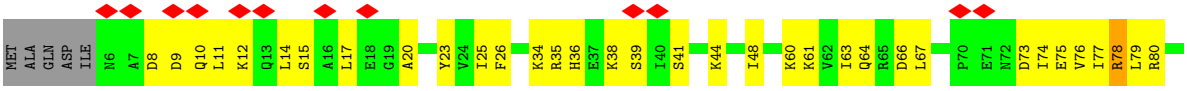


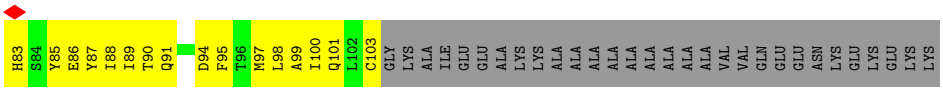


• Molecule 6: Dynein light chain roadblock-type 2 protein

Chain F:

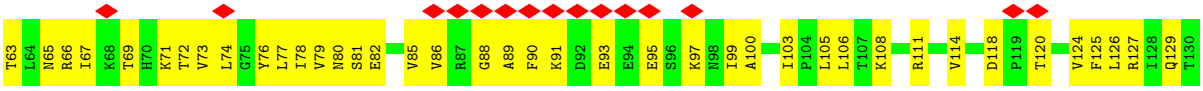






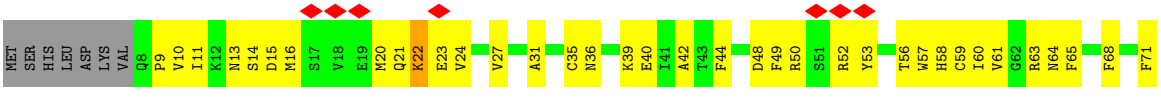
• Molecule 7: Dynein light chain roadblock-type 2 protein

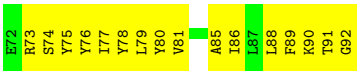
Chain G:



• Molecule 8: Dynein light chain

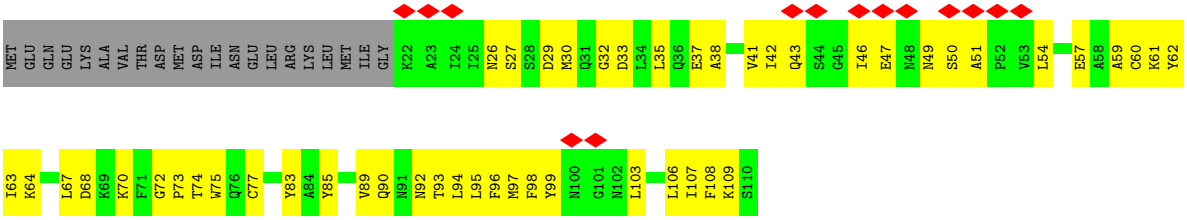
Chain H:





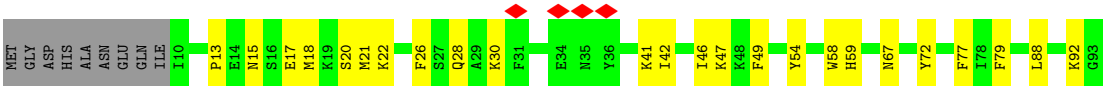
• Molecule 9: Dynein light chain

Chain I:



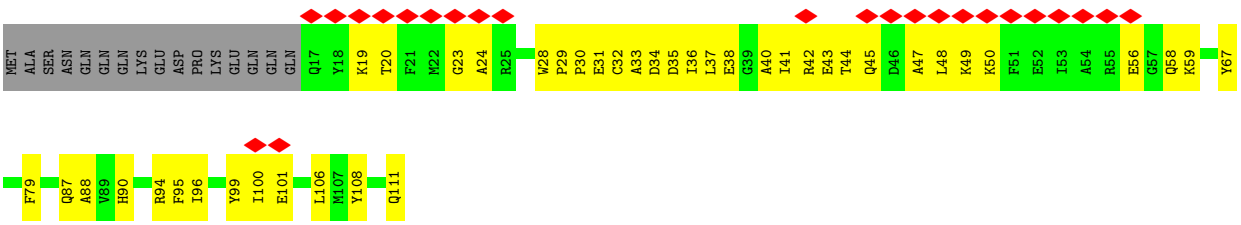
• Molecule 10: Dynein light chain

Chain J:



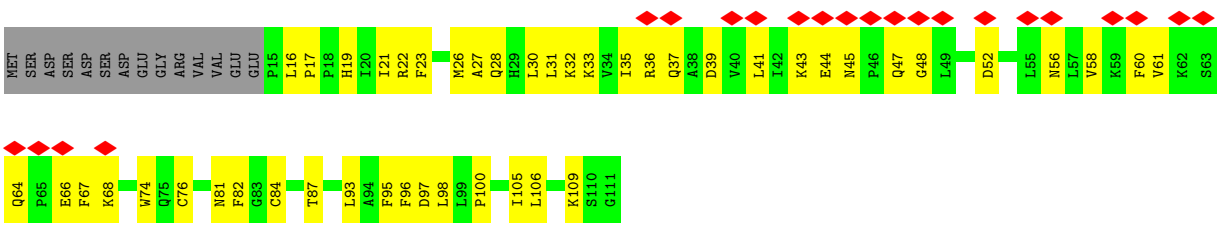
• Molecule 11: Dynein light chain

Chain K:



• Molecule 12: Dynein light chain

Chain L:

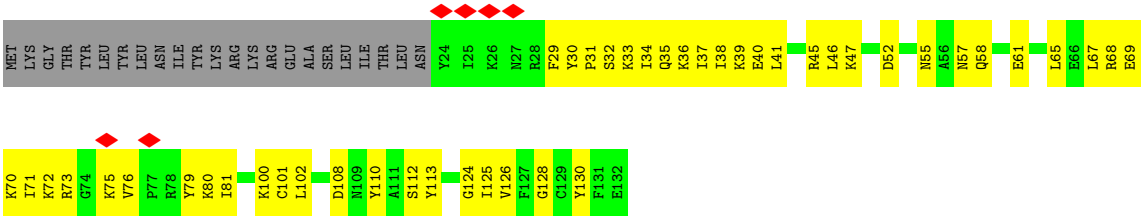


• Molecule 13: Dynein light chain

Chain M:

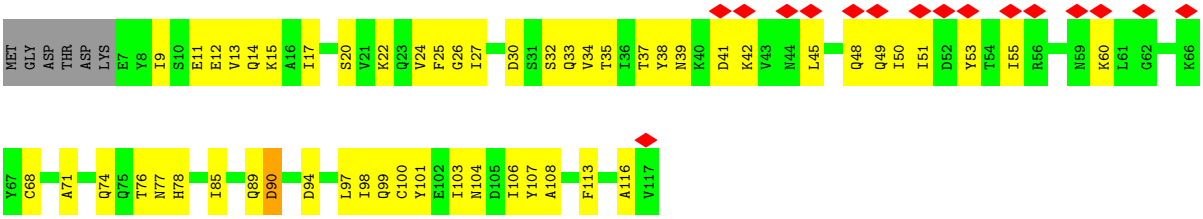
• Molecule 14: Dynein light chain 2A

Chain N:



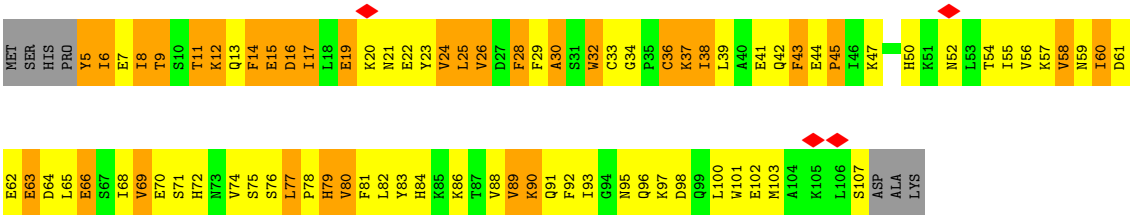
• Molecule 15: Dynein light chain tctex-type 1 protein

Chain O:



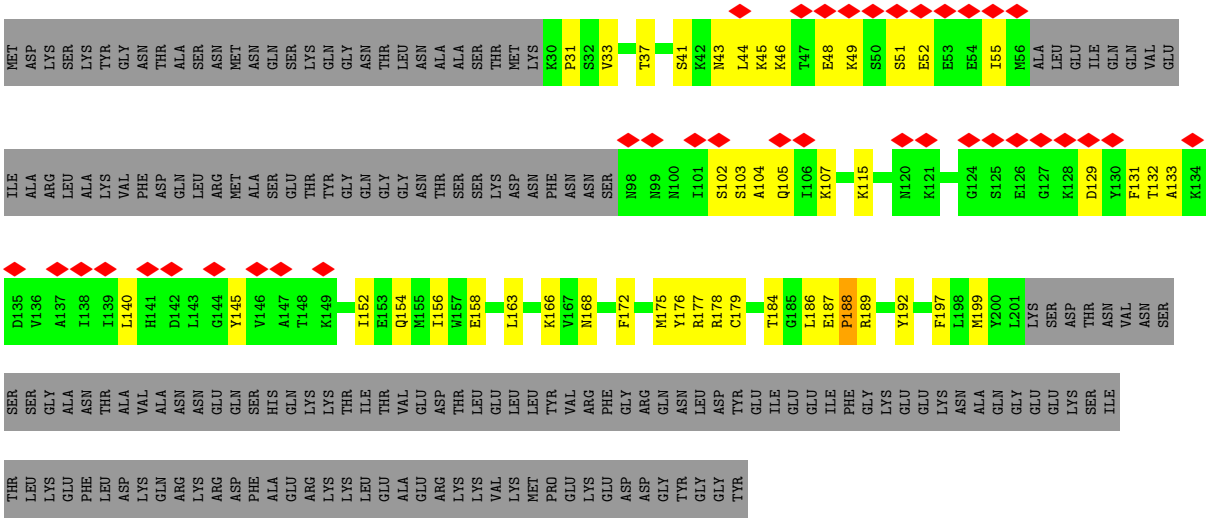
• Molecule 16: Thioredoxin

Chain P:

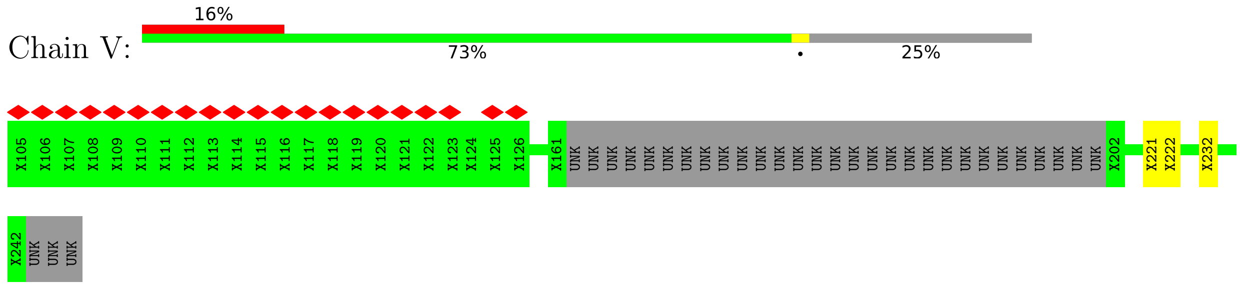


• Molecule 17: Calmodulin

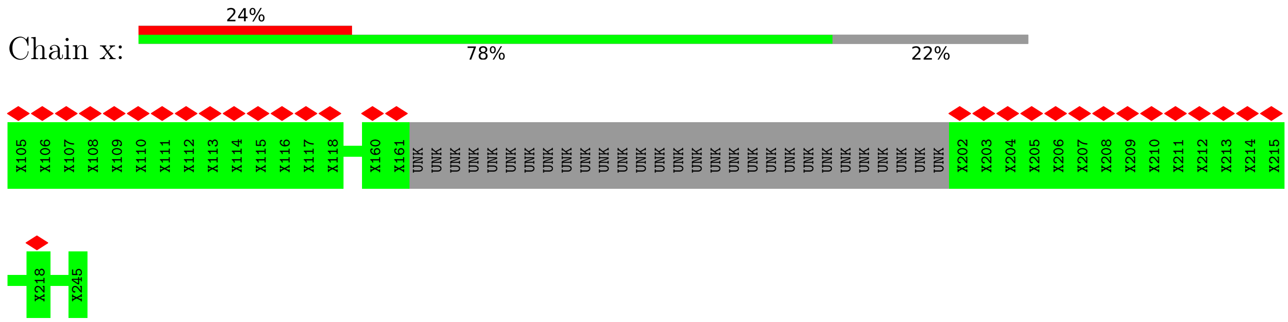
Chain T:



• Molecule 18: Docking complex 1/2 protein



• Molecule 18: Docking complex 1/2 protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	590	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80.0	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.383	Depositor
Minimum map value	-0.252	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.053	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	629.0, 629.0, 629.0	wwPDB
Map dimensions	74, 74, 74	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	8.5, 8.5, 8.5	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.31	0/18167	0.63	1/25169 (0.0%)
2	B	0.79	100/25709 (0.4%)	0.77	68/35300 (0.2%)
3	C	0.70	156/25227 (0.6%)	0.68	68/34687 (0.2%)
4	d	0.32	0/3710	0.51	0/5026
5	e	0.30	0/4021	0.55	6/5463 (0.1%)
6	F	0.29	0/793	0.51	0/1070
7	G	0.27	0/751	0.52	0/1014
8	H	0.28	0/718	0.47	0/965
9	I	0.28	0/705	0.51	0/954
10	J	0.29	0/723	0.45	0/966
11	K	0.29	0/828	0.50	0/1114
12	L	0.29	0/790	0.50	0/1063
13	M	0.27	0/743	0.45	0/996
14	N	0.32	0/915	0.55	0/1229
15	O	0.28	0/891	0.47	0/1209
16	P	2.95	64/866 (7.4%)	2.22	36/1171 (3.1%)
17	T	0.27	0/1070	0.44	0/1436
All	All	0.67	320/86627 (0.4%)	0.70	179/118832 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
3	C	0	5
All	All	0	8

All (320) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1075	TRP	C-O	16.60	1.54	1.23
3	C	3345	LYS	C-O	-12.11	1.00	1.23
3	C	3331	GLY	CA-C	10.79	1.69	1.51
16	P	41	GLU	CD-OE1	10.22	1.36	1.25
2	B	1255	GLU	CD-OE2	10.08	1.36	1.25
16	P	62	GLU	CD-OE1	9.86	1.36	1.25
2	B	77	GLN	N-CA	9.57	1.65	1.46
2	B	1232	GLU	CG-CD	9.35	1.66	1.51
16	P	66	GLU	CD-OE1	9.21	1.35	1.25
2	B	1261	TYR	CG-CD2	9.21	1.51	1.39
16	P	32	TRP	CD2-CE2	9.09	1.52	1.41
3	C	3217	SER	CA-CB	-9.08	1.39	1.52
2	B	1261	TYR	CE1-CZ	8.81	1.50	1.38
2	B	1367	GLU	CD-OE2	8.73	1.35	1.25
16	P	71	SER	CB-OG	8.69	1.53	1.42
3	C	3325	ALA	CA-CB	8.54	1.70	1.52
2	B	1224	ARG	CZ-NH1	8.51	1.44	1.33
3	C	3281	LEU	N-CA	8.45	1.63	1.46
3	C	3274	ASP	N-CA	8.44	1.63	1.46
2	B	1250	GLU	CD-OE1	8.44	1.34	1.25
16	P	70	GLU	CD-OE1	-8.24	1.16	1.25
3	C	3238	ASP	N-CA	8.18	1.62	1.46
2	B	1235	SER	CB-OG	8.15	1.52	1.42
3	C	3336	ALA	N-CA	8.15	1.62	1.46
3	C	3308	PRO	CA-CB	8.15	1.69	1.53
3	C	3355	GLN	C-N	8.09	1.52	1.34
2	B	1330	TRP	CD2-CE2	-8.08	1.31	1.41
16	P	63	GLU	CD-OE2	8.00	1.34	1.25
3	C	3343	HIS	N-CA	7.99	1.62	1.46
16	P	44	GLU	CD-OE1	7.92	1.34	1.25
3	C	3286	PHE	N-CA	-7.89	1.30	1.46
2	B	1312	TRP	CG-CD1	7.89	1.47	1.36
3	C	3332	ILE	N-CA	7.83	1.62	1.46
3	C	3230	LEU	N-CA	-7.83	1.30	1.46
3	C	3337	PHE	N-CA	-7.82	1.30	1.46
3	C	3209	GLN	N-CA	-7.80	1.30	1.46
16	P	14	PHE	CG-CD1	7.75	1.50	1.38
3	C	3312	GLN	C-O	7.75	1.38	1.23
16	P	101	TRP	NE1-CE2	-7.73	1.27	1.37
3	C	3335	TRP	CA-CB	-7.70	1.37	1.53
16	P	23	TYR	CE2-CZ	-7.70	1.28	1.38
3	C	3228	LYS	C-O	7.70	1.38	1.23
2	B	1355	GLU	CD-OE1	-7.69	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3208	ALA	CA-CB	7.69	1.68	1.52
3	C	3330	ALA	CA-CB	7.68	1.68	1.52
3	C	3281	LEU	C-O	7.66	1.37	1.23
3	C	3212	VAL	CA-CB	7.62	1.70	1.54
16	P	23	TYR	CG-CD1	-7.58	1.29	1.39
3	C	3322	ALA	N-CA	-7.55	1.31	1.46
16	P	5	TYR	CG-CD1	7.48	1.48	1.39
3	C	3205	LEU	N-CA	-7.45	1.31	1.46
2	B	1275	GLU	CG-CD	7.42	1.63	1.51
3	C	3313	SER	C-O	7.39	1.37	1.23
3	C	3229	PRO	CA-C	-7.38	1.38	1.52
16	P	19	GLU	CG-CD	-7.35	1.41	1.51
3	C	3210	GLU	N-CA	7.35	1.61	1.46
3	C	3334	LYS	CA-CB	7.35	1.70	1.53
3	C	3248	LEU	C-O	7.34	1.37	1.23
2	B	1330	TRP	CG-CD1	-7.32	1.26	1.36
3	C	3306	LEU	N-CA	7.30	1.60	1.46
16	P	5	TYR	CE2-CZ	7.28	1.48	1.38
3	C	3215	ILE	CA-CB	7.28	1.71	1.54
3	C	3220	ILE	N-CA	7.24	1.60	1.46
3	C	3224	LYS	C-O	7.23	1.37	1.23
3	C	3283	ASP	C-O	-7.22	1.09	1.23
3	C	3219	ASP	CA-CB	-7.18	1.38	1.53
3	C	3309	TYR	CA-CB	-7.15	1.38	1.53
3	C	3248	LEU	CA-CB	-7.14	1.37	1.53
3	C	3291	LYS	CA-CB	7.13	1.69	1.53
3	C	3296	ASP	C-O	7.13	1.36	1.23
2	B	1277	ARG	CZ-NH1	-7.05	1.23	1.33
3	C	3244	PHE	C-O	-7.04	1.09	1.23
2	B	1325	TRP	CD2-CE3	-7.03	1.29	1.40
3	C	3207	ARG	CA-CB	-7.03	1.38	1.53
3	C	3236	ILE	CA-CB	7.02	1.71	1.54
3	C	3296	ASP	N-CA	6.99	1.60	1.46
3	C	3305	LEU	CA-CB	-6.96	1.37	1.53
3	C	3328	ALA	CA-CB	-6.94	1.37	1.52
3	C	3275	GLU	N-CA	-6.94	1.32	1.46
16	P	32	TRP	CZ3-CH2	6.92	1.51	1.40
16	P	28	PHE	CG-CD2	6.90	1.49	1.38
3	C	3235	TYR	CA-CB	-6.89	1.38	1.53
3	C	3290	LEU	N-CA	-6.89	1.32	1.46
2	B	1245	PRO	CA-CB	6.88	1.67	1.53
3	C	3277	GLY	N-CA	6.88	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1289	GLU	CD-OE2	-6.88	1.18	1.25
3	C	3225	ALA	C-N	-6.87	1.18	1.34
3	C	3304	GLU	C-N	-6.86	1.18	1.34
3	C	3237	MET	N-CA	-6.85	1.32	1.46
16	P	44	GLU	CD-OE2	6.84	1.33	1.25
3	C	3216	GLU	N-CA	-6.84	1.32	1.46
3	C	3280	THR	CA-C	6.82	1.70	1.52
2	B	1239	GLU	CD-OE2	-6.82	1.18	1.25
3	C	3247	ARG	C-O	6.82	1.36	1.23
3	C	3240	VAL	CA-CB	6.81	1.69	1.54
3	C	3317	PHE	C-O	-6.81	1.10	1.23
3	C	3272	SER	C-N	-6.81	1.18	1.34
3	C	3207	ARG	C-N	6.79	1.49	1.34
3	C	3304	GLU	CA-CB	6.78	1.68	1.53
3	C	3310	LEU	N-CA	6.76	1.59	1.46
2	B	1268	TYR	CG-CD1	6.74	1.48	1.39
3	C	3235	TYR	C-N	6.74	1.49	1.34
2	B	1325	TRP	NE1-CE2	-6.74	1.28	1.37
3	C	3290	LEU	C-O	-6.72	1.10	1.23
3	C	3322	ALA	C-O	-6.72	1.10	1.23
3	C	3273	TYR	CA-C	6.71	1.70	1.52
2	B	1312	TRP	CD2-CE3	6.71	1.50	1.40
3	C	3234	LYS	C-N	-6.69	1.18	1.34
16	P	17	ILE	N-CA	6.69	1.59	1.46
3	C	3216	GLU	C-N	-6.68	1.18	1.34
3	C	3244	PHE	N-CA	-6.68	1.32	1.46
3	C	3218	LYS	CA-CB	6.68	1.68	1.53
3	C	3303	ILE	C-N	6.68	1.49	1.34
2	B	1229	PHE	CG-CD2	6.67	1.48	1.38
3	C	3226	ASN	CA-CB	-6.64	1.35	1.53
3	C	3334	LYS	C-N	-6.64	1.18	1.34
3	C	3299	ASN	N-CA	6.63	1.59	1.46
2	B	1237	ARG	NE-CZ	-6.60	1.24	1.33
2	B	1254	TYR	CD1-CE1	-6.60	1.29	1.39
3	C	3307	GLU	C-N	6.59	1.46	1.34
2	B	1362	TYR	CE1-CZ	-6.58	1.29	1.38
3	C	3324	LYS	C-N	6.58	1.49	1.34
3	C	3214	SER	CA-CB	-6.57	1.43	1.52
3	C	3307	GLU	N-CA	-6.57	1.33	1.46
16	P	36	CYS	CB-SG	-6.54	1.71	1.82
3	C	3208	ALA	CA-C	-6.54	1.35	1.52
2	B	1254	TYR	CB-CG	-6.53	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1254	TYR	CG-CD2	6.51	1.47	1.39
16	P	60	ILE	C-O	6.50	1.35	1.23
3	C	3234	LYS	N-CA	6.50	1.59	1.46
16	P	58	VAL	N-CA	6.49	1.59	1.46
2	B	1330	TRP	CZ3-CH2	-6.49	1.29	1.40
16	P	90	LYS	CA-CB	6.47	1.68	1.53
16	P	91	GLN	CG-CD	6.46	1.66	1.51
3	C	3282	GLY	N-CA	-6.44	1.36	1.46
3	C	3279	GLN	CA-CB	6.44	1.68	1.53
3	C	3227	LYS	C-N	-6.43	1.19	1.34
3	C	3285	ASN	CA-C	-6.42	1.36	1.52
16	P	80	VAL	CA-CB	6.41	1.68	1.54
2	B	1254	TYR	CE1-CZ	6.40	1.46	1.38
2	B	1254	TYR	CD2-CE2	-6.40	1.29	1.39
2	B	1217	GLU	CD-OE1	6.39	1.32	1.25
3	C	3335	TRP	CA-C	6.39	1.69	1.52
2	B	1366	VAL	CB-CG1	6.39	1.66	1.52
3	C	3220	ILE	C-O	6.38	1.35	1.23
3	C	3239	ALA	CA-CB	-6.38	1.39	1.52
16	P	14	PHE	CE2-CZ	6.35	1.49	1.37
2	B	1255	GLU	CB-CG	6.34	1.64	1.52
16	P	91	GLN	CA-CB	6.34	1.67	1.53
16	P	92	PHE	CA-CB	6.33	1.67	1.53
3	C	3321	PHE	CA-C	-6.33	1.36	1.52
3	C	3330	ALA	N-CA	-6.32	1.33	1.46
3	C	3292	GLU	CA-CB	-6.31	1.40	1.53
3	C	3311	ASN	C-N	-6.30	1.19	1.34
2	B	1267	TYR	CD2-CE2	-6.30	1.29	1.39
16	P	34	GLY	N-CA	-6.27	1.36	1.46
3	C	3286	PHE	C-O	-6.27	1.11	1.23
2	B	1330	TRP	C-O	6.25	1.35	1.23
2	B	1267	TYR	CB-CG	-6.25	1.42	1.51
3	C	3237	MET	CA-C	6.24	1.69	1.52
2	B	1267	TYR	CD1-CE1	-6.23	1.29	1.39
3	C	3314	GLU	C-O	6.23	1.35	1.23
16	P	30	ALA	C-O	6.21	1.35	1.23
2	B	1268	TYR	CE2-CZ	6.19	1.46	1.38
3	C	3214	SER	N-CA	6.19	1.58	1.46
3	C	3345	LYS	N-CA	-6.18	1.33	1.46
2	B	1357	ARG	CZ-NH2	-6.17	1.25	1.33
3	C	3336	ALA	CA-C	-6.17	1.36	1.52
3	C	3218	LYS	C-N	-6.16	1.19	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3227	LYS	C-O	6.15	1.35	1.23
2	B	1268	TYR	CE1-CZ	-6.13	1.30	1.38
2	B	1285	GLU	CD-OE2	-6.13	1.19	1.25
3	C	3339	ILE	CA-CB	-6.12	1.40	1.54
3	C	3300	GLU	N-CA	-6.09	1.34	1.46
16	P	22	GLU	CG-CD	6.08	1.61	1.51
2	B	1259	ASN	CB-CG	6.08	1.65	1.51
2	B	1362	TYR	CG-CD2	-6.07	1.31	1.39
3	C	3227	LYS	N-CA	6.06	1.58	1.46
3	C	3214	SER	C-N	6.06	1.48	1.34
2	B	1325	TRP	CD1-NE1	6.05	1.48	1.38
16	P	38	ILE	C-O	6.04	1.34	1.23
3	C	3342	TYR	CA-C	6.02	1.68	1.52
2	B	1368	LYS	CA-CB	6.01	1.67	1.53
2	B	1363	ASN	CB-CG	6.00	1.64	1.51
16	P	101	TRP	CD2-CE3	-5.98	1.31	1.40
3	C	3294	GLU	N-CA	-5.97	1.34	1.46
3	C	3221	VAL	N-CA	-5.97	1.34	1.46
16	P	28	PHE	CE1-CZ	5.97	1.48	1.37
2	B	1332	GLN	CG-CD	5.97	1.64	1.51
2	B	1234	GLU	CG-CD	-5.96	1.43	1.51
3	C	3204	ALA	CA-C	-5.96	1.37	1.52
2	B	1340	ASP	CB-CG	-5.96	1.39	1.51
2	B	1312	TRP	NE1-CE2	5.94	1.45	1.37
16	P	24	VAL	CA-CB	5.94	1.67	1.54
2	B	1252	MET	CA-CB	5.91	1.67	1.53
16	P	15	GLU	CA-CB	5.90	1.67	1.53
16	P	44	GLU	CB-CG	5.89	1.63	1.52
2	B	1370	LYS	N-CA	5.88	1.58	1.46
3	C	3223	LEU	C-O	5.88	1.34	1.23
2	B	1330	TRP	N-CA	5.87	1.58	1.46
2	B	1295	TYR	CB-CG	-5.86	1.42	1.51
2	B	1268	TYR	CG-CD2	-5.85	1.31	1.39
3	C	3333	LEU	C-O	5.84	1.34	1.23
3	C	3338	ALA	CA-CB	5.83	1.64	1.52
2	B	1252	MET	CG-SD	5.83	1.96	1.81
3	C	3219	ASP	CA-C	5.83	1.68	1.52
2	B	1297	GLN	N-CA	5.82	1.57	1.46
3	C	3312	GLN	CA-CB	-5.77	1.41	1.53
3	C	3274	ASP	C-O	5.76	1.34	1.23
3	C	3295	LYS	CA-C	5.75	1.68	1.52
3	C	3311	ASN	C-O	5.74	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1316	ALA	CA-CB	5.74	1.64	1.52
2	B	1366	VAL	N-CA	5.74	1.57	1.46
3	C	3209	GLN	C-O	-5.72	1.12	1.23
3	C	3339	ILE	N-CA	5.71	1.57	1.46
16	P	6	ILE	N-CA	5.69	1.57	1.46
3	C	3305	LEU	CA-C	5.67	1.67	1.52
2	B	1302	MET	N-CA	5.67	1.57	1.46
3	C	3245	LYS	N-CA	5.67	1.57	1.46
2	B	1295	TYR	CD2-CE2	-5.67	1.30	1.39
2	B	1325	TRP	CZ2-CH2	-5.67	1.26	1.37
3	C	3215	ILE	CA-C	-5.66	1.38	1.52
3	C	3309	TYR	CA-C	5.66	1.67	1.52
3	C	3333	LEU	C-N	5.65	1.47	1.34
3	C	3340	TYR	C-N	5.64	1.47	1.34
3	C	3289	LYS	CA-C	-5.63	1.38	1.52
2	B	1281	TYR	CD1-CE1	-5.63	1.30	1.39
2	B	1295	TYR	CD1-CE1	-5.62	1.30	1.39
16	P	21	ASN	N-CA	5.62	1.57	1.46
16	P	79	HIS	CA-CB	5.61	1.66	1.53
2	B	1329	PRO	CA-C	5.61	1.64	1.52
2	B	1362	TYR	CZ-OH	5.60	1.47	1.37
2	B	1358	ASN	CB-CG	5.59	1.64	1.51
3	C	3282	GLY	C-O	5.59	1.32	1.23
2	B	1229	PHE	CE1-CZ	5.57	1.48	1.37
2	B	1353	PRO	N-CD	5.57	1.55	1.47
16	P	81	PHE	CA-CB	5.55	1.66	1.53
16	P	26	VAL	CA-CB	5.54	1.66	1.54
3	C	3242	VAL	N-CA	5.54	1.57	1.46
3	C	3201	ALA	CA-CB	-5.53	1.40	1.52
3	C	3341	GLU	CA-CB	5.51	1.66	1.53
16	P	8	ILE	N-CA	5.50	1.57	1.46
16	P	29	PHE	CB-CG	-5.50	1.42	1.51
16	P	16	ASP	CA-C	5.50	1.67	1.52
2	B	1368	LYS	CE-NZ	5.50	1.62	1.49
2	B	1268	TYR	CB-CG	5.49	1.59	1.51
16	P	71	SER	CA-CB	-5.49	1.44	1.52
2	B	1254	TYR	CA-CB	5.47	1.66	1.53
3	C	3276	SER	CA-CB	5.46	1.61	1.52
16	P	102	GLU	CG-CD	-5.44	1.43	1.51
3	C	3211	ALA	C-N	5.43	1.46	1.34
3	C	3246	ALA	C-N	5.43	1.46	1.34
2	B	1274	ILE	N-CA	5.43	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1213	PRO	C-O	5.42	1.34	1.23
16	P	43	PHE	CA-CB	5.41	1.65	1.53
16	P	45	PRO	N-CA	5.40	1.56	1.47
3	C	3223	LEU	CA-CB	-5.40	1.41	1.53
2	B	1236	PHE	CG-CD1	-5.39	1.30	1.38
3	C	3310	LEU	C-O	-5.39	1.13	1.23
16	P	63	GLU	CB-CG	5.38	1.62	1.52
3	C	3279	GLN	C-N	-5.38	1.21	1.34
2	B	1251	SER	CA-CB	5.38	1.61	1.52
2	B	1342	ASN	N-CA	-5.37	1.35	1.46
3	C	3209	GLN	CA-C	5.36	1.66	1.52
2	B	1281	TYR	CB-CG	-5.35	1.43	1.51
3	C	3306	LEU	CA-C	-5.33	1.39	1.52
3	C	3226	ASN	CA-C	5.33	1.66	1.52
16	P	25	LEU	CA-CB	5.32	1.66	1.53
16	P	58	VAL	CB-CG2	5.31	1.64	1.52
2	B	1244	LEU	N-CA	-5.31	1.35	1.46
3	C	3290	LEU	CA-CB	5.31	1.66	1.53
3	C	3320	THR	CA-CB	-5.28	1.39	1.53
3	C	3298	ILE	CA-C	5.28	1.66	1.52
16	P	37	LYS	N-CA	-5.27	1.35	1.46
3	C	3230	LEU	CA-CB	5.27	1.65	1.53
3	C	3217	SER	C-O	5.26	1.33	1.23
3	C	3294	GLU	C-N	-5.26	1.22	1.34
3	C	3214	SER	C-O	5.26	1.33	1.23
3	C	3354	ILE	C-O	-5.25	1.13	1.23
2	B	1299	LYS	N-CA	5.24	1.56	1.46
2	B	1254	TYR	CZ-OH	-5.23	1.28	1.37
2	B	1332	GLN	CA-CB	5.23	1.65	1.53
3	C	3320	THR	N-CA	5.23	1.56	1.46
2	B	1250	GLU	C-N	5.22	1.46	1.34
16	P	50	HIS	C-O	5.21	1.33	1.23
2	B	1365	ILE	N-CA	-5.21	1.35	1.46
16	P	32	TRP	CG-CD1	5.21	1.44	1.36
3	C	3341	GLU	N-CA	-5.19	1.35	1.46
3	C	3243	PHE	CA-C	-5.17	1.39	1.52
3	C	3274	ASP	CA-C	-5.16	1.39	1.52
16	P	107	SER	CA-CB	-5.16	1.45	1.52
16	P	86	LYS	CB-CG	5.16	1.66	1.52
3	C	3308	PRO	C-N	-5.15	1.22	1.34
16	P	23	TYR	CA-CB	5.15	1.65	1.53
2	B	1309	LYS	CE-NZ	5.14	1.61	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1253	GLY	C-N	5.14	1.45	1.34
2	B	1360	LYS	CE-NZ	5.13	1.61	1.49
2	B	1242	GLN	CG-CD	5.12	1.62	1.51
2	B	1309	LYS	CA-CB	5.12	1.65	1.53
16	P	58	VAL	CB-CG1	-5.11	1.42	1.52
16	P	32	TRP	CG-CD2	-5.10	1.34	1.43
2	B	1302	MET	C-O	5.09	1.33	1.23
2	B	1336	ASP	N-CA	5.09	1.56	1.46
2	B	1367	GLU	CG-CD	5.08	1.59	1.51
2	B	1250	GLU	CB-CG	-5.07	1.42	1.52
3	C	3205	LEU	C-O	-5.07	1.13	1.23
16	P	69	VAL	C-N	5.06	1.45	1.34
3	C	3336	ALA	C-O	5.05	1.32	1.23
3	C	3273	TYR	CA-CB	-5.05	1.42	1.53
3	C	3216	GLU	CA-CB	5.05	1.65	1.53
3	C	3278	ILE	C-O	5.04	1.32	1.23
2	B	1288	PHE	CA-CB	-5.04	1.42	1.53
2	B	1357	ARG	CZ-NH1	-5.04	1.26	1.33
16	P	63	GLU	CD-OE1	-5.03	1.20	1.25
2	B	1312	TRP	CZ2-CH2	5.02	1.46	1.37
16	P	70	GLU	CD-OE2	5.02	1.31	1.25
3	C	3305	LEU	C-N	5.01	1.45	1.34
2	B	1281	TYR	N-CA	5.01	1.56	1.46
16	P	86	LYS	N-CA	5.01	1.56	1.46
2	B	1294	ASN	C-N	5.01	1.45	1.34

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3344	GLN	CA-C-N	-13.69	87.09	117.20
2	B	1224	ARG	NE-CZ-NH2	-12.33	114.14	120.30
2	B	1268	TYR	CB-CG-CD1	11.37	127.82	121.00
3	C	3345	LYS	N-CA-C	-11.25	80.62	111.00
16	P	14	PHE	CB-CG-CD2	-10.80	113.24	120.80
2	B	1254	TYR	CB-CG-CD1	-10.51	114.69	121.00
3	C	3355	GLN	C-N-CA	-10.39	95.72	121.70
2	B	1261	TYR	CB-CG-CD1	-9.97	115.02	121.00
2	B	1325	TRP	CE2-CD2-CG	9.81	115.15	107.30
2	B	1330	TRP	CA-CB-CG	9.76	132.24	113.70
2	B	1075	TRP	O-C-N	-9.62	107.31	122.70
2	B	1325	TRP	CD1-CG-CD2	-9.39	98.79	106.30
2	B	1229	PHE	CB-CG-CD2	9.28	127.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	822	LEU	CB-CG-CD1	-9.23	95.30	111.00
2	B	956	LEU	CA-CB-CG	-9.21	94.12	115.30
2	B	4432	PRO	N-CA-CB	8.77	113.83	103.30
2	B	1304	ASP	CB-CG-OD2	8.73	126.16	118.30
16	P	101	TRP	CD1-CG-CD2	-8.36	99.61	106.30
3	C	3345	LYS	CA-C-O	-8.30	102.67	120.10
16	P	32	TRP	CD1-NE1-CE2	-8.26	101.57	109.00
3	C	3345	LYS	CA-C-N	8.23	135.30	117.20
2	B	1320	PHE	CB-CG-CD1	-8.19	115.07	120.80
16	P	16	ASP	CB-CG-OD1	-8.13	110.98	118.30
2	B	1313	ASP	CB-CG-OD2	8.04	125.53	118.30
2	B	1268	TYR	CG-CD1-CE1	8.02	127.72	121.30
2	B	1362	TYR	CB-CG-CD1	8.02	125.81	121.00
16	P	5	TYR	CB-CG-CD2	-7.99	116.20	121.00
2	B	1322	TYR	CB-CG-CD1	7.92	125.75	121.00
2	B	1261	TYR	CG-CD1-CE1	-7.91	114.97	121.30
2	B	1237	ARG	NE-CZ-NH2	-7.68	116.46	120.30
16	P	98	ASP	CB-CG-OD1	7.62	125.16	118.30
16	P	32	TRP	CH2-CZ2-CE2	-7.52	109.88	117.40
2	B	164	LEU	CA-CB-CG	7.50	132.54	115.30
2	B	1268	TYR	CZ-CE2-CD2	7.44	126.50	119.80
16	P	61	ASP	CB-CG-OD2	7.41	124.97	118.30
2	B	1254	TYR	CG-CD1-CE1	-7.35	115.42	121.30
3	C	3297	SER	N-CA-CB	-7.32	99.52	110.50
3	C	3378	ALA	O-C-N	-7.29	111.03	122.70
2	B	1261	TYR	CZ-CE2-CD2	-7.29	113.24	119.80
3	C	3354	ILE	CA-C-O	-7.23	104.92	120.10
16	P	32	TRP	CG-CD1-NE1	7.22	117.32	110.10
3	C	3314	GLU	N-CA-CB	-7.21	97.62	110.60
5	e	822	LEU	CA-CB-CG	7.15	131.74	115.30
2	B	1362	TYR	CG-CD1-CE1	7.10	126.98	121.30
3	C	3295	LYS	N-CA-CB	-7.02	97.96	110.60
2	B	1229	PHE	CB-CG-CD1	-7.01	115.89	120.80
16	P	14	PHE	CB-CG-CD1	6.99	125.69	120.80
16	P	14	PHE	CG-CD2-CE2	-6.92	113.18	120.80
16	P	43	PHE	CB-CG-CD2	6.91	125.64	120.80
3	C	3328	ALA	CB-CA-C	-6.91	99.74	110.10
3	C	3213	ASP	O-C-N	-6.88	111.68	122.70
3	C	3312	GLN	N-CA-CB	-6.87	98.24	110.60
3	C	3354	ILE	N-CA-C	-6.82	92.59	111.00
2	B	1254	TYR	CZ-CE2-CD2	-6.80	113.68	119.80
2	B	1300	ASP	CB-CG-OD1	-6.79	112.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3211	ALA	CB-CA-C	-6.71	100.04	110.10
3	C	4188	PRO	N-CA-CB	6.69	111.33	103.30
3	C	3281	LEU	C-N-CA	-6.65	108.33	122.30
3	C	4182	PRO	N-CA-CB	6.63	111.25	103.30
2	B	1325	TRP	CE3-CZ3-CH2	6.57	128.43	121.20
16	P	64	ASP	CB-CG-OD2	-6.55	112.41	118.30
3	C	3354	ILE	CA-C-N	6.41	131.30	117.20
2	B	1248	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	B	1277	ARG	NE-CZ-NH2	6.36	123.48	120.30
3	C	3378	ALA	CA-C-N	6.36	131.19	117.20
3	C	3292	GLU	CB-CA-C	-6.33	97.73	110.40
2	B	1336	ASP	CB-CG-OD1	-6.33	112.61	118.30
3	C	2978	PRO	N-CA-CB	6.33	110.89	103.30
2	B	1300	ASP	CB-CG-OD2	6.31	123.98	118.30
16	P	14	PHE	CD1-CE1-CZ	-6.31	112.52	120.10
2	B	1268	TYR	CB-CG-CD2	-6.31	117.21	121.00
2	B	1237	ARG	NH1-CZ-NH2	6.29	126.31	119.40
2	B	4008	PRO	N-CA-CB	6.25	110.80	103.30
5	e	81	PRO	N-CA-CB	6.24	110.79	103.30
2	B	3703	PRO	N-CA-CB	6.24	110.79	103.30
3	C	4180	PRO	N-CA-CB	6.23	110.78	103.30
2	B	1364	VAL	CA-CB-CG1	6.20	120.20	110.90
3	C	3319	ASP	O-C-N	-6.19	112.79	122.70
3	C	4546	PRO	N-CA-CB	6.19	110.72	103.30
3	C	2979	PRO	N-CA-CB	6.18	110.72	103.30
2	B	1254	TYR	CD1-CG-CD2	6.15	124.66	117.90
2	B	1237	ARG	NE-CZ-NH1	-6.14	117.23	120.30
16	P	32	TRP	CG-CD2-CE3	-6.14	128.37	133.90
16	P	61	ASP	CB-CG-OD1	-6.14	112.77	118.30
16	P	32	TRP	NE1-CE2-CZ2	-6.11	123.68	130.40
3	C	3204	ALA	CB-CA-C	-6.04	101.05	110.10
3	C	3338	ALA	CB-CA-C	5.96	119.05	110.10
5	e	106	PRO	N-CA-CB	5.95	110.44	103.30
2	B	1325	TRP	CD2-CE2-CZ2	5.91	129.40	122.30
16	P	5	TYR	CG-CD2-CE2	-5.90	116.58	121.30
16	P	101	TRP	CE2-CD2-CG	5.89	112.01	107.30
16	P	32	TRP	CD1-CG-CD2	-5.88	101.60	106.30
2	B	1312	TRP	CE2-CD2-CG	-5.87	102.60	107.30
3	C	3244	PHE	C-N-CA	5.87	136.38	121.70
3	C	3284	MET	N-CA-CB	5.87	121.16	110.60
3	C	3287	MET	N-CA-CB	5.85	121.13	110.60
3	C	3272	SER	N-CA-CB	-5.82	101.77	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	101	TRP	CG-CD1-NE1	5.82	115.92	110.10
2	B	1652	PRO	N-CA-CB	5.79	110.25	103.30
3	C	3244	PHE	CA-C-N	5.77	129.90	117.20
3	C	3326	SER	N-CA-CB	-5.76	101.86	110.50
2	B	1248	TYR	CG-CD2-CE2	-5.75	116.70	121.30
3	C	3323	THR	N-CA-CB	5.75	121.22	110.30
16	P	32	TRP	CD2-CE3-CZ3	-5.74	111.34	118.80
5	e	1249	PRO	N-CA-CB	5.74	110.18	103.30
1	A	1185	PRO	N-CA-CB	5.72	110.16	103.30
3	C	3206	ARG	O-C-N	-5.65	113.66	122.70
2	B	1340	ASP	CB-CG-OD2	-5.64	113.23	118.30
3	C	2805	PRO	N-CA-CB	5.62	110.04	103.30
16	P	28	PHE	CB-CG-CD1	-5.62	116.87	120.80
5	e	1237	PRO	N-CA-CB	5.61	110.03	103.30
2	B	1362	TYR	CZ-CE2-CD2	5.59	124.83	119.80
16	P	23	TYR	CB-CG-CD2	5.58	124.35	121.00
2	B	1320	PHE	CG-CD1-CE1	-5.57	114.67	120.80
3	C	3203	PRO	CA-C-O	5.57	133.56	120.20
16	P	77	LEU	CB-CG-CD2	5.56	120.45	111.00
2	B	1229	PHE	CG-CD2-CE2	5.55	126.91	120.80
2	B	1325	TRP	NE1-CE2-CD2	-5.54	101.76	107.30
3	C	3331	GLY	O-C-N	-5.53	113.85	122.70
3	C	3483	PRO	N-CA-CB	5.53	109.94	103.30
3	C	3332	ILE	CB-CA-C	-5.52	100.56	111.60
3	C	3293	PHE	O-C-N	5.52	131.53	122.70
3	C	3307	GLU	N-CA-CB	-5.52	100.67	110.60
16	P	101	TRP	CG-CD2-CE3	-5.51	128.94	133.90
3	C	3237	MET	N-CA-CB	-5.49	100.71	110.60
3	C	3299	ASN	N-CA-CB	5.49	120.48	110.60
3	C	3209	GLN	O-C-N	-5.49	113.92	122.70
3	C	3217	SER	N-CA-CB	-5.49	102.27	110.50
16	P	5	TYR	CD1-CE1-CZ	-5.44	114.91	119.80
3	C	3311	ASN	CA-C-O	5.43	131.51	120.10
2	B	1249	THR	CA-CB-CG2	-5.42	104.82	112.40
3	C	3241	LEU	O-C-N	-5.41	114.05	122.70
2	B	1264	ILE	CG1-CB-CG2	-5.40	99.53	111.40
3	C	3325	ALA	N-CA-CB	5.39	117.65	110.10
3	C	3273	TYR	N-CA-CB	-5.39	100.89	110.60
3	C	3322	ALA	CA-C-N	5.39	129.06	117.20
3	C	3233	ILE	CB-CA-C	5.38	122.37	111.60
16	P	28	PHE	CB-CG-CD2	5.38	124.56	120.80
3	C	3275	GLU	N-CA-CB	-5.35	100.97	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3340	TYR	O-C-N	5.33	131.23	122.70
3	C	3216	GLU	CA-C-O	5.32	131.28	120.10
2	B	1322	TYR	CG-CD1-CE1	5.32	125.56	121.30
16	P	9	THR	CA-CB-CG2	-5.32	104.95	112.40
2	B	1246	PHE	CB-CG-CD1	5.31	124.52	120.80
16	P	64	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	3951	PRO	N-CA-CB	5.30	109.66	103.30
3	C	3239	ALA	CB-CA-C	-5.29	102.16	110.10
3	C	3329	ALA	O-C-N	5.29	131.16	122.70
2	B	1240	PHE	CB-CG-CD1	5.28	124.50	120.80
2	B	1320	PHE	CZ-CE2-CD2	-5.28	113.77	120.10
16	P	101	TRP	CH2-CZ2-CE2	-5.28	112.12	117.40
2	B	1164	MET	CB-CG-SD	-5.27	96.58	112.40
2	B	1229	PHE	CD1-CE1-CZ	5.27	126.43	120.10
2	B	1288	PHE	CB-CG-CD2	5.27	124.49	120.80
16	P	5	TYR	CD1-CG-CD2	5.27	123.69	117.90
2	B	1224	ARG	NH1-CZ-NH2	5.25	125.18	119.40
3	C	3229	PRO	O-C-N	5.25	131.09	122.70
16	P	11	THR	CA-CB-CG2	-5.24	105.06	112.40
3	C	3222	GLU	CB-CA-C	5.24	120.88	110.40
3	C	3276	SER	CB-CA-C	5.24	120.05	110.10
2	B	1245	PRO	N-CD-CG	5.19	110.99	103.20
2	B	1317	LEU	CB-CG-CD2	5.19	119.83	111.00
2	B	1261	TYR	CB-CG-CD2	5.19	124.11	121.00
3	C	3317	PHE	C-N-CA	5.17	134.64	121.70
3	C	3289	LYS	N-CA-CB	5.17	119.91	110.60
2	B	1369	VAL	O-C-N	-5.13	114.50	122.70
3	C	3313	SER	CA-C-N	-5.10	105.98	117.20
3	C	3227	LYS	CA-C-O	5.10	130.80	120.10
3	C	3230	LEU	CB-CA-C	5.09	119.88	110.20
16	P	89	VAL	CA-CB-CG1	5.09	118.54	110.90
2	B	1362	TYR	CD1-CG-CD2	-5.08	112.31	117.90
2	B	1232	GLU	OE1-CD-OE2	-5.07	117.21	123.30
16	P	98	ASP	CB-CG-OD2	-5.06	113.75	118.30
3	C	3355	GLN	CB-CA-C	5.05	120.50	110.40
16	P	78	PRO	N-CA-CB	5.04	109.35	103.30
2	B	1312	TRP	NE1-CE2-CD2	5.04	112.34	107.30
2	B	2557	PRO	N-CA-CB	5.04	109.34	103.30
3	C	3281	LEU	CB-CA-C	-5.04	100.63	110.20
2	B	1236	PHE	CB-CG-CD1	-5.00	117.30	120.80

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	282	ARG	Peptide
2	B	1075	TRP	Mainchain
2	B	966	LYS	Peptide
3	C	3201	ALA	Mainchain
3	C	3344	GLN	Mainchain
3	C	3354	ILE	Mainchain
3	C	3378	ALA	Mainchain
3	C	974	GLN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	18127	0	9379	311	0
2	B	25545	0	17415	935	0
3	C	25046	0	16443	674	0
4	d	3626	0	3455	0	0
5	e	3948	0	3485	0	0
6	F	781	0	791	46	0
7	G	744	0	771	42	0
8	H	702	0	686	50	0
9	I	694	0	684	44	0
10	J	702	0	671	18	0
11	K	803	0	766	67	0
12	L	773	0	806	51	0
13	M	726	0	726	29	0
14	N	897	0	911	70	0
15	O	878	0	868	36	0
16	P	847	0	836	76	0
17	T	1057	0	1033	35	0
18	V	490	0	102	5	0
18	x	505	0	105	0	0
19	C	81	0	36	0	0
20	C	31	0	12	0	0
All	All	87003	0	59981	2356	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 (2356) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1212:ILE:CG2	2:B:1213:PRO:HD3	1.22	1.64
2:B:814:TYR:CA	2:B:1075:TRP:CZ2	1.79	1.58
2:B:814:TYR:HB2	2:B:1075:TRP:CE2	1.39	1.56
2:B:1148:SER:CB	2:B:1214:LEU:HB2	1.35	1.56
2:B:1148:SER:H	2:B:1214:LEU:CD1	1.01	1.55
2:B:1212:ILE:CG2	2:B:1213:PRO:CD	1.88	1.51
2:B:814:TYR:HA	2:B:1075:TRP:CZ2	0.99	1.50
2:B:814:TYR:CB	2:B:1075:TRP:CE2	1.91	1.50
2:B:814:TYR:CA	2:B:1075:TRP:CE2	1.99	1.45
2:B:1148:SER:OG	2:B:1214:LEU:CB	1.75	1.34
3:C:3354:ILE:C	3:C:3358:ILE:H	1.25	1.34
2:B:1212:ILE:HG22	2:B:1213:PRO:CG	1.58	1.33
3:C:3343:HIS:HA	3:C:3346:SER:CB	1.58	1.32
2:B:813:ASP:OD2	2:B:1076:LEU:CD1	1.78	1.31
3:C:3194:ALA:HB2	3:C:3352:LYS:O	1.35	1.27
2:B:1136:ASP:OD2	2:B:1221:ASN:ND2	1.65	1.27
2:B:814:TYR:HB2	2:B:1075:TRP:CD2	1.20	1.24
2:B:814:TYR:N	2:B:1075:TRP:NE1	1.86	1.23
3:C:3187:ILE:CB	3:C:3360:GLU:N	2.03	1.21
3:C:3343:HIS:C	3:C:3346:SER:H	1.44	1.21
3:C:3343:HIS:CA	3:C:3346:SER:H	1.55	1.19
2:B:898:PRO:HG2	2:B:1074:SER:OG	1.43	1.19
2:B:813:ASP:OD2	2:B:1076:LEU:HD12	1.43	1.19
2:B:1212:ILE:HG23	2:B:1213:PRO:CD	1.60	1.18
1:A:357:ILE:HG21	1:A:379:LYS:C	1.64	1.17
2:B:1148:SER:N	2:B:1214:LEU:HD13	0.84	1.17
2:B:1148:SER:CB	2:B:1214:LEU:CB	2.20	1.16
2:B:1147:ILE:N	2:B:1214:LEU:HD11	1.63	1.11
1:A:357:ILE:CG2	1:A:379:LYS:O	1.99	1.10
3:C:3354:ILE:C	3:C:3358:ILE:N	2.06	1.08
2:B:813:ASP:OD2	2:B:1076:LEU:HD11	1.47	1.07
2:B:1148:SER:OG	2:B:1214:LEU:HB2	0.90	1.07
3:C:3354:ILE:O	3:C:3358:ILE:N	1.88	1.06
2:B:898:PRO:HG2	2:B:1074:SER:CB	1.87	1.05
2:B:814:TYR:N	2:B:1075:TRP:CE2	2.22	1.04
1:A:357:ILE:CG2	1:A:379:LYS:C	2.23	1.04
2:B:814:TYR:HA	2:B:1075:TRP:CH2	1.93	1.03
3:C:3194:ALA:HB1	3:C:3353:ARG:HA	1.38	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3194:ALA:CB	3:C:3353:ARG:HA	1.87	1.03
2:B:1148:SER:HB2	2:B:1214:LEU:HB2	1.39	1.03
2:B:2379:GLU:CB	3:C:1536:LEU:HA	1.89	1.02
3:C:3342:TYR:O	3:C:3346:SER:N	1.93	1.02
2:B:1148:SER:HB2	2:B:1214:LEU:CB	1.86	1.01
2:B:1212:ILE:HG22	2:B:1213:PRO:CD	1.73	1.01
3:C:3354:ILE:O	3:C:3357:ALA:N	1.93	1.01
2:B:1147:ILE:C	2:B:1214:LEU:HD13	1.81	1.00
3:C:3343:HIS:C	3:C:3346:SER:N	2.14	1.00
1:A:357:ILE:HG21	1:A:379:LYS:CA	1.58	0.99
2:B:814:TYR:CG	2:B:1075:TRP:CH2	2.16	0.99
2:B:814:TYR:CB	2:B:1075:TRP:CZ2	2.30	0.98
2:B:1212:ILE:HG22	2:B:1213:PRO:HG3	1.46	0.98
2:B:814:TYR:CB	2:B:1075:TRP:CD2	2.07	0.97
3:C:175:GLU:O	3:C:177:ARG:NH1	1.98	0.97
2:B:1148:SER:OG	2:B:1213:PRO:C	2.02	0.96
2:B:1214:LEU:HG	2:B:1215:GLN:HG3	1.47	0.96
2:B:814:TYR:HB2	2:B:1075:TRP:CG	2.00	0.96
3:C:3192:GLU:N	3:C:3356:VAL:CB	1.71	0.95
1:A:222:PHE:HB2	2:B:952:PRO:HB3	1.49	0.94
2:B:814:TYR:N	2:B:1075:TRP:HE1	1.60	0.94
2:B:1343:LYS:HA	2:B:1369:VAL:HG13	1.48	0.94
3:C:3194:ALA:CB	3:C:3352:LYS:O	2.14	0.94
2:B:1359:PHE:HB2	2:B:1362:TYR:HD2	1.32	0.94
3:C:3180:CYS:HA	3:C:3366:ALA:HB1	1.50	0.93
3:C:3344:GLN:H	3:C:3347:LYS:H	1.15	0.93
3:C:928:LYS:HD2	3:C:957:ARG:HH22	1.34	0.92
3:C:3344:GLN:C	3:C:3348:ILE:H	1.73	0.92
2:B:1147:ILE:H	2:B:1214:LEU:HD11	1.26	0.92
2:B:94:LEU:HD13	3:C:124:THR:HG23	1.49	0.91
2:B:1147:ILE:N	2:B:1214:LEU:CD1	2.33	0.91
3:C:3194:ALA:HB1	3:C:3353:ARG:CA	2.01	0.91
2:B:1243:LYS:HG3	2:B:1264:ILE:HG12	1.51	0.91
2:B:2379:GLU:CB	3:C:1536:LEU:CB	2.48	0.90
13:M:49:ASP:HB2	13:M:53:TRP:HE1	1.37	0.89
2:B:1283:ASN:HA	2:B:1286:LYS:HD2	1.54	0.89
3:C:3343:HIS:CA	3:C:3346:SER:N	2.36	0.89
2:B:1317:LEU:HB3	16:P:32:TRP:HH2	1.35	0.89
1:A:60:LEU:HD11	1:A:67:CYS:HB3	1.53	0.88
6:F:67:LEU:HD11	7:G:95:GLU:HB3	1.55	0.88
1:A:220:TRP:HE1	2:B:956:LEU:HD13	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1317:LEU:HD13	16:P:77:LEU:HB2	1.55	0.88
3:C:535:ASN:HA	3:C:548:LEU:HD23	1.56	0.87
2:B:435:GLN:HG3	2:B:533:ARG:HG3	1.55	0.87
2:B:1148:SER:N	2:B:1214:LEU:CD1	1.81	0.87
2:B:1359:PHE:HB2	2:B:1362:TYR:CD2	2.09	0.87
2:B:2379:GLU:CB	3:C:1536:LEU:CA	2.52	0.86
3:C:667:LYS:HA	3:C:671:GLN:HB2	1.58	0.86
3:C:3378:ALA:O	3:C:3380:ILE:N	2.09	0.85
2:B:483:LYS:HD3	2:B:484:LYS:HD3	1.56	0.85
3:C:633:GLU:HA	3:C:636:ARG:HD3	1.58	0.85
14:N:32:SER:HA	14:N:35:GLN:HB3	1.58	0.85
11:K:33:ALA:HA	14:N:36:LYS:HA	1.58	0.85
2:B:1135:HIS:CG	2:B:1217:GLU:OE2	2.18	0.85
1:A:357:ILE:HG21	1:A:379:LYS:O	1.65	0.85
2:B:1148:SER:HB2	2:B:1214:LEU:HD22	1.57	0.85
11:K:37:LEU:HD13	14:N:36:LYS:HZ3	1.42	0.85
1:A:342:ALA:HB3	1:A:346:LEU:HD21	1.56	0.85
3:C:3344:GLN:N	3:C:3347:LYS:H	1.73	0.84
2:B:1245:PRO:HA	2:B:1360:LYS:HB2	1.59	0.84
3:C:3190:GLU:CB	3:C:3355:GLN:C	2.46	0.84
3:C:3194:ALA:HB2	3:C:3352:LYS:C	1.98	0.84
11:K:36:ILE:HG22	11:K:96:ILE:HD11	1.59	0.84
3:C:862:LEU:HD13	3:C:972:TRP:HE1	1.40	0.84
2:B:157:TYR:HA	2:B:178:SER:HB2	1.60	0.84
3:C:3343:HIS:HA	3:C:3346:SER:CA	2.08	0.84
3:C:3344:GLN:N	3:C:3346:SER:N	2.25	0.83
11:K:34:ASP:HB3	14:N:40:GLU:HB2	1.59	0.83
2:B:1346:GLY:HA3	2:B:1369:VAL:HG11	1.59	0.83
3:C:89:GLN:HA	3:C:126:ASN:HD21	1.40	0.83
2:B:477:ILE:HG13	2:B:481:ALA:HA	1.61	0.83
2:B:1148:SER:OG	2:B:1214:LEU:CA	2.26	0.82
2:B:1176:VAL:HG13	2:B:1188:GLN:HG2	1.61	0.82
2:B:4318:LEU:O	2:B:4322:GLU:N	2.12	0.82
2:B:175:PRO:HG2	2:B:210:VAL:HG12	1.60	0.82
2:B:902:ILE:HA	2:B:915:PRO:HG2	1.60	0.82
3:C:242:GLU:HG3	3:C:368:LYS:HE3	1.58	0.82
1:A:282:ARG:O	1:A:284:ASN:N	2.11	0.82
3:C:3190:GLU:CB	3:C:3355:GLN:O	2.28	0.82
3:C:3202:LEU:O	3:C:3204:ALA:N	2.13	0.82
1:A:220:TRP:NE1	2:B:956:LEU:HD13	1.94	0.82
2:B:1148:SER:HB2	2:B:1214:LEU:CD2	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2229:LYS:O	2:B:2230:THR:N	2.13	0.82
3:C:3187:ILE:CB	3:C:3359:ALA:O	0.82	0.81
3:C:456:ARG:HA	3:C:459:LYS:HD2	1.62	0.81
1:A:357:ILE:HG22	1:A:379:LYS:O	1.79	0.81
2:B:1212:ILE:CB	2:B:1213:PRO:CD	2.39	0.81
2:B:898:PRO:HG2	2:B:1074:SER:HB3	1.62	0.81
2:B:898:PRO:CG	2:B:1074:SER:OG	2.28	0.80
3:C:3194:ALA:CB	3:C:3352:LYS:C	2.50	0.80
2:B:1317:LEU:HB3	16:P:32:TRP:CH2	2.16	0.80
2:B:509:GLN:HA	2:B:512:ASP:HB2	1.62	0.80
11:K:34:ASP:HB2	14:N:36:LYS:C	2.02	0.80
3:C:1071:ILE:HG13	3:C:1074:MET:HB2	1.64	0.80
1:A:2611:LYS:O	1:A:2613:THR:N	2.15	0.80
1:A:250:LYS:HD3	1:A:251:TRP:HB2	1.62	0.79
2:B:1146:VAL:CG1	2:B:1215:GLN:CD	2.50	0.79
2:B:4032:GLY:O	2:B:4036:GLY:N	2.15	0.79
16:P:37:LYS:O	16:P:95:ASN:ND2	2.15	0.79
1:A:4124:TYR:N	1:A:4146:MET:O	2.15	0.79
2:B:94:LEU:HD11	2:B:109:VAL:HG23	1.64	0.79
2:B:814:TYR:HA	2:B:1075:TRP:HZ2	0.99	0.79
1:A:4048:THR:O	1:A:4110:ALA:N	2.16	0.79
2:B:3830:PHE:O	2:B:3839:ASP:N	2.16	0.78
3:C:3194:ALA:CB	3:C:3353:ARG:CA	2.60	0.78
3:C:31:SER:O	3:C:37:ASN:ND2	2.14	0.78
3:C:269:LYS:HD2	3:C:281:GLN:HA	1.66	0.78
1:A:5:LEU:HB2	1:A:352:LEU:HD11	1.64	0.78
3:C:502:LEU:HB2	3:C:509:LYS:HD2	1.64	0.78
2:B:1147:ILE:H	2:B:1214:LEU:CD1	1.94	0.78
15:O:22:LYS:HD2	15:O:26:GLY:HA3	1.64	0.78
1:A:256:ILE:HD11	1:A:322:GLU:HB2	1.66	0.78
1:A:2631:ALA:O	1:A:2635:LYS:N	2.16	0.78
3:C:3202:LEU:O	3:C:3205:LEU:N	2.16	0.78
11:K:30:PRO:HD2	14:N:33:LYS:HB2	1.65	0.78
2:B:112:GLU:O	2:B:120:HIS:NE2	2.16	0.78
2:B:137:LEU:HB3	2:B:142:TRP:HD1	1.49	0.78
3:C:60:GLN:HB3	3:C:62:GLN:HE22	1.47	0.78
3:C:381:ILE:O	3:C:396:MET:N	2.17	0.77
3:C:3344:GLN:O	3:C:3348:ILE:N	2.18	0.77
3:C:101:PRO:HG2	3:C:104:ASP:HB3	1.67	0.77
2:B:1148:SER:OG	2:B:1213:PRO:O	2.02	0.77
2:B:1360:LYS:O	2:B:1364:VAL:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:708:TYR:HE1	2:B:756:ARG:HB3	1.51	0.76
2:B:1340:ASP:OD2	2:B:1343:LYS:HB3	1.86	0.76
2:B:3546:ARG:O	2:B:3550:GLY:N	2.19	0.76
2:B:3552:ASN:O	2:B:3553:LEU:N	2.18	0.76
1:A:6:VAL:HB	1:A:353:ASN:HB3	1.68	0.76
2:B:1178:ILE:HA	2:B:1181:LYS:HE2	1.66	0.76
2:B:841:LYS:HA	2:B:844:LEU:HD12	1.66	0.76
1:A:344:ASN:HD21	2:B:969:LEU:HB3	1.50	0.76
2:B:2201:TYR:O	2:B:2205:GLY:N	2.19	0.76
2:B:1148:SER:HG	2:B:1214:LEU:HB2	1.46	0.76
3:C:477:ASN:HD22	3:C:528:LEU:HD23	1.49	0.76
2:B:1107:ARG:HD3	2:B:1190:ILE:HG12	1.67	0.76
2:B:459:ILE:HG23	2:B:499:LEU:HD22	1.68	0.76
2:B:1120:THR:OG1	2:B:1157:ARG:NH1	2.19	0.76
2:B:794:LEU:HD21	2:B:867:VAL:HA	1.68	0.75
2:B:1146:VAL:HG13	2:B:1215:GLN:HG3	1.68	0.75
3:C:542:ILE:HD13	3:C:576:TYR:HA	1.68	0.75
2:B:215:PRO:HA	2:B:218:LEU:HD12	1.67	0.75
1:A:22:SER:OG	1:A:321:ARG:NH1	2.20	0.75
3:C:973:ASP:HB3	3:C:981:ASP:HB3	1.69	0.75
3:C:3187:ILE:CB	3:C:3359:ALA:C	0.85	0.75
3:C:3342:TYR:O	3:C:3346:SER:CA	2.34	0.75
2:B:67:GLN:H	2:B:85:LYS:HZ3	1.33	0.75
16:P:36:CYS:HB2	16:P:95:ASN:HD21	1.51	0.75
1:A:221:SER:HB2	1:A:226:TYR:HE1	1.52	0.74
3:C:3344:GLN:CA	3:C:3347:LYS:H	2.00	0.74
3:C:1146:GLN:HB3	3:C:1187:TRP:CH2	2.22	0.74
2:B:373:THR:HA	2:B:376:ALA:HB3	1.70	0.74
3:C:1105:ARG:NH2	3:C:1176:GLU:OE2	2.19	0.74
3:C:3343:HIS:HA	3:C:3346:SER:H	1.50	0.74
3:C:3354:ILE:HA	3:C:3357:ALA:HB3	1.70	0.74
14:N:102:LEU:HD23	15:O:90:ASP:O	1.88	0.74
2:B:1146:VAL:HG13	2:B:1215:GLN:CG	2.18	0.74
2:B:814:TYR:CG	2:B:1075:TRP:CZ2	2.61	0.74
1:A:332:GLU:O	1:A:334:ARG:NH1	2.21	0.74
2:B:1148:SER:CA	2:B:1214:LEU:HD13	2.09	0.74
1:A:2297:GLY:N	1:A:2375:PHE:O	2.21	0.73
3:C:948:LEU:HA	3:C:951:ILE:HD12	1.68	0.73
2:B:2228:THR:O	2:B:2231:LYS:N	2.21	0.73
3:C:1141:GLN:HA	3:C:1144:LYS:HD2	1.70	0.73
1:A:2496:MET:O	1:A:2500:ALA:N	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1148:SER:H	2:B:1214:LEU:CG	1.96	0.73
2:B:1240:PHE:O	2:B:1244:LEU:HB2	1.88	0.73
2:B:2396:MET:N	2:B:2447:PRO:O	2.22	0.73
3:C:801:ILE:HD13	3:C:868:LEU:HD21	1.69	0.73
2:B:1148:SER:HB2	2:B:1214:LEU:CG	2.17	0.73
2:B:1136:ASP:CG	2:B:1221:ASN:HD21	1.91	0.73
3:C:859:VAL:HA	3:C:975:GLN:HE22	1.53	0.73
12:L:87:THR:OG1	13:M:54:ASN:ND2	2.19	0.73
2:B:802:ILE:HG12	2:B:877:THR:HG21	1.69	0.73
2:B:1148:SER:OG	2:B:1214:LEU:N	2.22	0.73
2:B:1568:SER:O	2:B:1572:ALA:N	2.21	0.73
2:B:1136:ASP:CG	2:B:1221:ASN:ND2	2.40	0.73
2:B:1219:THR:HA	2:B:1222:ILE:HD12	1.71	0.73
9:I:89:VAL:HG21	9:I:94:LEU:HB2	1.69	0.73
1:A:4004:LEU:O	1:A:4008:CYS:N	2.21	0.72
3:C:880:PRO:HB2	3:C:883:THR:HB	1.71	0.72
7:G:136:MET:O	7:G:146:ILE:HA	1.89	0.72
2:B:301:LYS:HE3	2:B:320:ILE:HG21	1.70	0.72
2:B:924:LEU:HD12	2:B:926:VAL:H	1.53	0.72
2:B:1149:ASP:OD1	2:B:1214:LEU:CD2	2.37	0.72
3:C:210:GLU:OE1	3:C:277:ASN:ND2	2.23	0.72
2:B:548:LEU:HD21	2:B:613:ILE:HD13	1.71	0.72
2:B:1285:GLU:HG3	2:B:1290:LEU:HD12	1.70	0.72
3:C:895:TYR:HA	3:C:898:LEU:HD12	1.72	0.72
9:I:51:ALA:H	9:I:54:LEU:HD23	1.54	0.72
3:C:14:LYS:HG3	3:C:24:LYS:HE3	1.70	0.72
3:C:971:ASN:ND2	3:C:986:TYR:OH	2.23	0.72
1:A:343:ASN:HD21	2:B:931:ARG:HE	1.38	0.72
2:B:64:VAL:HG13	2:B:86:LYS:HD3	1.72	0.72
2:B:1650:ALA:N	2:B:1653:ALA:O	2.22	0.72
2:B:2221:ASP:O	2:B:2225:GLY:N	2.23	0.72
3:C:3344:GLN:HA	3:C:3347:LYS:CB	2.19	0.72
11:K:20:THR:O	14:N:75:LYS:NZ	2.22	0.72
1:A:1954:SER:O	1:A:1957:SER:N	2.22	0.72
2:B:1360:LYS:HD2	2:B:1363:ASN:HB3	1.71	0.71
3:C:534:ASN:HA	3:C:537:ASN:HB2	1.70	0.71
3:C:3194:ALA:HB3	3:C:3353:ARG:HA	1.70	0.71
16:P:28:PHE:CZ	16:P:74:VAL:HG21	2.25	0.71
1:A:2627:LYS:O	1:A:2631:ALA:N	2.23	0.71
2:B:62:LEU:O	2:B:77:GLN:NE2	2.24	0.71
2:B:1271:LEU:HD21	2:B:1301:CYS:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3180:CYS:HA	3:C:3366:ALA:CB	2.20	0.71
14:N:41:LEU:HD11	14:N:70:LYS:HG3	1.73	0.71
3:C:3187:ILE:O	3:C:3356:VAL:O	2.07	0.71
6:F:14:LEU:HA	6:F:17:LEU:HD23	1.71	0.71
2:B:64:VAL:HA	2:B:83:LYS:HZ1	1.55	0.71
1:A:322:GLU:HG3	1:A:340:GLY:HA3	1.71	0.71
2:B:734:GLU:HB2	2:B:737:VAL:HG22	1.73	0.71
2:B:1315:ILE:HD13	2:B:1318:ILE:HD12	1.70	0.71
7:G:76:TYR:H	7:G:89:ALA:HB3	1.56	0.70
1:A:22:SER:HB3	1:A:340:GLY:HA2	1.72	0.70
2:B:1136:ASP:OD2	2:B:1218:GLU:OE1	1.80	0.70
3:C:853:VAL:O	3:C:857:ARG:HD3	1.90	0.70
3:C:3343:HIS:C	3:C:3345:LYS:N	2.44	0.70
2:B:117:LEU:HD13	3:C:146:ILE:HG13	1.71	0.70
2:B:3848:ASP:O	2:B:3853:CYS:N	2.25	0.70
1:A:3895:MET:O	1:A:3899:THR:N	2.24	0.70
2:B:173:MET:HE1	2:B:218:LEU:HD23	1.72	0.70
3:C:3194:ALA:HB1	3:C:3353:ARG:N	2.06	0.70
1:A:319:ARG:HB2	1:A:322:GLU:OE2	1.91	0.70
1:A:1400:ALA:N	1:A:1524:ARG:O	2.22	0.70
2:B:1048:ASP:OD1	2:B:1173:LYS:NZ	2.25	0.70
2:B:1249:THR:OG1	2:B:1259:ASN:ND2	2.24	0.70
2:B:2209:GLU:N	2:B:2258:HIS:O	2.25	0.70
2:B:208:LYS:HB3	2:B:212:LYS:HE2	1.73	0.70
2:B:1147:ILE:CA	2:B:1214:LEU:CD1	2.70	0.70
2:B:1301:CYS:SG	2:B:1302:MET:N	2.65	0.70
2:B:422:ARG:HD3	2:B:478:MET:HG3	1.74	0.69
2:B:1310:THR:O	16:P:76:SER:HB3	1.92	0.69
3:C:3343:HIS:HA	3:C:3346:SER:N	2.05	0.69
2:B:1277:ARG:HH12	2:B:1280:GLU:HB2	1.57	0.69
12:L:28:GLN:HG3	12:L:32:LYS:HE3	1.72	0.69
2:B:1150:VAL:HA	2:B:1153:VAL:HG12	1.72	0.69
3:C:248:SER:O	3:C:252:LYS:HB2	1.92	0.69
1:A:124:PRO:HB3	1:A:185:PHE:HE2	1.57	0.69
1:A:3594:ARG:O	1:A:3621:TRP:N	2.26	0.69
1:A:208:MET:HG3	1:A:296:ILE:HD13	1.73	0.69
1:A:2044:TYR:O	1:A:2086:GLN:N	2.26	0.69
1:A:3519:LEU:O	1:A:3523:LEU:N	2.26	0.69
2:B:533:ARG:HE	2:B:535:ILE:HD11	1.57	0.69
2:B:3833:MET:O	2:B:3839:ASP:N	2.25	0.69
10:J:26:PHE:O	10:J:30:LYS:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:LEU:HD11	2:B:427:LEU:HB2	1.74	0.69
1:A:3384:SER:O	1:A:3388:ARG:N	2.26	0.69
2:B:493:ARG:NH2	2:B:500:GLU:OE2	2.26	0.69
3:C:784:VAL:O	3:C:788:LEU:HG	1.92	0.69
2:B:169:LYS:HZ1	3:C:150:LYS:HB2	1.59	0.68
2:B:1137:LYS:HB3	2:B:1215:GLN:NE2	2.08	0.68
2:B:1310:THR:HA	16:P:93:ILE:HG21	1.75	0.68
2:B:4123:ASP:O	2:B:4126:ILE:N	2.26	0.68
1:A:3221:SER:O	1:A:3225:ARG:N	2.25	0.68
2:B:20:GLN:HG2	3:C:16:THR:HG22	1.75	0.68
2:B:445:GLY:HA2	2:B:506:VAL:HG21	1.73	0.68
2:B:1070:PRO:HB3	2:B:1079:ASN:HA	1.74	0.68
2:B:420:LEU:O	2:B:424:GLN:HG2	1.93	0.68
3:C:177:ARG:HE	3:C:259:GLN:HA	1.59	0.68
3:C:871:LEU:HD22	3:C:875:VAL:HG23	1.75	0.68
2:B:536:ILE:HG22	2:B:540:LEU:HG	1.74	0.68
3:C:3192:GLU:H	3:C:3356:VAL:CB	2.01	0.68
6:F:20:ALA:HA	6:F:101:GLN:HA	1.74	0.68
12:L:26:MET:HB2	12:L:30:LEU:HD22	1.75	0.68
2:B:510:GLY:HA2	2:B:523:LEU:HD23	1.74	0.68
1:A:2893:LEU:O	1:A:2898:ARG:N	2.26	0.68
2:B:1229:PHE:O	2:B:1233:VAL:HG23	1.94	0.68
1:A:3470:LEU:O	1:A:3473:ILE:N	2.28	0.67
1:A:189:ARG:NH1	1:A:190:LEU:O	2.27	0.67
1:A:3:GLN:N	1:A:305:ASN:O	2.23	0.67
1:A:3835:GLU:O	1:A:3839:LYS:N	2.27	0.67
3:C:1065:ILE:HD13	3:C:1082:CYS:HB2	1.76	0.67
3:C:3741:ASN:O	3:C:3745:GLU:N	2.27	0.67
1:A:1931:LYS:O	1:A:1939:LYS:N	2.28	0.67
2:B:596:ARG:NH1	2:B:597:ASP:OD1	2.27	0.67
3:C:79:PHE:O	3:C:82:THR:OG1	2.11	0.67
3:C:3344:GLN:H	3:C:3347:LYS:N	1.90	0.67
1:A:329:ASP:O	1:A:334:ARG:NH1	2.27	0.67
2:B:1054:ILE:HD13	2:B:1057:LEU:HD12	1.77	0.67
2:B:1113:LEU:HD21	2:B:1160:ILE:HB	1.76	0.67
2:B:1226:LEU:HD11	2:B:1285:GLU:OE2	1.93	0.67
3:C:935:VAL:HG21	3:C:1076:LEU:HB2	1.75	0.67
2:B:439:LEU:HB3	2:B:533:ARG:HH11	1.59	0.67
2:B:1047:LEU:HD22	2:B:1106:PHE:HE2	1.60	0.67
2:B:1146:VAL:HG13	2:B:1215:GLN:CD	2.14	0.67
3:C:96:LEU:HB3	3:C:119:ILE:HB	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4441:ILE:N	2:B:4494:TYR:O	2.28	0.67
17:T:33:VAL:O	17:T:37:THR:HG23	1.94	0.67
1:A:3781:TYR:O	1:A:3785:GLU:N	2.26	0.67
3:C:57:TYR:HB2	3:C:91:LYS:HB2	1.77	0.67
3:C:531:PHE:HA	3:C:534:ASN:HB2	1.76	0.67
2:B:470:PHE:CE1	2:B:488:ASP:HB3	2.29	0.67
2:B:1047:LEU:HD22	2:B:1106:PHE:CE2	2.30	0.67
3:C:3353:ARG:O	3:C:3354:ILE:O	2.13	0.67
2:B:1149:ASP:H	2:B:1214:LEU:HD22	1.58	0.66
3:C:1112:THR:HG21	3:C:1179:ALA:HA	1.78	0.66
1:A:1484:GLU:O	1:A:1495:LEU:N	2.27	0.66
1:A:2495:ASP:O	1:A:2496:MET:N	2.29	0.66
9:I:73:PRO:O	9:I:109:LYS:NZ	2.27	0.66
9:I:99:TYR:HD2	9:I:103:LEU:HB2	1.61	0.66
2:B:1277:ARG:NH1	2:B:1280:GLU:HB2	2.10	0.66
2:B:1343:LYS:HA	2:B:1369:VAL:CG1	2.24	0.66
3:C:3187:ILE:C	3:C:3360:GLU:N	2.49	0.66
7:G:62:ASP:HB3	7:G:66:ARG:HH21	1.61	0.66
16:P:24:VAL:HG22	16:P:54:THR:HB	1.78	0.66
1:A:274:GLY:O	1:A:282:ARG:NH1	2.27	0.66
1:A:1592:ARG:O	1:A:1593:SER:N	2.29	0.66
2:B:2890:GLY:N	2:B:3022:PHE:O	2.29	0.66
15:O:51:ILE:O	15:O:55:ILE:HG12	1.96	0.66
2:B:1315:ILE:HG12	2:B:1362:TYR:HD1	1.61	0.66
3:C:621:ILE:HA	3:C:624:PHE:CD2	2.31	0.66
3:C:884:LYS:HG3	3:C:885:ARG:HD2	1.78	0.66
3:C:243:LEU:HD22	3:C:320:LEU:HD13	1.78	0.66
2:B:1212:ILE:HG23	2:B:1213:PRO:HD3	0.66	0.66
3:C:210:GLU:HG3	3:C:280:ASN:ND2	2.11	0.66
3:C:624:PHE:HB3	3:C:634:ILE:HG23	1.77	0.66
2:B:132:VAL:HG11	3:C:77:VAL:HG22	1.78	0.66
2:B:674:ASP:HB3	2:B:675:PRO:HD3	1.76	0.66
2:B:677:LEU:HD11	2:B:712:ILE:HD12	1.79	0.66
3:C:608:ILE:HD13	3:C:705:GLN:HG2	1.77	0.66
3:C:3353:ARG:O	3:C:3357:ALA:N	2.28	0.65
1:A:166:GLY:HA2	1:A:171:ARG:H	1.59	0.65
3:C:903:GLN:NE2	3:C:994:GLU:OE2	2.28	0.65
2:B:217:GLN:HA	2:B:220:LYS:HD3	1.77	0.65
3:C:336:ILE:O	3:C:340:PRO:HD2	1.97	0.65
2:B:572:MET:HG3	2:B:575:ASN:H	1.61	0.65
2:B:1283:ASN:CA	2:B:1286:LYS:HD2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1804:PHE:O	2:B:1808:LYS:N	2.28	0.65
3:C:52:LYS:NZ	3:C:75:ASP:OD2	2.29	0.65
1:A:283:THR:HG21	2:B:939:ASN:HB3	1.78	0.65
2:B:2465:TRP:O	2:B:2469:ALA:N	2.30	0.65
11:K:30:PRO:O	14:N:32:SER:HB3	1.97	0.65
1:A:339:GLY:C	1:A:346:LEU:HB2	2.17	0.65
2:B:454:GLU:O	2:B:458:GLN:CB	2.45	0.65
2:B:716:ASP:HA	2:B:719:VAL:HG12	1.78	0.65
2:B:752:ILE:HD13	2:B:765:PHE:HB3	1.77	0.65
2:B:806:ASN:OD1	2:B:881:HIS:NE2	2.30	0.65
2:B:851:LYS:HD2	2:B:851:LYS:O	1.97	0.65
2:B:1107:ARG:HG3	2:B:1111:LYS:HE3	1.78	0.65
2:B:1317:LEU:HD22	16:P:32:TRP:HZ3	1.62	0.65
3:C:1182:LEU:HD12	3:C:1185:ARG:HE	1.62	0.65
3:C:2492:ILE:O	3:C:2634:MET:N	2.29	0.65
16:P:47:LYS:HD3	16:P:55:ILE:CG1	2.27	0.65
1:A:2374:SER:O	1:A:2378:GLY:N	2.29	0.65
2:B:663:LYS:HG2	2:B:664:ASP:H	1.61	0.65
2:B:1346:GLY:HA2	2:B:1349:ILE:HD12	1.78	0.65
3:C:601:PRO:HD2	3:C:701:CYS:SG	2.37	0.65
9:I:30:MET:HG3	9:I:35:LEU:HD22	1.78	0.65
2:B:652:SER:O	2:B:672:ASN:ND2	2.30	0.65
3:C:542:ILE:HG23	3:C:575:ASN:HB2	1.79	0.65
9:I:59:ALA:O	9:I:63:ILE:HG12	1.97	0.65
2:B:65:SER:HB2	2:B:87:LYS:H	1.62	0.65
2:B:530:LEU:HD21	2:B:536:ILE:HG21	1.77	0.65
2:B:1243:LYS:HE2	2:B:1264:ILE:HA	1.78	0.65
2:B:1802:GLU:O	2:B:1806:ILE:N	2.30	0.65
2:B:1176:VAL:O	2:B:1179:THR:OG1	2.12	0.64
3:C:696:ILE:HG23	3:C:700:LYS:HE2	1.79	0.64
2:B:688:LEU:O	2:B:691:ARG:NH1	2.30	0.64
3:C:313:ASN:HD21	3:C:355:PHE:HB3	1.62	0.64
3:C:942:VAL:HB	3:C:1017:LEU:HD11	1.80	0.64
7:G:103:ILE:HD13	7:G:106:LEU:HD12	1.79	0.64
2:B:1244:LEU:HB3	2:B:1245:PRO:HD3	1.78	0.64
17:T:43:ASN:HA	17:T:46:LYS:HE3	1.79	0.64
3:C:819:VAL:HG12	3:C:909:MET:HG2	1.78	0.64
6:F:75:GLU:OE2	7:G:131:LYS:NZ	2.31	0.64
2:B:1245:PRO:CA	2:B:1360:LYS:HB2	2.27	0.64
1:A:256:ILE:HG23	1:A:324:ALA:HB2	1.78	0.64
2:B:1243:LYS:HZ3	2:B:1264:ILE:HG23	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1283:ASN:O	2:B:1287:LEU:HG	1.98	0.64
2:B:1359:PHE:O	2:B:1363:ASN:N	2.31	0.64
3:C:3870:GLU:O	3:C:3874:TRP:N	2.31	0.64
2:B:345:ARG:HG3	2:B:414:VAL:HG12	1.79	0.64
2:B:656:LEU:HD22	2:B:756:ARG:HD2	1.78	0.64
2:B:2285:LEU:N	2:B:2293:ILE:O	2.30	0.64
3:C:77:VAL:HG11	3:C:94:TRP:HZ2	1.63	0.64
3:C:3354:ILE:CA	3:C:3358:ILE:N	2.61	0.64
11:K:111:GLN:OE1	11:K:111:GLN:N	2.30	0.64
16:P:60:ILE:HG23	16:P:69:VAL:HG21	1.80	0.64
2:B:165:LEU:HA	2:B:168:ILE:HB	1.78	0.64
16:P:6:ILE:O	16:P:57:LYS:N	2.26	0.64
2:B:1161:ILE:HG13	2:B:1197:PHE:CZ	2.33	0.63
3:C:2910:PHE:O	3:C:2914:GLY:N	2.31	0.63
3:C:3353:ARG:O	3:C:3357:ALA:CB	2.46	0.63
3:C:3354:ILE:O	3:C:3357:ALA:CA	2.45	0.63
1:A:222:PHE:O	1:A:223:THR:OG1	2.14	0.63
3:C:1026:LEU:HD13	3:C:1088:TRP:CG	2.33	0.63
10:J:67:ASN:HB2	11:K:58:GLN:HB2	1.80	0.63
13:M:5:PRO:HA	13:M:77:ILE:HG22	1.80	0.63
2:B:1748:ASP:O	2:B:1752:GLY:N	2.31	0.63
3:C:601:PRO:HG3	3:C:697:ARG:HD3	1.80	0.63
3:C:1227:ARG:HG3	3:C:1228:ARG:HH22	1.62	0.63
14:N:76:VAL:HB	14:N:79:TYR:HB2	1.79	0.63
2:B:658:GLN:NE2	2:B:746:GLU:OE1	2.32	0.63
3:C:546:LEU:HD12	3:C:549:LEU:HD23	1.79	0.63
1:A:220:TRP:HB2	1:A:253:LEU:HD13	1.81	0.63
2:B:161:VAL:O	2:B:164:LEU:HB3	1.98	0.63
1:A:2175:SER:O	1:A:2177:ILE:N	2.32	0.63
2:B:64:VAL:HG22	2:B:83:LYS:HZ2	1.63	0.63
3:C:862:LEU:HB2	3:C:972:TRP:CD1	2.33	0.63
12:L:21:ILE:HG12	12:L:31:LEU:HD21	1.80	0.63
1:A:42:ASP:HB2	1:A:48:ASP:HB3	1.80	0.63
2:B:66:GLY:HA2	2:B:86:LYS:HG2	1.81	0.63
2:B:1147:ILE:HB	2:B:1214:LEU:HD12	1.81	0.63
3:C:317:LEU:HD23	3:C:356:TYR:HD2	1.64	0.63
3:C:667:LYS:HD2	3:C:716:ILE:HD12	1.81	0.63
3:C:872:ASP:O	3:C:888:ARG:NH2	2.31	0.63
8:H:10:VAL:N	8:H:80:TYR:O	2.29	0.63
1:A:341:TRP:CE2	1:A:344:ASN:HA	2.34	0.63
2:B:92:ILE:HB	2:B:109:VAL:HB	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ASN:HB2	2:B:180:LYS:HE2	1.81	0.63
2:B:228:LEU:O	2:B:232:GLU:HG2	1.98	0.63
1:A:223:THR:HA	2:B:956:LEU:HD11	1.81	0.63
1:A:1398:GLY:O	1:A:1524:ARG:N	2.32	0.63
2:B:55:GLN:O	2:B:93:LYS:NZ	2.25	0.63
2:B:425:ASP:OD1	2:B:426:ILE:N	2.32	0.62
8:H:9:PRO:HA	8:H:81:VAL:HA	1.80	0.62
2:B:801:ILE:HG21	2:B:874:ALA:HB1	1.79	0.62
3:C:3180:CYS:CA	3:C:3366:ALA:HB1	2.26	0.62
11:K:37:LEU:HD13	14:N:36:LYS:NZ	2.12	0.62
2:B:1318:ILE:HG12	2:B:1345:LEU:HD13	1.79	0.62
3:C:343:MET:HG2	3:C:422:CYS:HB2	1.80	0.62
3:C:618:THR:HA	3:C:621:ILE:HG12	1.81	0.62
16:P:26:VAL:O	16:P:80:VAL:HA	1.99	0.62
1:A:264:TRP:HB3	1:A:296:ILE:HD12	1.81	0.62
2:B:797:PHE:CE1	2:B:829:VAL:HA	2.34	0.62
3:C:56:TYR:OH	3:C:74:GLN:NE2	2.32	0.62
3:C:177:ARG:NH2	3:C:258:GLU:HB2	2.14	0.62
2:B:1365:ILE:O	2:B:1369:VAL:HG23	2.00	0.62
2:B:3590:LEU:O	2:B:3594:LEU:N	2.31	0.62
3:C:3344:GLN:CA	3:C:3347:LYS:N	2.62	0.62
8:H:40:GLU:OE1	8:H:40:GLU:N	2.32	0.62
9:I:99:TYR:CD2	9:I:103:LEU:HB2	2.35	0.62
2:B:196:PHE:O	2:B:200:ILE:HG12	2.00	0.62
2:B:507:ILE:HD11	2:B:536:ILE:HG23	1.80	0.62
2:B:701:ILE:HA	2:B:704:LYS:HD2	1.80	0.62
3:C:28:VAL:HG22	3:C:69:LYS:HD3	1.81	0.62
3:C:85:LEU:HG	3:C:87:LYS:H	1.63	0.62
3:C:805:ARG:HG3	3:C:806:ILE:HG13	1.81	0.62
2:B:439:LEU:HB3	2:B:533:ARG:NH1	2.15	0.62
2:B:565:GLY:HA2	2:B:571:SER:H	1.63	0.62
2:B:1284:LEU:HD23	2:B:1287:LEU:HD12	1.81	0.62
2:B:3516:PRO:O	2:B:3519:LEU:N	2.32	0.62
12:L:82:PHE:HB3	13:M:60:ASN:O	1.99	0.62
2:B:30:LYS:HA	2:B:33:LEU:HD23	1.81	0.62
2:B:1138:LYS:HG2	2:B:1145:LYS:O	2.00	0.62
2:B:1340:ASP:CG	2:B:1343:LYS:HB3	2.21	0.62
3:C:244:ILE:HG23	3:C:247:ARG:HH21	1.64	0.62
3:C:317:LEU:HA	3:C:352:ILE:HG23	1.80	0.62
1:A:345:TRP:CD1	2:B:970:ALA:HB1	2.34	0.62
11:K:32:CYS:SG	11:K:33:ALA:N	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:74:GLN:HB3	15:O:107:TYR:HB2	1.82	0.62
17:T:166:LYS:HE3	17:T:168:ASN:HD21	1.65	0.62
2:B:833:GLY:HA2	2:B:836:ILE:HG12	1.81	0.61
1:A:96:LEU:HD23	1:A:113:ILE:HG22	1.81	0.61
2:B:875:ILE:HB	2:B:962:PHE:CZ	2.35	0.61
2:B:2189:GLY:O	2:B:2193:VAL:N	2.31	0.61
2:B:677:LEU:HD11	2:B:712:ILE:CD1	2.30	0.61
2:B:1079:ASN:OD1	2:B:1080:LEU:N	2.33	0.61
3:C:952:GLN:HG2	3:C:1006:ILE:HD13	1.81	0.61
3:C:3344:GLN:N	3:C:3347:LYS:N	2.45	0.61
1:A:144:GLN:HE21	1:A:171:ARG:HH11	1.48	0.61
2:B:503:LEU:O	2:B:507:ILE:HG13	2.01	0.61
2:B:665:GLU:HB3	2:B:726:LYS:HG3	1.82	0.61
3:C:243:LEU:HB3	3:C:322:LYS:HD2	1.82	0.61
17:T:104:ALA:O	17:T:177:ARG:HD3	2.00	0.61
1:A:334:ARG:HD3	1:A:351:ALA:HB1	1.82	0.61
2:B:123:SER:O	2:B:127:GLU:HB2	2.01	0.61
8:H:16:MET:HB3	8:H:20:MET:HB2	1.82	0.61
8:H:77:ILE:HG12	8:H:79:LEU:HD22	1.82	0.61
2:B:454:GLU:O	2:B:458:GLN:HB2	2.00	0.61
2:B:1148:SER:CB	2:B:1214:LEU:CG	2.76	0.61
2:B:1311:MET:O	2:B:1314:ALA:HB3	2.00	0.61
2:B:1340:ASP:O	2:B:1344:THR:OG1	2.14	0.61
3:C:398:TRP:CD1	3:C:496:LYS:HB2	2.36	0.61
3:C:596:LEU:HD11	3:C:598:ARG:HE	1.65	0.61
3:C:3354:ILE:CB	3:C:3358:ILE:CB	2.79	0.61
3:C:3355:GLN:O	3:C:3359:ALA:CB	2.49	0.61
7:G:81:SER:N	7:G:142:GLU:O	2.33	0.61
3:C:562:LYS:HA	3:C:565:LEU:HB2	1.81	0.61
7:G:138:ALA:HB3	7:G:145:LEU:HB2	1.82	0.61
2:B:315:GLU:O	2:B:319:PRO:HD2	2.00	0.61
2:B:531:LEU:HD13	2:B:609:LEU:HB3	1.83	0.61
3:C:511:ASP:O	3:C:515:VAL:HG23	2.01	0.61
16:P:60:ILE:HA	16:P:65:LEU:HD22	1.83	0.61
1:A:5:LEU:H	1:A:306:LEU:HD22	1.66	0.61
2:B:422:ARG:HG2	2:B:477:ILE:HG23	1.83	0.61
2:B:439:LEU:HD22	2:B:530:LEU:HA	1.82	0.61
3:C:535:ASN:HB3	3:C:568:ARG:HH12	1.66	0.61
11:K:37:LEU:HB2	14:N:36:LYS:HD2	1.81	0.61
2:B:115:ASN:HD21	3:C:98:ILE:HG23	1.66	0.60
2:B:2904:THR:O	2:B:2908:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:82:LEU:HG	16:P:89:VAL:HB	1.83	0.60
1:A:3487:VAL:O	1:A:3491:LYS:N	2.33	0.60
3:C:3344:GLN:O	3:C:3348:ILE:CB	2.50	0.60
6:F:88:ILE:O	6:F:98:LEU:HA	2.01	0.60
11:K:29:PRO:HG2	14:N:30:TYR:H	1.65	0.60
2:B:26:LYS:H	2:B:29:ILE:HD12	1.67	0.60
2:B:161:VAL:HG13	2:B:164:LEU:HD13	1.83	0.60
2:B:433:ILE:HA	2:B:463:PHE:CZ	2.36	0.60
2:B:435:GLN:HA	2:B:438:LYS:HE2	1.83	0.60
2:B:1149:ASP:N	2:B:1214:LEU:HD22	2.15	0.60
1:A:124:PRO:HB3	1:A:185:PHE:CE2	2.34	0.60
3:C:405:LEU:HD21	3:C:464:PHE:HB3	1.83	0.60
6:F:76:VAL:HG22	6:F:90:THR:HG23	1.84	0.60
12:L:22:ARG:NH1	12:L:97:ASP:OD2	2.33	0.60
12:L:33:LYS:HD3	12:L:60:PHE:CZ	2.36	0.60
1:A:192:PRO:HA	1:A:239:TRP:HE1	1.65	0.60
1:A:1616:ALA:O	1:A:1620:LEU:N	2.32	0.60
1:A:1915:ALA:O	1:A:1919:SER:N	2.33	0.60
2:B:165:LEU:O	2:B:169:LYS:N	2.27	0.60
2:B:555:LEU:HD21	2:B:602:PRO:HG2	1.83	0.60
2:B:1328:LYS:HG2	2:B:1332:GLN:HE21	1.65	0.60
3:C:1081:ILE:O	3:C:1085:LEU:HG	2.01	0.60
6:F:9:ASP:OD1	6:F:10:GLN:N	2.34	0.60
1:A:1348:TYR:O	1:A:1355:LYS:N	2.34	0.60
2:B:473:VAL:HG23	2:B:488:ASP:OD1	2.02	0.60
3:C:678:HIS:HD2	3:C:686:VAL:HA	1.65	0.60
3:C:678:HIS:CD2	3:C:686:VAL:HA	2.36	0.60
1:A:3214:GLU:O	1:A:3218:ASN:N	2.35	0.60
2:B:1196:ASN:O	2:B:1200:ILE:HG12	2.02	0.60
8:H:14:SER:HA	8:H:77:ILE:HA	1.83	0.60
9:I:67:LEU:HB3	9:I:75:TRP:CD1	2.37	0.60
12:L:37:GLN:HE22	12:L:41:LEU:HD12	1.65	0.60
1:A:341:TRP:NE1	1:A:343:ASN:O	2.34	0.60
3:C:143:ILE:HG21	3:C:162:VAL:HG21	1.83	0.60
2:B:1106:PHE:HD2	2:B:1171:LEU:HB2	1.65	0.60
2:B:3393:ARG:O	2:B:3396:GLU:N	2.34	0.60
17:T:45:LYS:O	17:T:49:LYS:HG2	2.00	0.60
2:B:433:ILE:HA	2:B:463:PHE:HZ	1.67	0.60
2:B:1126:LYS:HZ2	2:B:1134:LEU:HD22	1.67	0.60
3:C:24:LYS:HZ1	3:C:29:GLU:HB2	1.67	0.60
7:G:126:LEU:O	7:G:137:VAL:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:PHE:HD1	2:B:302:LEU:HD12	1.67	0.59
3:C:316:TYR:HB2	3:C:353:ALA:HB2	1.84	0.59
3:C:3353:ARG:O	3:C:3357:ALA:HB3	2.02	0.59
2:B:814:TYR:HB2	2:B:1075:TRP:NE1	2.07	0.59
3:C:3343:HIS:O	3:C:3345:LYS:N	2.34	0.59
2:B:429:LEU:O	2:B:433:ILE:HG13	2.01	0.59
2:B:1068:LYS:HD3	2:B:1069:THR:O	2.02	0.59
2:B:1240:PHE:HE1	2:B:1267:TYR:HB3	1.68	0.59
16:P:58:VAL:HG22	16:P:65:LEU:HD21	1.83	0.59
3:C:750:ASN:HB2	3:C:887:LYS:HD3	1.85	0.59
3:C:1039:SER:HB3	3:C:1103:ARG:NH2	2.18	0.59
14:N:108:ASP:OD1	14:N:130:TYR:N	2.28	0.59
1:A:200:ARG:HH22	1:A:228:ASN:ND2	2.01	0.59
1:A:288:VAL:HG12	1:A:290:ASP:H	1.66	0.59
1:A:3406:ARG:O	1:A:3688:ALA:N	2.33	0.59
2:B:359:VAL:HG21	2:B:419:PHE:HZ	1.68	0.59
2:B:1311:MET:SD	2:B:1356:ILE:HG13	2.43	0.59
3:C:321:GLU:HB2	3:C:345:ALA:HB1	1.82	0.59
3:C:3354:ILE:CA	3:C:3357:ALA:HB3	2.32	0.59
3:C:3194:ALA:HB1	3:C:3352:LYS:C	2.23	0.59
7:G:127:ARG:HG2	7:G:129:GLN:HE22	1.67	0.59
9:I:93:THR:HB	9:I:109:LYS:HB2	1.85	0.59
16:P:65:LEU:O	16:P:69:VAL:HG23	2.02	0.59
3:C:77:VAL:HG11	3:C:94:TRP:CZ2	2.38	0.59
3:C:812:THR:HA	3:C:815:LYS:HE3	1.85	0.59
3:C:970:TYR:CE1	3:C:977:LYS:HD2	2.38	0.59
3:C:3343:HIS:CA	3:C:3346:SER:CB	2.54	0.59
16:P:90:LYS:HD2	16:P:103:MET:HE3	1.84	0.59
3:C:577:ALA:HA	3:C:641:TYR:OH	2.03	0.59
3:C:755:HIS:CE1	3:C:794:LEU:HD13	2.37	0.59
1:A:144:GLN:HE21	1:A:171:ARG:NH1	2.01	0.59
1:A:320:PRO:HD2	1:A:341:TRP:O	2.03	0.59
1:A:3206:LYS:O	1:A:3210:ALA:N	2.33	0.59
2:B:203:TRP:HZ3	2:B:253:VAL:HG13	1.68	0.59
2:B:367:LEU:HD11	2:B:375:GLU:HB2	1.84	0.59
2:B:433:ILE:HG23	2:B:463:PHE:HE2	1.67	0.59
3:C:346:ILE:O	3:C:349:ILE:HG13	2.03	0.59
3:C:495:PHE:CE1	3:C:513:ASP:HB3	2.38	0.59
16:P:42:GLN:C	16:P:45:PRO:HD2	2.24	0.59
2:B:336:GLN:OE1	2:B:406:LYS:NZ	2.36	0.58
2:B:586:ALA:HB1	2:B:686:TYR:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1246:PHE:CG	2:B:1360:LYS:HB3	2.38	0.58
2:B:2657:LYS:O	2:B:2660:SER:N	2.36	0.58
3:C:1009:THR:HA	3:C:1012:LYS:HE2	1.85	0.58
3:C:3354:ILE:C	3:C:3358:ILE:CB	2.71	0.58
2:B:1660:ILE:O	2:B:1672:PHE:N	2.35	0.58
1:A:2628:GLN:O	1:A:2632:GLU:N	2.34	0.58
2:B:273:LYS:HB3	2:B:282:ARG:HH12	1.66	0.58
8:H:13:ASN:O	8:H:78:TYR:N	2.33	0.58
11:K:19:LYS:HG2	11:K:28:TRP:HB2	1.86	0.58
11:K:38:GLU:O	11:K:42:ARG:HG2	2.04	0.58
1:A:357:ILE:HG23	1:A:379:LYS:C	2.23	0.58
2:B:671:VAL:HG11	2:B:673:PHE:CE2	2.38	0.58
2:B:1218:GLU:O	2:B:1222:ILE:HG13	2.04	0.58
3:C:21:LEU:HD22	3:C:91:LYS:HG3	1.85	0.58
3:C:934:GLU:O	3:C:945:ASN:N	2.24	0.58
14:N:33:LYS:HD3	14:N:36:LYS:HG3	1.84	0.58
1:A:10:LEU:HG	1:A:65:ASN:HB3	1.86	0.58
1:A:38:GLY:O	1:A:53:PRO:HB3	2.04	0.58
1:A:2928:VAL:O	1:A:2932:SER:N	2.29	0.58
2:B:1175:ASN:O	2:B:1179:THR:HG23	2.03	0.58
7:G:71:LYS:HD3	7:G:72:THR:HG23	1.85	0.58
7:G:111:ARG:HA	7:G:114:VAL:HG12	1.84	0.58
7:G:136:MET:HB3	7:G:147:VAL:HG12	1.85	0.58
12:L:31:LEU:O	12:L:35:ILE:HG12	2.03	0.58
1:A:284:ASN:HA	2:B:935:ASN:HD21	1.68	0.58
1:A:3023:ARG:O	1:A:3027:LYS:N	2.37	0.58
2:B:1250:GLU:HA	2:B:1256:ASN:HB3	1.86	0.58
3:C:561:LEU:O	3:C:565:LEU:N	2.23	0.58
3:C:561:LEU:HG	3:C:565:LEU:HG	1.84	0.58
3:C:899:LEU:HD13	3:C:989:ILE:HD11	1.85	0.58
3:C:1095:GLN:O	3:C:1098:GLN:HG3	2.03	0.58
7:G:71:LYS:O	7:G:72:THR:OG1	2.21	0.58
1:A:3135:LEU:O	1:A:3139:VAL:N	2.35	0.58
2:B:64:VAL:O	2:B:74:TYR:HA	2.03	0.58
2:B:1224:ARG:O	2:B:1228:ILE:HG12	2.02	0.58
2:B:4547:VAL:O	2:B:4558:VAL:N	2.36	0.58
8:H:9:PRO:HG3	8:H:81:VAL:HG13	1.86	0.58
2:B:336:GLN:HG3	2:B:338:PRO:HG2	1.85	0.58
2:B:814:TYR:HB2	2:B:1075:TRP:CD1	2.36	0.58
2:B:1072:ASP:HB3	2:B:1077:ARG:HA	1.86	0.58
2:B:1215:GLN:HB3	2:B:1218:GLU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:933:VAL:HG21	3:C:944:LEU:HB3	1.86	0.58
3:C:2912:ASP:O	3:C:2918:LYS:N	2.37	0.58
6:F:34:LYS:HE3	6:F:36:HIS:CE1	2.39	0.58
8:H:16:MET:O	8:H:21:GLN:NE2	2.36	0.58
11:K:23:GLY:HA3	11:K:41:ILE:HG23	1.85	0.58
16:P:32:TRP:CH2	16:P:77:LEU:HG	2.38	0.58
1:A:225:GLN:HG3	1:A:282:ARG:HH11	1.69	0.58
2:B:429:LEU:HB2	2:B:470:PHE:CE2	2.39	0.58
2:B:2781:ASP:O	2:B:3047:TRP:N	2.37	0.58
3:C:1095:GLN:OE1	3:C:1098:GLN:NE2	2.37	0.58
3:C:3344:GLN:C	3:C:3345:LYS:O	2.23	0.58
2:B:55:GLN:HE21	2:B:57:ASN:HB3	1.68	0.57
2:B:503:LEU:HD11	2:B:533:ARG:HH21	1.68	0.57
2:B:1734:THR:O	2:B:1737:VAL:N	2.37	0.57
3:C:36:LYS:NZ	3:C:71:THR:O	2.29	0.57
3:C:3203:PRO:O	3:C:3204:ALA:HB2	2.04	0.57
1:A:1701:GLN:O	1:A:1705:ASN:N	2.35	0.57
2:B:134:GLN:HE21	3:C:79:PHE:HZ	1.51	0.57
3:C:210:GLU:HG3	3:C:280:ASN:HD21	1.69	0.57
3:C:580:LEU:HD22	3:C:641:TYR:CE1	2.39	0.57
1:A:51:ILE:HA	1:A:82:ARG:HG3	1.86	0.57
1:A:161:PHE:HD1	1:A:177:LEU:HB3	1.70	0.57
1:A:3615:CYS:O	1:A:3619:GLY:N	2.37	0.57
2:B:200:ILE:HG21	2:B:257:LEU:HD21	1.85	0.57
2:B:1354:LYS:HG2	2:B:1357:ARG:NH1	2.19	0.57
1:A:195:ASN:N	1:A:196:PRO:HD2	2.19	0.57
2:B:2376:SER:CB	3:C:1540:GLN:HA	2.34	0.57
3:C:104:ASP:OD2	3:C:107:LYS:HE3	2.05	0.57
16:P:47:LYS:HD3	16:P:55:ILE:HG12	1.86	0.57
2:B:422:ARG:NE	2:B:478:MET:HA	2.20	0.57
2:B:1315:ILE:HG23	2:B:1365:ILE:HG13	1.86	0.57
2:B:1325:TRP:HA	2:B:1328:LYS:HG3	1.86	0.57
12:L:96:PHE:CE2	12:L:105:ILE:HD11	2.39	0.57
16:P:11:THR:O	16:P:15:GLU:HG2	2.05	0.57
1:A:276:PHE:HE2	1:A:284:ASN:HB2	1.70	0.57
1:A:1400:ALA:O	1:A:1526:ILE:N	2.38	0.57
2:B:609:LEU:HD13	2:B:614:THR:HG23	1.86	0.57
2:B:810:SER:HB3	2:B:815:ASP:HA	1.87	0.57
2:B:1357:ARG:HG3	2:B:1358:ASN:OD1	2.05	0.57
2:B:653:GLN:HG3	2:B:655:LYS:H	1.69	0.57
2:B:1268:TYR:HB3	2:B:1305:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:529:GLN:HA	3:C:532:ILE:HD12	1.87	0.57
7:G:78:ILE:HG23	7:G:86:VAL:HB	1.87	0.57
11:K:41:ILE:O	11:K:45:GLN:NE2	2.37	0.57
1:A:99:GLY:HA3	1:A:149:HIS:HE1	1.69	0.57
1:A:225:GLN:HB2	1:A:251:TRP:CD1	2.40	0.57
2:B:956:LEU:O	2:B:960:ARG:HD3	2.05	0.57
3:C:1111:LEU:HB3	3:C:1183:LEU:HD21	1.87	0.57
3:C:1195:GLU:O	3:C:1199:LYS:HD3	2.04	0.57
3:C:3186:GLN:O	3:C:3359:ALA:CB	2.52	0.57
14:N:32:SER:O	14:N:36:LYS:HG2	2.05	0.57
1:A:69:TRP:O	1:A:70:ARG:NE	2.30	0.57
1:A:2417:PHE:N	1:A:2487:ALA:O	2.38	0.57
2:B:738:LYS:O	2:B:741:ILE:HG22	2.05	0.57
2:B:1107:ARG:NH1	2:B:1111:LYS:HB3	2.19	0.57
2:B:1117:ILE:HG22	2:B:1200:ILE:HG22	1.87	0.57
2:B:2818:LEU:N	2:B:2835:THR:O	2.38	0.57
3:C:972:TRP:HA	3:C:975:GLN:HE21	1.70	0.57
13:M:23:ILE:HG22	13:M:41:ILE:HG12	1.87	0.57
2:B:227:PRO:HD3	2:B:346:GLU:HB3	1.86	0.57
2:B:929:THR:HG22	2:B:930:ILE:H	1.68	0.57
3:C:1223:VAL:HG22	3:C:1259:LYS:HE2	1.87	0.57
9:I:38:ALA:O	9:I:42:ILE:HG13	2.04	0.57
1:A:203:HIS:HB3	1:A:219:GLY:HA3	1.87	0.56
2:B:1145:LYS:HZ1	2:B:1150:VAL:HG11	1.69	0.56
2:B:1225:ASP:HB3	2:B:1281:TYR:CZ	2.40	0.56
2:B:1250:GLU:OE2	2:B:1256:ASN:ND2	2.38	0.56
2:B:4191:GLY:O	2:B:4196:GLY:N	2.38	0.56
3:C:278:HIS:HD2	3:C:282:ARG:NH1	2.03	0.56
9:I:57:GLU:O	9:I:61:LYS:HG2	2.05	0.56
11:K:31:GLU:HA	14:N:32:SER:HB3	1.87	0.56
2:B:1276:GLY:O	2:B:1280:GLU:HG2	2.05	0.56
3:C:1116:LYS:O	3:C:1120:THR:HG23	2.05	0.56
1:A:232:TYR:HB2	1:A:239:TRP:CZ3	2.39	0.56
2:B:16:ASN:HB2	2:B:17:ARG:HH11	1.71	0.56
2:B:51:GLY:HA2	2:B:54:GLN:HE21	1.71	0.56
2:B:310:PHE:HA	2:B:313:LEU:HD12	1.86	0.56
2:B:425:ASP:OD1	2:B:426:ILE:HG13	2.04	0.56
2:B:1051:ASP:OD1	2:B:1174:HIS:NE2	2.38	0.56
3:C:1057:GLN:NE2	3:C:1061:GLU:OE2	2.36	0.56
11:K:45:GLN:O	11:K:49:LYS:HG2	2.04	0.56
1:A:62:LEU:HD13	1:A:327:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:707:THR:O	2:B:710:THR:OG1	2.18	0.56
2:B:988:ALA:O	2:B:992:THR:HG23	2.04	0.56
6:F:74:ILE:HD12	6:F:77:ILE:HD11	1.87	0.56
1:A:3492:LYS:O	1:A:3496:GLU:N	2.39	0.56
1:A:4135:GLY:O	1:A:4140:PHE:N	2.38	0.56
2:B:380:LEU:HD21	2:B:427:LEU:HA	1.86	0.56
2:B:839:LEU:O	2:B:842:GLU:HG2	2.06	0.56
2:B:3579:ILE:O	2:B:3625:MET:N	2.39	0.56
3:C:562:LYS:HA	3:C:565:LEU:HD12	1.88	0.56
12:L:74:TRP:CD2	12:L:109:LYS:HD3	2.41	0.56
13:M:76:LYS:HA	13:M:80:LEU:O	2.05	0.56
15:O:99:GLN:NE2	15:O:100:CYS:O	2.39	0.56
16:P:33:CYS:SG	16:P:38:ILE:HG23	2.45	0.56
1:A:255:GLY:HA3	1:A:268:ILE:HD11	1.87	0.56
1:A:341:TRP:HH2	2:B:967:GLN:HE22	1.53	0.56
2:B:658:GLN:HB3	2:B:667:ASP:HB3	1.86	0.56
2:B:918:GLY:HA2	2:B:921:SER:HB2	1.87	0.56
2:B:1325:TRP:HE1	2:B:1333:ILE:HG23	1.71	0.56
3:C:910:LYS:HB3	3:C:998:VAL:HG11	1.87	0.56
15:O:32:SER:HA	15:O:35:THR:OG1	2.05	0.56
2:B:133:MET:HB3	2:B:137:LEU:HD11	1.86	0.56
2:B:541:GLU:HA	2:B:616:ARG:HH12	1.71	0.56
3:C:874:HIS:HB3	3:C:884:LYS:HD2	1.87	0.56
3:C:1055:PHE:HE2	3:C:1093:LYS:HE3	1.70	0.56
14:N:80:LYS:O	14:N:128:GLY:HA2	2.05	0.56
16:P:43:PHE:HD1	16:P:100:LEU:HD21	1.69	0.56
2:B:110:VAL:HG12	3:C:122:GLU:HG2	1.86	0.56
2:B:928:ASN:OD1	2:B:932:ASN:ND2	2.39	0.56
2:B:1037:LEU:O	2:B:1041:ARG:HG2	2.06	0.56
2:B:1117:ILE:HG13	2:B:1197:PHE:CE2	2.41	0.56
2:B:1124:ILE:HG22	2:B:1207:VAL:HG12	1.88	0.56
3:C:78:LEU:HD12	3:C:131:LEU:HD12	1.88	0.56
15:O:45:LEU:HA	15:O:48:GLN:HE21	1.70	0.56
2:B:158:VAL:HA	2:B:161:VAL:HB	1.88	0.56
2:B:1047:LEU:HG	2:B:1047:LEU:O	2.06	0.56
3:C:3117:PHE:CB	3:C:3433:ALA:HB2	2.36	0.56
3:C:3355:GLN:O	3:C:3359:ALA:HB3	2.05	0.56
11:K:33:ALA:C	14:N:36:LYS:HD3	2.27	0.56
16:P:39:LEU:HG	16:P:95:ASN:HB2	1.87	0.56
2:B:176:LEU:HD22	2:B:243:LEU:HD21	1.87	0.56
2:B:544:HIS:CG	2:B:613:ILE:HG22	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1243:LYS:NZ	2:B:1264:ILE:HG23	2.21	0.56
3:C:807:GLU:N	3:C:807:GLU:OE2	2.39	0.56
8:H:22:LYS:NZ	8:H:23:GLU:OE2	2.38	0.56
16:P:36:CYS:CB	16:P:95:ASN:HD21	2.19	0.56
1:A:44:ASN:HB2	1:A:48:ASP:OD2	2.05	0.55
2:B:656:LEU:HD12	2:B:752:ILE:O	2.05	0.55
2:B:721:ASN:OD1	2:B:770:LYS:NZ	2.39	0.55
3:C:40:LEU:HD11	3:C:73:ALA:HB2	1.87	0.55
3:C:542:ILE:HD12	3:C:576:TYR:CD1	2.41	0.55
11:K:100:ILE:HG12	11:K:101:GLU:OE1	2.05	0.55
16:P:42:GLN:HG2	16:P:97:LYS:HG3	1.87	0.55
1:A:194:GLY:H	1:A:239:TRP:HD1	1.54	0.55
2:B:1172:LYS:HA	2:B:1176:VAL:HB	1.87	0.55
2:B:1240:PHE:HA	2:B:1243:LYS:HZ2	1.71	0.55
2:B:52:PHE:O	2:B:93:LYS:NZ	2.40	0.55
2:B:134:GLN:HB2	3:C:79:PHE:CZ	2.41	0.55
2:B:247:GLN:O	2:B:250:SER:OG	2.24	0.55
2:B:327:ILE:HD11	2:B:397:TYR:CE1	2.40	0.55
12:L:21:ILE:HA	12:L:96:PHE:HB3	1.88	0.55
12:L:33:LYS:HD3	12:L:60:PHE:HZ	1.70	0.55
1:A:170:GLN:HB2	2:B:861:ASP:HB3	1.88	0.55
1:A:272:SER:HA	1:A:287:PHE:HD1	1.72	0.55
1:A:1689:GLY:O	1:A:1693:THR:N	2.38	0.55
2:B:625:LEU:O	2:B:628:SER:OG	2.23	0.55
3:C:430:VAL:O	3:C:434:PRO:HD3	2.06	0.55
3:C:541:ASN:HB2	3:C:544:TYR:CD2	2.41	0.55
16:P:28:PHE:HB2	16:P:79:HIS:HB3	1.88	0.55
1:A:75:GLN:O	1:A:121:TRP:N	2.39	0.55
1:A:272:SER:HA	1:A:287:PHE:CD1	2.42	0.55
2:B:275:GLN:OE1	2:B:275:GLN:N	2.40	0.55
2:B:962:PHE:O	2:B:967:GLN:N	2.40	0.55
2:B:1099:THR:O	2:B:1103:VAL:HG23	2.07	0.55
12:L:84:CYS:HA	13:M:56:ILE:HG23	1.88	0.55
1:A:169:TYR:HB2	1:A:171:ARG:NE	2.22	0.55
2:B:67:GLN:H	2:B:85:LYS:NZ	2.02	0.55
2:B:326:LEU:HD22	2:B:330:LYS:HG3	1.89	0.55
2:B:1277:ARG:HH11	2:B:1277:ARG:HA	1.71	0.55
3:C:405:LEU:HD23	3:C:468:GLN:HE21	1.72	0.55
3:C:1032:GLN:HG3	3:C:1036:LYS:HG2	1.89	0.55
1:A:4080:ALA:HB1	1:A:4092:TYR:O	2.07	0.55
2:B:84:PHE:HZ	3:C:150:LYS:HD3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:ILE:HD13	2:B:394:TYR:OH	2.05	0.55
2:B:429:LEU:HD13	2:B:470:PHE:CG	2.42	0.55
2:B:1285:GLU:HG3	2:B:1290:LEU:CD1	2.36	0.55
3:C:135:MET:HG3	3:C:165:PHE:HE2	1.71	0.55
11:K:37:LEU:CD1	14:N:36:LYS:HZ3	2.18	0.55
13:M:17:ILE:O	13:M:21:LYS:HG2	2.06	0.55
1:A:199:PRO:O	1:A:221:SER:OG	2.16	0.55
1:A:2176:THR:O	1:A:2177:ILE:N	2.40	0.55
2:B:118:LEU:HD13	2:B:158:VAL:HG12	1.88	0.55
2:B:123:SER:HB3	3:C:96:LEU:HD21	1.88	0.55
2:B:269:THR:HB	2:B:270:PRO:HD3	1.89	0.55
2:B:589:LEU:HD21	2:B:640:LYS:HB2	1.89	0.55
2:B:615:GLU:HA	2:B:619:TYR:CD2	2.42	0.55
2:B:987:ARG:HA	2:B:990:PHE:CD2	2.41	0.55
2:B:1123:GLY:O	2:B:1138:LYS:NZ	2.40	0.55
3:C:624:PHE:HB3	3:C:634:ILE:CG2	2.37	0.55
12:L:81:ASN:HB3	13:M:60:ASN:HD21	1.72	0.55
16:P:8:ILE:HD11	16:P:14:PHE:HD1	1.72	0.55
2:B:1154:GLU:HB3	2:B:1155:PRO:HD3	1.87	0.55
3:C:536:PHE:HD1	3:C:545:SER:HG	1.54	0.55
3:C:1112:THR:OG1	3:C:1179:ALA:O	2.20	0.55
3:C:1211:GLU:HG3	3:C:1214:GLN:HE21	1.72	0.55
2:B:179:HIS:HB3	2:B:203:TRP:CE2	2.42	0.54
3:C:457:LEU:HD23	3:C:460:LEU:HD12	1.89	0.54
3:C:1253:GLU:HA	3:C:1256:TYR:CE1	2.42	0.54
7:G:125:PHE:HA	7:G:139:PRO:HD2	1.88	0.54
15:O:13:VAL:O	15:O:17:ILE:HG12	2.07	0.54
1:A:1727:ASN:O	1:A:1731:LYS:N	2.39	0.54
2:B:718:ILE:HD11	2:B:766:ILE:O	2.07	0.54
2:B:862:TYR:O	2:B:866:ILE:HG12	2.07	0.54
2:B:1109:THR:HG23	2:B:1164:MET:HG3	1.89	0.54
3:C:936:GLN:HB3	3:C:1080:ASN:ND2	2.23	0.54
12:L:39:ASP:O	12:L:43:LYS:HG2	2.08	0.54
1:A:99:GLY:HA3	1:A:149:HIS:CE1	2.42	0.54
1:A:2406:CYS:O	1:A:2410:GLU:N	2.38	0.54
2:B:190:LYS:O	2:B:194:HIS:HB2	2.07	0.54
2:B:1061:GLN:HA	2:B:1064:ILE:HD12	1.89	0.54
3:C:928:LYS:HD2	3:C:957:ARG:NH2	2.15	0.54
2:B:344:ILE:HD11	2:B:397:TYR:HE2	1.70	0.54
2:B:1317:LEU:HD22	16:P:32:TRP:CZ3	2.43	0.54
9:I:30:MET:HE1	9:I:75:TRP:HH2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:GLN:HB3	2:B:178:SER:OG	2.06	0.54
2:B:198:GLY:O	2:B:202:THR:HG23	2.06	0.54
2:B:836:ILE:HD13	2:B:839:LEU:HD21	1.90	0.54
2:B:939:ASN:OD1	2:B:940:ILE:N	2.40	0.54
2:B:1325:TRP:NE1	2:B:1333:ILE:HG23	2.22	0.54
2:B:1814:SER:O	2:B:1818:LEU:N	2.39	0.54
3:C:134:LEU:O	3:C:138:VAL:HG12	2.08	0.54
6:F:25:ILE:HD11	6:F:95:PHE:HB3	1.88	0.54
1:A:3438:HIS:O	1:A:3442:GLY:N	2.41	0.54
2:B:843:VAL:HG11	2:B:859:TYR:CE2	2.43	0.54
2:B:1240:PHE:CE2	2:B:1271:LEU:HD22	2.43	0.54
2:B:1317:LEU:CD1	16:P:77:LEU:H	2.20	0.54
3:C:349:ILE:HG23	3:C:357:ASN:HD21	1.73	0.54
3:C:970:TYR:HE1	3:C:977:LYS:HD2	1.73	0.54
1:A:2102:LEU:O	1:A:2106:GLY:N	2.40	0.54
2:B:137:LEU:HG	2:B:145:LEU:HB2	1.90	0.54
3:C:3378:ALA:O	3:C:3381:GLN:N	2.39	0.54
16:P:13:GLN:HA	16:P:16:ASP:OD1	2.08	0.54
17:T:179:CYS:HB3	17:T:192:TYR:CZ	2.42	0.54
1:A:194:GLY:N	1:A:239:TRP:HD1	2.06	0.54
1:A:219:GLY:O	1:A:226:TYR:N	2.41	0.54
2:B:335:ASN:HD21	2:B:340:LEU:HD13	1.73	0.54
2:B:1280:GLU:HA	2:B:1283:ASN:OD1	2.07	0.54
3:C:3187:ILE:CB	3:C:3360:GLU:CA	2.84	0.54
7:G:93:GLU:O	7:G:97:LYS:HG2	2.08	0.54
8:H:57:TRP:CE2	8:H:90:LYS:HD2	2.43	0.54
1:A:169:TYR:HB2	1:A:171:ARG:HE	1.73	0.54
1:A:2499:ARG:O	1:A:2503:PHE:N	2.40	0.54
2:B:118:LEU:HD12	2:B:162:TYR:HD1	1.72	0.54
2:B:527:PHE:HB3	2:B:530:LEU:HD13	1.90	0.54
2:B:1107:ARG:HG3	2:B:1111:LYS:CE	2.38	0.54
2:B:1245:PRO:C	2:B:1360:LYS:HB2	2.28	0.54
3:C:580:LEU:HD13	3:C:641:TYR:CD2	2.42	0.54
8:H:24:VAL:HA	8:H:49:PHE:HZ	1.73	0.54
15:O:9:ILE:HG23	15:O:12:GLU:HB3	1.90	0.54
2:B:164:LEU:O	2:B:168:ILE:HG12	2.08	0.54
2:B:1054:ILE:HD11	2:B:1098:TYR:HB2	1.90	0.54
3:C:123:ILE:HD11	3:C:134:LEU:HD12	1.90	0.54
3:C:325:GLU:HB3	3:C:338:THR:OG1	2.08	0.54
3:C:352:ILE:HB	3:C:357:ASN:HD22	1.72	0.54
3:C:715:ILE:HD11	18:V:222:UNK:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:716:ILE:O	3:C:720:GLU:HG2	2.07	0.54
3:C:1124:LYS:HB3	3:C:1125:PRO:HD3	1.90	0.54
3:C:3342:TYR:O	3:C:3346:SER:HA	2.06	0.54
2:B:1110:GLN:HA	2:B:1164:MET:SD	2.48	0.53
2:B:1264:ILE:HG22	2:B:1268:TYR:CE2	2.43	0.53
3:C:410:GLY:O	3:C:414:LYS:HG2	2.06	0.53
3:C:1037:LYS:HA	3:C:1040:LYS:HE2	1.90	0.53
3:C:1139:LEU:O	3:C:1143:ARG:HG3	2.08	0.53
1:A:18:PRO:HB2	1:A:338:PHE:CE2	2.43	0.53
2:B:240:ASN:O	2:B:243:LEU:HG	2.07	0.53
2:B:449:GLY:HA2	2:B:452:LEU:HG	1.89	0.53
2:B:730:LEU:HG	2:B:731:PRO:HD3	1.89	0.53
2:B:812:ASP:HB2	2:B:900:PHE:CE2	2.42	0.53
2:B:904:LEU:HG	2:B:913:PHE:CE1	2.43	0.53
2:B:936:ASP:HA	2:B:939:ASN:ND2	2.23	0.53
2:B:1229:PHE:HE2	2:B:1277:ARG:HG3	1.72	0.53
2:B:1314:ALA:HB2	16:P:75:SER:C	2.29	0.53
3:C:1184:ARG:HA	3:C:1187:TRP:HD1	1.72	0.53
3:C:2324:GLY:O	3:C:2327:LEU:N	2.41	0.53
12:L:52:ASP:OD1	12:L:56:ASN:ND2	2.41	0.53
15:O:38:TYR:HD1	15:O:106:ILE:HG22	1.73	0.53
17:T:131:PHE:CD1	17:T:172:PHE:HE2	2.25	0.53
1:A:3048:SER:O	1:A:3052:GLY:N	2.41	0.53
1:A:4006:GLU:O	1:A:4011:LEU:N	2.41	0.53
2:B:133:MET:HG3	2:B:148:LYS:HG3	1.90	0.53
2:B:671:VAL:HG11	2:B:673:PHE:CZ	2.43	0.53
2:B:1057:LEU:HD13	2:B:1094:TRP:HB3	1.90	0.53
2:B:1212:ILE:HG22	2:B:1213:PRO:HG2	1.73	0.53
3:C:17:ILE:O	3:C:20:SER:OG	2.26	0.53
3:C:674:LEU:HB2	18:V:232:UNK:CB	2.38	0.53
3:C:982:LYS:HG3	3:C:984:THR:HG22	1.91	0.53
14:N:34:ILE:HD12	14:N:71:ILE:HG13	1.90	0.53
16:P:16:ASP:OD2	16:P:17:ILE:N	2.41	0.53
17:T:107:LYS:HB2	17:T:177:ARG:HG2	1.90	0.53
2:B:16:ASN:HB2	2:B:17:ARG:NH1	2.24	0.53
2:B:84:PHE:CZ	3:C:150:LYS:HD3	2.44	0.53
2:B:197:GLU:O	2:B:201:ILE:HG12	2.08	0.53
2:B:653:GLN:HG2	2:B:671:VAL:HA	1.90	0.53
2:B:1366:VAL:HA	2:B:1369:VAL:HB	1.89	0.53
3:C:478:LEU:HD23	3:C:484:LEU:HB2	1.88	0.53
17:T:152:ILE:O	17:T:156:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LEU:HD23	1:A:304:ILE:O	2.09	0.53
1:A:316:CYS:HB3	1:A:350:TRP:CD2	2.44	0.53
1:A:3733:SER:O	1:A:3737:GLY:N	2.41	0.53
3:C:135:MET:HG2	3:C:139:TYR:HD2	1.73	0.53
3:C:1235:PRO:HB3	3:C:1249:LEU:HD11	1.90	0.53
9:I:64:LYS:HE2	9:I:75:TRP:O	2.09	0.53
11:K:42:ARG:NH2	11:K:67:TYR:OH	2.42	0.53
11:K:95:PHE:CZ	11:K:106:LEU:HD11	2.43	0.53
1:A:60:LEU:HD13	1:A:69:TRP:CE2	2.44	0.53
2:B:203:TRP:CZ3	2:B:253:VAL:HG13	2.43	0.53
2:B:893:ARG:NH1	2:B:895:ASP:O	2.40	0.53
2:B:1325:TRP:HA	2:B:1328:LYS:CG	2.37	0.53
3:C:44:PHE:HE1	3:C:51:ASN:C	2.12	0.53
3:C:596:LEU:HD21	3:C:598:ARG:HD2	1.90	0.53
3:C:1140:GLU:HA	3:C:1143:ARG:HD2	1.91	0.53
6:F:61:LYS:HB2	8:H:36:ASN:ND2	2.24	0.53
8:H:71:PHE:O	8:H:73:ARG:NH2	2.41	0.53
11:K:44:THR:O	11:K:48:LEU:HG	2.09	0.53
14:N:33:LYS:O	14:N:36:LYS:HB2	2.08	0.53
15:O:14:GLN:HB2	15:O:97:LEU:HD11	1.91	0.53
16:P:25:LEU:HB2	16:P:55:ILE:HD13	1.89	0.53
2:B:915:PRO:HA	2:B:927:ARG:HH21	1.74	0.53
2:B:1260:ALA:O	2:B:1264:ILE:HG13	2.08	0.53
3:C:547:LYS:O	3:C:551:LYS:HG2	2.09	0.53
3:C:750:ASN:HD21	3:C:886:ILE:HG22	1.74	0.53
3:C:945:ASN:HB3	3:C:946:PRO:HD3	1.91	0.53
8:H:16:MET:SD	8:H:76:TYR:N	2.82	0.53
13:M:71:LYS:O	13:M:85:TRP:HA	2.07	0.53
2:B:105:ALA:HA	2:B:108:VAL:HG22	1.91	0.53
2:B:537:ALA:HA	2:B:540:LEU:HB2	1.91	0.53
2:B:1350:LYS:HE2	2:B:1370:LYS:HE3	1.91	0.53
3:C:1091:GLU:O	3:C:1094:LEU:HG	2.08	0.53
12:L:67:PHE:HB3	12:L:74:TRP:HZ2	1.74	0.53
16:P:80:VAL:HG12	16:P:103:MET:SD	2.48	0.53
1:A:266:TYR:O	1:A:293:VAL:HA	2.09	0.53
2:B:814:TYR:N	2:B:1075:TRP:CZ2	2.57	0.53
2:B:1285:GLU:HG3	2:B:1290:LEU:HB2	1.90	0.53
3:C:98:ILE:HG13	3:C:116:ASN:O	2.09	0.53
6:F:44:LYS:HE3	6:F:48:ILE:HD11	1.91	0.53
14:N:29:PHE:HD1	14:N:76:VAL:HG11	1.74	0.53
16:P:65:LEU:HG	16:P:68:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:O	1:A:268:ILE:HA	2.08	0.53
2:B:436:PHE:O	2:B:533:ARG:NH1	2.42	0.53
2:B:470:PHE:CZ	2:B:488:ASP:HB3	2.43	0.53
2:B:1170:LYS:O	2:B:1173:LYS:HE2	2.09	0.53
3:C:127:THR:HB	3:C:130:MET:HB3	1.90	0.53
3:C:3378:ALA:O	3:C:3379:GLN:C	2.48	0.53
11:K:24:ALA:HB2	11:K:100:ILE:HD12	1.91	0.53
1:A:283:THR:HA	2:B:955:PHE:CZ	2.44	0.52
2:B:1090:ARG:HA	2:B:1093:ARG:HE	1.74	0.52
2:B:1271:LEU:HD12	2:B:1274:ILE:HG21	1.91	0.52
11:K:28:TRP:CE2	14:N:33:LYS:HE3	2.43	0.52
1:A:345:TRP:CZ2	2:B:967:GLN:HG2	2.45	0.52
1:A:3764:LEU:O	1:A:3768:LEU:N	2.38	0.52
1:A:3991:SER:O	1:A:3995:ALA:HB3	2.10	0.52
3:C:269:LYS:HE3	3:C:284:ARG:HD3	1.92	0.52
3:C:1055:PHE:CE2	3:C:1093:LYS:HE3	2.45	0.52
1:A:143:PRO:HD3	1:A:187:TRP:CD1	2.44	0.52
2:B:60:ASN:ND2	3:C:137:SER:O	2.42	0.52
2:B:67:GLN:HA	2:B:71:CYS:O	2.10	0.52
2:B:1356:ILE:HA	2:B:1359:PHE:HD2	1.75	0.52
3:C:48:GLU:HG3	3:C:100:ASN:O	2.08	0.52
3:C:478:LEU:HB3	3:C:484:LEU:HD22	1.90	0.52
3:C:944:LEU:HD11	3:C:1071:ILE:HD11	1.92	0.52
6:F:86:GLU:O	6:F:100:ILE:HA	2.10	0.52
7:G:79:VAL:HG11	7:G:100:ALA:HB1	1.91	0.52
12:L:28:GLN:O	12:L:32:LYS:HG2	2.09	0.52
2:B:88:GLY:O	2:B:89:ILE:HD13	2.10	0.52
2:B:545:ILE:O	2:B:549:GLU:HG2	2.09	0.52
2:B:1151:LYS:HG3	2:B:1208:LYS:HE3	1.90	0.52
2:B:1315:ILE:CG1	2:B:1362:TYR:HD1	2.22	0.52
2:B:1982:THR:O	2:B:1994:LEU:N	2.42	0.52
2:B:2372:ARG:CB	3:C:1543:GLY:HA2	2.39	0.52
2:B:3874:ILE:O	2:B:3878:ILE:N	2.40	0.52
3:C:696:ILE:O	3:C:700:LYS:HD3	2.10	0.52
11:K:29:PRO:HD2	14:N:30:TYR:HD2	1.75	0.52
11:K:30:PRO:HG3	14:N:36:LYS:NZ	2.24	0.52
1:A:10:LEU:HD22	1:A:349:LEU:HD22	1.91	0.52
1:A:22:SER:HB3	1:A:340:GLY:CA	2.39	0.52
2:B:656:LEU:O	2:B:756:ARG:NH2	2.42	0.52
2:B:813:ASP:CG	2:B:1075:TRP:HE1	2.12	0.52
2:B:885:GLN:HA	2:B:894:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1130:ASP:OD1	2:B:1135:HIS:NE2	2.39	0.52
3:C:269:LYS:CD	3:C:281:GLN:HA	2.38	0.52
3:C:470:PHE:CZ	3:C:524:LEU:HD13	2.45	0.52
3:C:548:LEU:HD12	3:C:551:LYS:HG3	1.91	0.52
3:C:853:VAL:HG23	3:C:854:GLU:H	1.74	0.52
3:C:1099:ASP:O	3:C:1103:ARG:HG2	2.10	0.52
6:F:83:HIS:N	6:F:103:CYS:SG	2.83	0.52
2:B:596:ARG:HB3	2:B:633:ILE:HG21	1.91	0.52
2:B:1052:GLU:O	2:B:1056:HIS:ND1	2.43	0.52
3:C:200:LEU:HB3	3:C:275:HIS:NE2	2.24	0.52
3:C:969:LEU:HB2	3:C:974:GLN:HE22	1.75	0.52
11:K:47:ALA:HA	11:K:50:LYS:HE2	1.91	0.52
16:P:28:PHE:HA	16:P:58:VAL:O	2.10	0.52
17:T:186:LEU:HA	17:T:189:ARG:HG2	1.90	0.52
1:A:322:GLU:OE2	1:A:341:TRP:N	2.42	0.52
2:B:418:SER:O	2:B:422:ARG:HG3	2.10	0.52
2:B:1256:ASN:OD1	2:B:1257:ILE:N	2.43	0.52
3:C:624:PHE:HE2	3:C:641:TYR:CD2	2.27	0.52
6:F:34:LYS:HG2	6:F:35:ARG:H	1.74	0.52
11:K:35:ASP:OD2	14:N:39:LYS:HE2	2.10	0.52
2:B:319:PRO:HA	2:B:322:HIS:HB2	1.91	0.52
2:B:523:LEU:O	2:B:526:ASN:HB2	2.10	0.52
3:C:542:ILE:HD11	3:C:579:GLU:OE1	2.10	0.52
3:C:566:THR:HA	3:C:569:TYR:CD2	2.45	0.52
16:P:39:LEU:HD11	16:P:96:GLN:N	2.25	0.52
1:A:7:TRP:CZ3	1:A:350:TRP:HB3	2.45	0.52
1:A:220:TRP:HE1	2:B:956:LEU:CD1	2.16	0.52
1:A:1327:ARG:O	1:A:1330:ASN:N	2.42	0.52
2:B:28:LYS:HD3	2:B:73:PHE:HD1	1.75	0.52
2:B:1291:GLN:OE1	2:B:1291:GLN:N	2.38	0.52
2:B:3985:PHE:N	2:B:4076:LEU:O	2.42	0.52
2:B:4390:SER:O	2:B:4394:SER:N	2.43	0.52
3:C:1133:GLY:HA3	3:C:1268:ARG:HD3	1.92	0.52
9:I:99:TYR:HB2	9:I:103:LEU:H	1.75	0.52
13:M:67:HIS:HB3	13:M:85:TRP:HB2	1.91	0.52
16:P:24:VAL:HA	16:P:54:THR:O	2.09	0.52
1:A:60:LEU:HD13	1:A:69:TRP:CD2	2.45	0.52
1:A:3615:CYS:O	1:A:3620:HIS:N	2.43	0.52
2:B:525:ASP:O	2:B:528:GLU:HG3	2.10	0.52
2:B:737:VAL:HG12	2:B:740:LYS:HD2	1.92	0.52
2:B:789:LYS:HE2	2:B:839:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:THR:HB	3:C:334:GLN:HG3	1.92	0.52
6:F:78:ARG:HB2	6:F:88:ILE:HG22	1.91	0.52
7:G:65:ASN:O	7:G:69:THR:HG23	2.10	0.52
9:I:30:MET:HE1	9:I:75:TRP:CH2	2.45	0.52
2:B:260:LEU:HD13	2:B:268:THR:HG21	1.91	0.51
2:B:503:LEU:O	2:B:506:VAL:HG12	2.10	0.51
2:B:1318:ILE:HG22	2:B:1322:TYR:CE2	2.45	0.51
3:C:785:HIS:C	3:C:789:LYS:HZ2	2.14	0.51
13:M:74:PHE:HD2	13:M:83:LEU:HB2	1.74	0.51
16:P:6:ILE:HB	16:P:56:VAL:HG22	1.92	0.51
17:T:103:SER:O	17:T:107:LYS:HG3	2.10	0.51
1:A:162:GLY:HA2	1:A:174:PHE:O	2.10	0.51
1:A:344:ASN:ND2	2:B:969:LEU:HB3	2.23	0.51
2:B:544:HIS:O	2:B:548:LEU:HD13	2.10	0.51
2:B:1148:SER:CB	2:B:1214:LEU:HD22	2.33	0.51
3:C:81:THR:HA	3:C:126:ASN:HA	1.91	0.51
3:C:1076:LEU:HD23	3:C:1076:LEU:H	1.74	0.51
3:C:1164:ASP:HA	3:C:1167:LEU:O	2.10	0.51
3:C:3342:TYR:O	3:C:3345:LYS:C	2.48	0.51
6:F:87:TYR:OH	6:F:98:LEU:HD13	2.11	0.51
2:B:671:VAL:HG12	2:B:673:PHE:H	1.75	0.51
2:B:709:ARG:O	2:B:713:VAL:HG23	2.10	0.51
2:B:862:TYR:O	2:B:865:VAL:HG12	2.10	0.51
3:C:488:PHE:HA	3:C:491:ILE:HD12	1.91	0.51
3:C:3378:ALA:C	3:C:3380:ILE:N	2.63	0.51
8:H:63:ARG:HH21	8:H:85:ALA:N	2.09	0.51
16:P:15:GLU:O	16:P:19:GLU:HG2	2.11	0.51
1:A:329:ASP:H	1:A:334:ARG:NH1	2.08	0.51
1:A:1302:ASP:O	1:A:1304:SER:N	2.44	0.51
1:A:3409:PHE:O	1:A:3413:LYS:N	2.43	0.51
3:C:9:ARG:NH2	3:C:117:ASP:OD2	2.40	0.51
3:C:234:GLU:O	3:C:368:LYS:NZ	2.43	0.51
14:N:81:ILE:HG23	14:N:126:VAL:HG13	1.91	0.51
2:B:1145:LYS:HE2	2:B:1150:VAL:HG21	1.93	0.51
2:B:1271:LEU:O	2:B:1274:ILE:HB	2.11	0.51
3:C:203:SER:O	3:C:207:GLN:HG2	2.11	0.51
3:C:582:THR:O	3:C:585:ARG:HG3	2.11	0.51
3:C:789:LYS:O	3:C:793:GLN:HG2	2.11	0.51
3:C:2397:GLY:O	3:C:2633:ASN:N	2.43	0.51
15:O:20:SER:HA	15:O:53:TYR:HE2	1.75	0.51
3:C:53:ILE:HB	3:C:95:PHE:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:752:LEU:HD13	3:C:795:ILE:HG12	1.93	0.51
3:C:1120:THR:O	3:C:1124:LYS:HB2	2.11	0.51
6:F:73:ASP:OD1	6:F:74:ILE:N	2.43	0.51
15:O:94:ASP:OD1	15:O:116:ALA:N	2.43	0.51
2:B:91:VAL:HA	2:B:109:VAL:O	2.10	0.51
2:B:173:MET:HE1	2:B:218:LEU:HA	1.93	0.51
2:B:1459:THR:N	2:B:1466:THR:O	2.43	0.51
3:C:12:TRP:O	3:C:16:THR:HG23	2.10	0.51
1:A:209:ALA:HB3	1:A:264:TRP:CD1	2.46	0.51
2:B:1250:GLU:HG3	2:B:1256:ASN:HD22	1.74	0.51
3:C:902:THR:O	3:C:905:SER:OG	2.27	0.51
3:C:3180:CYS:CB	3:C:3366:ALA:C	2.79	0.51
7:G:80:ASN:HA	7:G:143:PHE:HA	1.92	0.51
17:T:186:LEU:H	17:T:189:ARG:HH11	1.58	0.51
1:A:2891:ARG:O	1:A:2895:LEU:N	2.44	0.51
1:A:3850:PRO:O	1:A:3855:MET:N	2.43	0.51
2:B:563:LEU:HB2	2:B:564:GLU:OE1	2.09	0.51
2:B:653:GLN:HE21	2:B:655:LYS:H	1.57	0.51
2:B:927:ARG:NH1	2:B:929:THR:OG1	2.44	0.51
3:C:420:LYS:HB3	3:C:421:LYS:HZ2	1.75	0.51
16:P:28:PHE:CD2	16:P:74:VAL:HG11	2.45	0.51
3:C:78:LEU:HD23	3:C:78:LEU:O	2.11	0.51
3:C:336:ILE:O	3:C:339:LEU:N	2.44	0.51
3:C:374:ILE:HD11	3:C:453:PHE:CE2	2.46	0.51
3:C:596:LEU:HG	3:C:598:ARG:HG2	1.92	0.51
11:K:37:LEU:HB2	14:N:36:LYS:CD	2.41	0.51
14:N:37:ILE:HG23	14:N:70:LYS:HZ3	1.76	0.51
16:P:63:GLU:HA	16:P:66:GLU:CD	2.30	0.51
2:B:155:ASN:OD1	2:B:180:LYS:NZ	2.44	0.50
2:B:720:ASP:HB3	2:B:724:HIS:CE1	2.45	0.50
2:B:876:GLN:HG3	2:B:966:LYS:HD2	1.93	0.50
3:C:193:ASP:OD1	3:C:267:ILE:HG21	2.10	0.50
3:C:807:GLU:O	3:C:811:LYS:NZ	2.35	0.50
3:C:892:TRP:O	3:C:896:GLN:HG2	2.11	0.50
11:K:94:ARG:O	11:K:108:TYR:HA	2.11	0.50
2:B:1240:PHE:HD1	2:B:1243:LYS:NZ	2.08	0.50
2:B:1361:GLY:O	2:B:1364:VAL:HG12	2.12	0.50
3:C:263:LYS:HG3	3:C:264:ASP:N	2.26	0.50
3:C:576:TYR:CD1	3:C:624:PHE:HE1	2.29	0.50
3:C:790:LYS:O	3:C:793:GLN:HB2	2.11	0.50
6:F:85:TYR:HE2	6:F:87:TYR:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ASP:N	8:H:76:TYR:O	2.36	0.50
16:P:9:THR:HA	16:P:65:LEU:HD12	1.94	0.50
1:A:190:LEU:HD13	1:A:232:TYR:CZ	2.47	0.50
2:B:110:VAL:H	3:C:122:GLU:HG2	1.75	0.50
2:B:301:LYS:HA	2:B:316:LEU:HD23	1.93	0.50
2:B:449:GLY:HA2	2:B:452:LEU:CG	2.41	0.50
2:B:859:TYR:CE2	2:B:863:VAL:HG21	2.47	0.50
3:C:1109:ASP:O	3:C:1113:GLU:HG2	2.11	0.50
6:F:97:MET:N	6:F:97:MET:SD	2.84	0.50
1:A:4036:THR:O	1:A:4040:GLN:N	2.45	0.50
3:C:260:LEU:HD22	3:C:307:LEU:HD22	1.93	0.50
3:C:1107:LEU:HB3	3:C:1156:VAL:HG21	1.93	0.50
7:G:72:THR:HB	7:G:150:THR:OG1	2.12	0.50
16:P:17:ILE:HD13	16:P:20:LYS:HE3	1.93	0.50
2:B:135:ASN:HB3	3:C:82:THR:HG21	1.93	0.50
2:B:797:PHE:HE1	2:B:829:VAL:HA	1.77	0.50
2:B:1311:MET:C	2:B:1362:TYR:HE1	2.14	0.50
9:I:43:GLN:NE2	9:I:47:GLU:OE2	2.33	0.50
12:L:28:GLN:HE22	12:L:31:LEU:HD23	1.75	0.50
15:O:101:TYR:HB3	15:O:108:ALA:HB3	1.93	0.50
17:T:41:SER:O	17:T:45:LYS:HG2	2.11	0.50
1:A:18:PRO:HB2	1:A:338:PHE:HE2	1.77	0.50
1:A:192:PRO:CA	1:A:239:TRP:HE1	2.25	0.50
1:A:334:ARG:CB	1:A:353:ASN:HA	2.42	0.50
2:B:462:GLU:HG2	2:B:499:LEU:HD21	1.92	0.50
2:B:533:ARG:HB3	2:B:535:ILE:HG12	1.94	0.50
2:B:877:THR:HG22	2:B:881:HIS:CE1	2.47	0.50
3:C:177:ARG:NE	3:C:259:GLN:HA	2.25	0.50
3:C:1026:LEU:HD12	3:C:1027:CYS:N	2.25	0.50
3:C:1228:ARG:HA	3:C:1228:ARG:NE	2.27	0.50
1:A:213:GLN:HB2	1:A:232:TYR:O	2.12	0.50
1:A:3840:TYR:O	1:A:3844:LYS:N	2.45	0.50
2:B:1114:LEU:O	2:B:1118:GLU:HG2	2.12	0.50
2:B:1328:LYS:HG2	2:B:1332:GLN:HG2	1.93	0.50
3:C:44:PHE:HB2	3:C:53:ILE:HD11	1.92	0.50
3:C:91:LYS:HD3	3:C:125:PRO:HD3	1.93	0.50
3:C:250:MET:HA	3:C:314:VAL:HG11	1.93	0.50
3:C:499:GLY:HA2	3:C:509:LYS:HG3	1.93	0.50
3:C:1211:GLU:HG3	3:C:1214:GLN:NE2	2.27	0.50
6:F:25:ILE:HD13	6:F:97:MET:HG3	1.93	0.50
9:I:33:ASP:N	9:I:33:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:27:ILE:HG21	15:O:32:SER:OG	2.10	0.50
1:A:310:GLU:HG3	1:A:311:THR:H	1.76	0.50
1:A:3552:ILE:O	1:A:3556:PHE:N	2.43	0.50
2:B:387:CYS:O	2:B:391:LYS:HD2	2.10	0.50
3:C:44:PHE:CZ	3:C:97:ARG:HB3	2.46	0.50
3:C:1235:PRO:HD3	3:C:1252:PHE:CE2	2.47	0.50
2:B:45:ASN:HD21	2:B:48:GLU:CD	2.15	0.50
2:B:119:GLU:O	2:B:122:ASN:HB3	2.12	0.50
2:B:332:LYS:HB3	2:B:405:TRP:CD1	2.46	0.50
2:B:454:GLU:O	2:B:458:GLN:HB3	2.10	0.50
2:B:1138:LYS:HE3	2:B:1145:LYS:HD3	1.93	0.50
2:B:1222:ILE:HG12	2:B:1284:LEU:HD13	1.93	0.50
2:B:1252:MET:HB3	2:B:1255:GLU:OE1	2.11	0.50
3:C:27:ILE:HG12	3:C:68:ILE:HA	1.93	0.50
3:C:370:THR:HG21	3:C:450:PHE:HB2	1.94	0.50
3:C:971:ASN:H	3:C:974:GLN:HE21	1.60	0.50
3:C:1184:ARG:HA	3:C:1187:TRP:CD1	2.47	0.50
6:F:77:ILE:O	6:F:89:ILE:HB	2.11	0.50
11:K:37:LEU:HD22	14:N:33:LYS:HZ2	1.76	0.50
14:N:39:LYS:HA	14:N:113:TYR:CE2	2.47	0.50
2:B:26:LYS:HD3	2:B:74:TYR:HE1	1.77	0.49
2:B:309:ASP:HA	2:B:358:PHE:CE2	2.47	0.49
2:B:1040:CYS:O	2:B:1045:PRO:HD3	2.11	0.49
2:B:1317:LEU:HD13	16:P:77:LEU:H	1.76	0.49
3:C:254:THR:O	3:C:258:GLU:HG3	2.12	0.49
3:C:278:HIS:HB2	3:C:282:ARG:HD3	1.94	0.49
3:C:532:ILE:HG21	3:C:564:ASN:HB3	1.94	0.49
3:C:633:GLU:HA	3:C:636:ARG:HH11	1.77	0.49
3:C:1035:ILE:HG21	3:C:1095:GLN:HG2	1.94	0.49
12:L:16:LEU:HD22	12:L:17:PRO:HD2	1.93	0.49
1:A:144:GLN:NE2	1:A:145:PRO:O	2.46	0.49
1:A:276:PHE:HB2	1:A:282:ARG:CG	2.41	0.49
2:B:187:THR:HB	2:B:188:PRO:HD3	1.95	0.49
2:B:876:GLN:CD	2:B:966:LYS:HB3	2.31	0.49
2:B:1148:SER:HG	2:B:1213:PRO:C	1.93	0.49
2:B:1261:TYR:O	2:B:1265:MET:N	2.44	0.49
3:C:45:LEU:O	3:C:106:LYS:NZ	2.45	0.49
6:F:87:TYR:HA	6:F:99:ALA:O	2.12	0.49
1:A:221:SER:HB2	1:A:226:TYR:CE1	2.40	0.49
1:A:2827:ILE:O	1:A:2831:GLU:N	2.45	0.49
1:A:3217:ILE:O	1:A:3221:SER:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4001:ASN:O	1:A:4005:GLN:N	2.39	0.49
1:A:4085:GLY:O	1:A:4088:GLY:N	2.46	0.49
2:B:137:LEU:HB3	2:B:142:TRP:CD1	2.37	0.49
2:B:606:LEU:HD13	2:B:612:GLY:HA2	1.94	0.49
2:B:663:LYS:HD3	2:B:666:ASN:HB3	1.94	0.49
2:B:688:LEU:HD12	2:B:691:ARG:HH22	1.77	0.49
3:C:89:GLN:HE22	3:C:91:LYS:NZ	2.09	0.49
3:C:443:ASP:OD2	3:C:443:ASP:N	2.45	0.49
3:C:3332:ILE:O	3:C:3333:LEU:C	2.49	0.49
8:H:73:ARG:HH11	8:H:73:ARG:HG2	1.76	0.49
1:A:53:PRO:O	1:A:82:ARG:HB3	2.12	0.49
1:A:4155:LYS:O	1:A:4159:SER:N	2.45	0.49
2:B:127:GLU:OE1	2:B:127:GLU:N	2.45	0.49
2:B:132:VAL:HG22	3:C:75:ASP:O	2.12	0.49
2:B:892:LYS:HG2	2:B:893:ARG:H	1.78	0.49
2:B:1324:ASP:O	2:B:1328:LYS:HG3	2.12	0.49
3:C:591:LYS:HE3	3:C:596:LEU:HD22	1.95	0.49
3:C:715:ILE:HG12	18:V:221:UNK:O	2.13	0.49
3:C:896:GLN:O	3:C:900:ASN:ND2	2.39	0.49
3:C:1101:HIS:O	3:C:1105:ARG:HG2	2.12	0.49
11:K:30:PRO:HG3	14:N:36:LYS:HZ2	1.77	0.49
1:A:48:ASP:HA	1:A:51:ILE:HG12	1.94	0.49
1:A:2324:ASN:HA	1:A:2327:ASN:O	2.13	0.49
2:B:96:LEU:HD23	2:B:99:LEU:HD23	1.94	0.49
2:B:337:PRO:HD3	2:B:404:ASN:HB2	1.93	0.49
2:B:351:ILE:HG21	2:B:416:LEU:HD22	1.95	0.49
2:B:876:GLN:CG	2:B:966:LYS:HD2	2.42	0.49
2:B:1034:ASN:O	2:B:1038:LYS:HG2	2.13	0.49
3:C:21:LEU:HD21	3:C:57:TYR:CD1	2.48	0.49
3:C:46:SER:HA	3:C:106:LYS:NZ	2.28	0.49
3:C:805:ARG:O	3:C:809:ASN:ND2	2.46	0.49
3:C:1054:LYS:O	3:C:1058:ILE:HG12	2.12	0.49
3:C:1143:ARG:O	3:C:1146:GLN:HB2	2.13	0.49
3:C:1146:GLN:HA	3:C:1149:ILE:HD12	1.94	0.49
8:H:49:PHE:HA	8:H:52:ARG:HG2	1.93	0.49
8:H:60:ILE:HG21	8:H:65:PHE:CE2	2.47	0.49
17:T:163:LEU:HD22	17:T:166:LYS:HB2	1.94	0.49
2:B:211:LEU:HD12	2:B:277:GLU:HB3	1.94	0.49
2:B:436:PHE:HA	2:B:533:ARG:NH1	2.28	0.49
2:B:524:LEU:HB3	2:B:611:GLN:HG3	1.93	0.49
2:B:1152:ASP:O	2:B:1155:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1325:TRP:HA	2:B:1328:LYS:CD	2.42	0.49
3:C:241:THR:HA	3:C:244:ILE:HD12	1.95	0.49
3:C:409:LEU:HD11	3:C:461:ILE:HG12	1.93	0.49
3:C:482:ASP:OD1	3:C:483:VAL:N	2.45	0.49
3:C:805:ARG:HG3	3:C:806:ILE:N	2.27	0.49
3:C:948:LEU:HD13	3:C:1010:LYS:HG2	1.95	0.49
3:C:3439:GLN:O	3:C:3443:LEU:N	2.42	0.49
1:A:225:GLN:HG3	1:A:282:ARG:NH1	2.27	0.49
2:B:17:ARG:NH1	3:C:19:ASP:OD2	2.46	0.49
2:B:839:LEU:O	2:B:843:VAL:HG23	2.12	0.49
3:C:663:ILE:HG22	3:C:667:LYS:NZ	2.28	0.49
6:F:94:ASP:OD1	6:F:94:ASP:N	2.46	0.49
9:I:83:TYR:CE2	9:I:85:TYR:HD1	2.30	0.49
16:P:72:HIS:HB2	16:P:74:VAL:HG23	1.95	0.49
2:B:285:ALA:O	2:B:288:ASN:HB2	2.13	0.49
2:B:736:LEU:HA	2:B:739:LYS:HD2	1.94	0.49
2:B:811:PRO:HB3	2:B:900:PHE:HA	1.94	0.49
2:B:872:SER:HB3	2:B:966:LYS:HE3	1.94	0.49
3:C:135:MET:HA	3:C:139:TYR:CD2	2.47	0.49
3:C:1116:LYS:HG2	3:C:1182:LEU:HD21	1.95	0.49
17:T:154:GLN:O	17:T:158:GLU:HG2	2.13	0.49
1:A:158:VAL:HB	1:A:180:LEU:HB3	1.93	0.49
2:B:137:LEU:HD21	2:B:145:LEU:HD22	1.94	0.49
2:B:248:LEU:HA	2:B:253:VAL:HG11	1.94	0.49
2:B:500:GLU:HG2	2:B:535:ILE:HB	1.95	0.49
2:B:788:GLN:HA	2:B:791:HIS:CD2	2.47	0.49
2:B:1291:GLN:H	2:B:1291:GLN:CD	2.15	0.49
3:C:52:LYS:HA	3:C:95:PHE:O	2.11	0.49
3:C:56:TYR:HE1	3:C:76:PRO:HD2	1.78	0.49
3:C:626:GLU:H	3:C:629:ILE:HG13	1.78	0.49
3:C:3194:ALA:CB	3:C:3353:ARG:N	2.71	0.49
12:L:95:PHE:HD1	12:L:106:LEU:HB2	1.78	0.49
13:M:5:PRO:HD3	13:M:25:ILE:HD11	1.94	0.49
16:P:7:GLU:HA	16:P:57:LYS:O	2.12	0.49
1:A:334:ARG:HB3	1:A:353:ASN:HA	1.95	0.49
1:A:1300:GLN:O	1:A:1302:ASP:N	2.44	0.49
2:B:467:VAL:O	2:B:471:THR:HG23	2.13	0.49
2:B:1315:ILE:HG12	2:B:1362:TYR:CD1	2.46	0.49
3:C:572:ILE:O	3:C:576:TYR:HD2	1.95	0.49
3:C:580:LEU:HD13	3:C:641:TYR:CE2	2.48	0.49
11:K:29:PRO:HB2	14:N:30:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:14:GLU:OE2	13:M:18:LYS:HD3	2.13	0.49
15:O:68:CYS:SG	15:O:113:PHE:HB2	2.53	0.49
1:A:205:ALA:HA	1:A:215:MET:O	2.13	0.48
2:B:1126:LYS:HZ1	2:B:1138:LYS:HB3	1.76	0.48
3:C:136:GLU:OE2	3:C:166:GLN:NE2	2.45	0.48
3:C:674:LEU:HD21	3:C:769:THR:HG21	1.95	0.48
3:C:820:HIS:HB3	3:C:920:GLY:O	2.12	0.48
7:G:74:LEU:HD11	7:G:150:THR:HG23	1.95	0.48
8:H:16:MET:HG3	8:H:74:SER:O	2.13	0.48
9:I:68:ASP:HA	9:I:72:GLY:O	2.12	0.48
11:K:29:PRO:HD2	14:N:30:TYR:CD2	2.48	0.48
16:P:59:ASN:O	16:P:65:LEU:HD13	2.13	0.48
2:B:92:ILE:HD13	2:B:109:VAL:HG12	1.94	0.48
2:B:144:ASP:O	2:B:148:LYS:HG2	2.13	0.48
2:B:2888:LEU:O	2:B:3022:PHE:N	2.46	0.48
2:B:3533:LEU:N	2:B:3642:THR:O	2.43	0.48
3:C:426:THR:O	3:C:430:VAL:HG23	2.14	0.48
3:C:446:ILE:HG23	3:C:450:PHE:CZ	2.48	0.48
3:C:818:LEU:HB3	3:C:962:VAL:HG11	1.93	0.48
9:I:26:ASN:HD21	9:I:98:PHE:HB2	1.79	0.48
10:J:20:SER:O	10:J:54:TYR:OH	2.28	0.48
1:A:2287:GLU:N	1:A:2305:ASP:O	2.43	0.48
2:B:13:PHE:O	2:B:17:ARG:HG2	2.13	0.48
2:B:500:GLU:HA	2:B:503:LEU:HD12	1.94	0.48
2:B:968:CYS:O	2:B:972:ILE:HG12	2.14	0.48
2:B:1113:LEU:HA	2:B:1116:PHE:CD1	2.48	0.48
3:C:102:ALA:O	3:C:106:LYS:HE2	2.13	0.48
3:C:358:THR:HB	3:C:361:LYS:HG3	1.94	0.48
3:C:876:ASP:HB2	3:C:877:PRO:HD3	1.94	0.48
3:C:1227:ARG:HG3	3:C:1228:ARG:NH2	2.27	0.48
11:K:48:LEU:HB2	11:K:49:LYS:NZ	2.28	0.48
12:L:68:LYS:H	12:L:68:LYS:HD2	1.77	0.48
2:B:873:THR:O	2:B:876:GLN:HB2	2.13	0.48
2:B:1120:THR:HG21	2:B:1154:GLU:OE1	2.14	0.48
2:B:1271:LEU:O	2:B:1275:GLU:HG2	2.12	0.48
3:C:100:ASN:OD1	3:C:101:PRO:HD3	2.14	0.48
3:C:493:ASP:O	3:C:496:LYS:HG2	2.13	0.48
3:C:1200:GLU:HA	3:C:1203:HIS:CD2	2.48	0.48
3:C:2864:LEU:N	3:C:3023:THR:O	2.45	0.48
6:F:87:TYR:HD1	6:F:100:ILE:HG13	1.79	0.48
2:B:105:ALA:HB3	3:C:20:SER:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:613:ILE:HD12	2:B:616:ARG:HB2	1.96	0.48
2:B:729:LEU:HB3	2:B:737:VAL:HG23	1.95	0.48
2:B:1568:SER:O	2:B:1571:GLU:N	2.44	0.48
3:C:29:GLU:OE2	3:C:33:GLN:NE2	2.46	0.48
3:C:446:ILE:HG23	3:C:450:PHE:HZ	1.78	0.48
3:C:935:VAL:H	3:C:1077:MET:HB2	1.78	0.48
1:A:277:GLU:HG2	1:A:280:GLY:H	1.79	0.48
1:A:4124:TYR:O	1:A:4146:MET:N	2.46	0.48
2:B:228:LEU:HD13	2:B:302:LEU:HD13	1.95	0.48
2:B:469:ALA:O	2:B:473:VAL:HG22	2.13	0.48
2:B:477:ILE:HB	2:B:484:LYS:HB2	1.96	0.48
2:B:1069:THR:OG1	2:B:1070:PRO:HD2	2.13	0.48
3:C:257:SER:O	3:C:261:LYS:HG2	2.13	0.48
3:C:339:LEU:O	3:C:343:MET:HG3	2.13	0.48
8:H:50:ARG:HH22	8:H:56:THR:HG23	1.78	0.48
14:N:102:LEU:HG	15:O:89:GLN:HE21	1.79	0.48
1:A:3468:LYS:O	1:A:3472:THR:N	2.44	0.48
2:B:21:ALA:C	3:C:115:ASP:HB3	2.34	0.48
2:B:615:GLU:HA	2:B:619:TYR:HD2	1.78	0.48
2:B:725:ILE:HD12	2:B:728:CYS:HB3	1.95	0.48
2:B:1106:PHE:CD2	2:B:1171:LEU:HB2	2.48	0.48
2:B:1126:LYS:NZ	2:B:1134:LEU:HD22	2.29	0.48
2:B:1271:LEU:HA	2:B:1274:ILE:HB	1.95	0.48
3:C:276:LYS:O	3:C:278:HIS:N	2.46	0.48
3:C:314:VAL:HA	3:C:317:LEU:HG	1.94	0.48
3:C:818:LEU:HB3	3:C:962:VAL:CG1	2.44	0.48
3:C:1108:LEU:HD21	3:C:1180:ARG:HB2	1.95	0.48
6:F:60:LYS:NZ	6:F:64:GLN:OE1	2.47	0.48
12:L:33:LYS:HZ1	12:L:67:PHE:HE2	1.61	0.48
12:L:81:ASN:HD21	13:M:59:ARG:NE	2.11	0.48
15:O:20:SER:HA	15:O:53:TYR:CE2	2.49	0.48
2:B:56:ASP:HA	2:B:97:HIS:NE2	2.28	0.48
2:B:128:ILE:O	2:B:132:VAL:HG23	2.14	0.48
2:B:156:ASN:HA	2:B:159:ALA:CB	2.44	0.48
2:B:447:THR:OG1	2:B:448:LYS:N	2.46	0.48
2:B:1148:SER:HG	2:B:1214:LEU:CB	2.12	0.48
3:C:160:GLU:O	3:C:164:GLU:HG2	2.14	0.48
14:N:38:ILE:HD11	14:N:124:GLY:HA3	1.96	0.48
2:B:120:HIS:CE1	3:C:119:ILE:HD13	2.48	0.48
2:B:191:ASP:O	2:B:195:VAL:HG13	2.14	0.48
2:B:790:ILE:HG13	2:B:859:TYR:OH	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:885:GLN:HA	2:B:894:ASN:HD21	1.79	0.48
2:B:1318:ILE:HG23	2:B:1345:LEU:HD13	1.96	0.48
3:C:172:PHE:HA	3:C:175:GLU:HB2	1.95	0.48
3:C:603:GLU:HA	3:C:606:LYS:HE2	1.96	0.48
3:C:973:ASP:O	3:C:981:ASP:N	2.47	0.48
7:G:79:VAL:HG23	7:G:144:SER:HB2	1.95	0.48
7:G:124:VAL:HG12	7:G:125:PHE:CE1	2.48	0.48
16:P:6:ILE:HB	16:P:56:VAL:HA	1.95	0.48
1:A:322:GLU:HG3	1:A:339:GLY:O	2.14	0.48
2:B:335:ASN:ND2	2:B:340:LEU:HD13	2.28	0.48
2:B:706:GLU:O	2:B:710:THR:HG23	2.14	0.48
2:B:1147:ILE:C	2:B:1214:LEU:CD1	2.59	0.48
2:B:1256:ASN:OD1	2:B:1257:ILE:HG13	2.13	0.48
3:C:314:VAL:O	3:C:317:LEU:HG	2.13	0.48
3:C:1185:ARG:HA	3:C:1188:ASP:OD2	2.13	0.48
7:G:77:LEU:HD22	7:G:146:ILE:HB	1.95	0.48
1:A:154:PHE:CE1	1:A:234:ILE:HD11	2.49	0.47
2:B:507:ILE:HG22	2:B:543:LYS:HD2	1.96	0.47
2:B:521:PHE:HA	2:B:524:LEU:HB2	1.96	0.47
2:B:1120:THR:O	2:B:1124:ILE:HG13	2.14	0.47
2:B:1329:PRO:HD2	2:B:1332:GLN:OE1	2.14	0.47
3:C:80:PHE:CD2	3:C:90:ASP:HB2	2.49	0.47
7:G:63:THR:O	7:G:66:ARG:HG2	2.14	0.47
14:N:41:LEU:HB3	14:N:45:ARG:CZ	2.44	0.47
1:A:157:LYS:HB2	1:A:159:TYR:HE1	1.80	0.47
1:A:256:ILE:CD1	1:A:322:GLU:HB2	2.41	0.47
2:B:26:LYS:HB2	2:B:29:ILE:HG13	1.95	0.47
2:B:663:LYS:HE3	2:B:666:ASN:HD22	1.79	0.47
2:B:930:ILE:O	2:B:934:ILE:HG12	2.14	0.47
2:B:1102:LEU:HA	2:B:1105:GLN:HG2	1.95	0.47
2:B:1107:ARG:CD	2:B:1190:ILE:HG12	2.41	0.47
2:B:1360:LYS:HG3	2:B:1364:VAL:N	2.28	0.47
3:C:1129:ILE:O	3:C:1201:TYR:OH	2.31	0.47
8:H:58:HIS:HB2	8:H:89:PHE:CZ	2.48	0.47
9:I:29:ASP:OD2	9:I:92:ASN:N	2.42	0.47
9:I:97:MET:HE1	9:I:99:TYR:CE1	2.49	0.47
12:L:81:ASN:HD21	13:M:59:ARG:HE	1.62	0.47
15:O:27:ILE:HD13	15:O:32:SER:OG	2.14	0.47
16:P:28:PHE:CE1	16:P:74:VAL:HG21	2.49	0.47
2:B:136:PRO:HG3	3:C:78:LEU:HD13	1.96	0.47
2:B:156:ASN:HA	2:B:159:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:ILE:HG23	2:B:463:PHE:CE2	2.47	0.47
3:C:1143:ARG:HG2	3:C:1190:LEU:HD11	1.96	0.47
3:C:1180:ARG:HA	3:C:1183:LEU:HD12	1.94	0.47
3:C:3592:ASP:O	3:C:3595:LEU:N	2.47	0.47
9:I:83:TYR:HE2	9:I:85:TYR:HD1	1.61	0.47
2:B:118:LEU:HD12	2:B:162:TYR:CD1	2.49	0.47
2:B:368:ILE:HG12	2:B:371:LYS:HB2	1.96	0.47
2:B:524:LEU:HD13	2:B:611:GLN:HG3	1.96	0.47
2:B:1352:LEU:HB3	2:B:1353:PRO:HD2	1.96	0.47
3:C:256:TRP:HA	3:C:259:GLN:HG3	1.96	0.47
3:C:507:ASN:O	3:C:511:ASP:HB2	2.14	0.47
3:C:1096:TYR:HA	3:C:1099:ASP:OD2	2.15	0.47
3:C:1112:THR:HG23	3:C:1182:LEU:HB3	1.97	0.47
7:G:76:TYR:CE2	7:G:78:ILE:HB	2.50	0.47
7:G:82:GLU:OE1	7:G:82:GLU:N	2.46	0.47
9:I:37:GLU:O	9:I:41:VAL:HG23	2.14	0.47
10:J:15:ASN:HD21	10:J:22:LYS:HB2	1.80	0.47
12:L:41:LEU:HA	12:L:44:GLU:HG3	1.94	0.47
12:L:74:TRP:CE2	12:L:109:LYS:HD3	2.50	0.47
14:N:52:ASP:HB3	14:N:55:ASN:OD1	2.13	0.47
17:T:186:LEU:H	17:T:189:ARG:HD3	1.79	0.47
1:A:317:LYS:HG3	1:A:342:ALA:HB1	1.96	0.47
1:A:4037:ALA:O	1:A:4041:GLY:N	2.41	0.47
2:B:26:LYS:HE2	2:B:72:THR:HG21	1.96	0.47
2:B:126:ASN:HB2	2:B:156:ASN:HD21	1.78	0.47
2:B:137:LEU:HD21	2:B:145:LEU:HD13	1.97	0.47
2:B:653:GLN:H	2:B:757:TRP:HE1	1.62	0.47
2:B:721:ASN:HB3	2:B:777:PHE:HE2	1.78	0.47
2:B:851:LYS:NZ	2:B:854:ASN:OD1	2.47	0.47
2:B:1171:LEU:HG	2:B:1176:VAL:HG23	1.96	0.47
3:C:317:LEU:HD23	3:C:356:TYR:CD2	2.46	0.47
3:C:456:ARG:HG2	3:C:502:LEU:HD11	1.95	0.47
3:C:936:GLN:O	3:C:942:VAL:HA	2.15	0.47
3:C:944:LEU:HD11	3:C:948:LEU:HD12	1.97	0.47
6:F:26:PHE:CE1	6:F:98:LEU:HD11	2.50	0.47
16:P:79:HIS:CG	16:P:93:ILE:HG22	2.50	0.47
17:T:44:LEU:O	17:T:48:GLU:HG2	2.13	0.47
1:A:95:MET:O	1:A:113:ILE:HA	2.14	0.47
1:A:200:ARG:HA	1:A:220:TRP:O	2.13	0.47
1:A:342:ALA:HB2	1:A:346:LEU:HD11	1.96	0.47
1:A:3996:ASP:HA	1:A:4168:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:524:LEU:HA	2:B:524:LEU:HD23	1.68	0.47
2:B:656:LEU:HB3	2:B:756:ARG:CZ	2.44	0.47
2:B:1145:LYS:CE	2:B:1150:VAL:HG21	2.45	0.47
3:C:51:ASN:HA	3:C:97:ARG:HD2	1.95	0.47
3:C:869:TYR:CG	3:C:869:TYR:O	2.68	0.47
3:C:951:ILE:HG21	3:C:1074:MET:SD	2.54	0.47
3:C:1115:THR:HG21	3:C:1183:LEU:HD23	1.96	0.47
9:I:73:PRO:O	9:I:74:THR:HG22	2.15	0.47
10:J:21:MET:HG2	10:J:54:TYR:CZ	2.50	0.47
11:K:35:ASP:OD1	11:K:36:ILE:N	2.48	0.47
15:O:76:THR:HG22	15:O:78:HIS:H	1.79	0.47
17:T:176:TYR:OH	17:T:199:MET:SD	2.60	0.47
1:A:196:PRO:N	1:A:197:PRO:HD2	2.30	0.47
1:A:208:MET:SD	1:A:266:TYR:OH	2.66	0.47
2:B:157:TYR:H	2:B:180:LYS:CE	2.27	0.47
2:B:271:PHE:HA	2:B:275:GLN:OE1	2.15	0.47
2:B:439:LEU:CD2	2:B:530:LEU:HA	2.45	0.47
2:B:505:SER:O	2:B:509:GLN:HG3	2.15	0.47
2:B:697:THR:O	2:B:701:ILE:HG13	2.15	0.47
2:B:854:ASN:HA	2:B:857:LYS:HE2	1.95	0.47
2:B:969:LEU:O	2:B:972:ILE:HB	2.15	0.47
2:B:1040:CYS:HA	2:B:1043:LYS:HD2	1.97	0.47
2:B:1057:LEU:O	2:B:1091:VAL:HG11	2.15	0.47
3:C:464:PHE:O	3:C:468:GLN:HG2	2.13	0.47
3:C:535:ASN:O	3:C:545:SER:HA	2.15	0.47
3:C:663:ILE:HG21	3:C:698:GLU:OE1	2.14	0.47
3:C:903:GLN:HE21	3:C:994:GLU:CD	2.18	0.47
8:H:59:CYS:HB2	8:H:88:LEU:HD13	1.96	0.47
10:J:13:PRO:HG2	10:J:79:PHE:HB3	1.96	0.47
17:T:51:SER:O	17:T:55:ILE:HG12	2.14	0.47
1:A:3894:VAL:O	1:A:3898:LEU:N	2.39	0.47
2:B:1073:ILE:HG23	2:B:1078:ILE:HD12	1.97	0.47
3:C:459:LYS:HD3	3:C:510:PHE:CG	2.50	0.47
3:C:688:PHE:O	3:C:692:ILE:HG13	2.15	0.47
3:C:948:LEU:HD22	3:C:1010:LYS:HD3	1.97	0.47
3:C:1006:ILE:O	3:C:1009:THR:OG1	2.26	0.47
3:C:1105:ARG:NH1	3:C:1175:ASP:HB2	2.30	0.47
8:H:35:CYS:SG	8:H:40:GLU:HB3	2.55	0.47
1:A:220:TRP:CE2	2:B:956:LEU:HD13	2.50	0.47
2:B:473:VAL:O	2:B:484:LYS:HD2	2.15	0.47
2:B:1303:ASN:O	2:B:1307:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:331:THR:HG22	3:C:333:GLN:H	1.78	0.47
2:B:117:LEU:CD1	3:C:146:ILE:HG13	2.43	0.47
2:B:813:ASP:C	2:B:1075:TRP:HE1	2.15	0.47
2:B:917:ILE:HG12	2:B:983:CYS:HB3	1.97	0.47
2:B:1146:VAL:CG1	2:B:1215:GLN:HG3	2.42	0.47
3:C:177:ARG:HE	3:C:259:GLN:CA	2.27	0.47
3:C:213:PHE:O	3:C:217:ILE:HG12	2.15	0.47
3:C:321:GLU:OE2	3:C:321:GLU:N	2.48	0.47
3:C:1107:LEU:HD13	3:C:1156:VAL:HG22	1.97	0.47
3:C:1209:LEU:O	3:C:1213:LYS:HG2	2.15	0.47
3:C:3203:PRO:O	3:C:3204:ALA:CB	2.63	0.47
8:H:31:ALA:HB2	8:H:44:PHE:CD2	2.50	0.47
12:L:22:ARG:HD2	12:L:95:PHE:CE2	2.50	0.47
1:A:2955:MET:O	1:A:2959:LYS:N	2.47	0.46
1:A:3817:ASN:O	1:A:3821:ALA:N	2.41	0.46
2:B:164:LEU:HD22	2:B:165:LEU:HD22	1.96	0.46
2:B:443:GLU:O	2:B:444:LEU:HD23	2.16	0.46
2:B:856:TRP:O	2:B:860:ASN:ND2	2.48	0.46
2:B:1126:LYS:NZ	2:B:1138:LYS:HB3	2.30	0.46
2:B:1154:GLU:CD	2:B:1204:VAL:HG11	2.35	0.46
3:C:601:PRO:HG3	3:C:697:ARG:HB3	1.96	0.46
3:C:751:LEU:HD13	3:C:869:TYR:O	2.14	0.46
14:N:32:SER:CA	14:N:35:GLN:HB3	2.38	0.46
14:N:57:ASN:HD22	14:N:58:GLN:NE2	2.13	0.46
14:N:68:ARG:O	14:N:72:LYS:HG2	2.16	0.46
16:P:84:HIS:HB3	16:P:89:VAL:HG21	1.96	0.46
1:A:283:THR:HG23	2:B:955:PHE:HE1	1.79	0.46
1:A:329:ASP:H	1:A:334:ARG:HH11	1.62	0.46
1:A:4077:LEU:O	1:A:4102:HIS:N	2.47	0.46
2:B:605:LYS:HB3	2:B:611:GLN:HB3	1.96	0.46
2:B:1285:GLU:CG	2:B:1290:LEU:HB2	2.44	0.46
2:B:1311:MET:O	2:B:1362:TYR:HE1	1.98	0.46
2:B:4412:GLN:O	2:B:4414:TRP:N	2.49	0.46
2:B:4548:TYR:HA	2:B:4557:TYR:HA	1.97	0.46
3:C:937:LEU:HD12	3:C:940:ASP:O	2.15	0.46
3:C:1145:GLU:O	3:C:1148:GLU:N	2.48	0.46
12:L:36:ARG:HD2	12:L:37:GLN:N	2.31	0.46
2:B:157:TYR:H	2:B:180:LYS:HE2	1.80	0.46
2:B:1302:MET:HA	2:B:1305:LEU:HD12	1.97	0.46
3:C:365:LEU:HA	3:C:368:LYS:HZ1	1.80	0.46
3:C:477:ASN:ND2	3:C:528:LEU:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:854:GLU:HA	3:C:857:ARG:HB2	1.97	0.46
6:F:60:LYS:HA	6:F:63:ILE:HG22	1.96	0.46
14:N:35:GLN:O	14:N:38:ILE:HG22	2.15	0.46
2:B:91:VAL:HG13	2:B:108:VAL:HB	1.97	0.46
2:B:613:ILE:HD11	2:B:619:TYR:HB2	1.96	0.46
2:B:1255:GLU:OE1	2:B:1255:GLU:N	2.48	0.46
3:C:80:PHE:CD1	3:C:87:LYS:HB3	2.51	0.46
3:C:874:HIS:CD2	3:C:881:GLU:HG3	2.50	0.46
3:C:896:GLN:O	3:C:900:ASN:HB2	2.15	0.46
9:I:89:VAL:HG11	9:I:94:LEU:HD22	1.98	0.46
1:A:32:THR:HG22	1:A:34:ILE:HG12	1.96	0.46
1:A:2077:TYR:N	1:A:2123:GLN:O	2.43	0.46
2:B:173:MET:CE	2:B:218:LEU:HA	2.45	0.46
2:B:786:SER:O	2:B:790:ILE:HG12	2.15	0.46
2:B:2631:GLY:O	2:B:2645:LEU:N	2.42	0.46
3:C:940:ASP:O	3:C:941:LYS:HE2	2.15	0.46
3:C:1111:LEU:HG	3:C:1153:PHE:CD1	2.51	0.46
12:L:81:ASN:O	13:M:60:ASN:N	2.48	0.46
1:A:345:TRP:O	1:A:346:LEU:HD23	2.16	0.46
2:B:28:LYS:HD3	2:B:73:PHE:CD1	2.51	0.46
2:B:122:ASN:HB2	2:B:159:ALA:HB2	1.98	0.46
2:B:633:ILE:HA	2:B:636:TYR:HD2	1.81	0.46
2:B:670:LYS:HD3	2:B:670:LYS:HA	1.69	0.46
2:B:718:ILE:HD13	2:B:769:SER:HB3	1.98	0.46
2:B:1121:LYS:NZ	2:B:1200:ILE:HD12	2.31	0.46
2:B:1236:PHE:HA	2:B:1239:GLU:OE1	2.14	0.46
2:B:1328:LYS:CG	2:B:1332:GLN:HG2	2.45	0.46
2:B:1577:ARG:O	2:B:1579:ASP:N	2.45	0.46
3:C:24:LYS:NZ	3:C:29:GLU:HB2	2.30	0.46
3:C:25:ASP:HB2	3:C:28:VAL:HG23	1.97	0.46
3:C:568:ARG:HD2	3:C:572:ILE:HG13	1.97	0.46
3:C:972:TRP:O	3:C:975:GLN:HG2	2.15	0.46
7:G:99:ILE:HG23	7:G:103:ILE:HG13	1.97	0.46
12:L:58:VAL:HG23	12:L:76:CYS:SG	2.55	0.46
1:A:26:ILE:HG13	1:A:323:SER:OG	2.16	0.46
1:A:248:ILE:HG22	1:A:301:TRP:HD1	1.79	0.46
2:B:593:LYS:HA	2:B:596:ARG:HG2	1.97	0.46
2:B:2446:GLY:O	2:B:2675:SER:N	2.43	0.46
3:C:326:PRO:HG2	3:C:372:GLN:OE1	2.15	0.46
3:C:786:GLN:HA	3:C:789:LYS:HG2	1.97	0.46
3:C:1187:TRP:O	3:C:1190:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:33:LYS:O	12:L:36:ARG:HG3	2.16	0.46
14:N:70:LYS:O	14:N:73:ARG:HG3	2.16	0.46
15:O:24:VAL:HG22	15:O:49:GLN:HE22	1.81	0.46
2:B:66:GLY:O	2:B:72:THR:HA	2.16	0.46
2:B:419:PHE:HA	2:B:422:ARG:CD	2.46	0.46
2:B:540:LEU:O	2:B:544:HIS:N	2.45	0.46
2:B:913:PHE:HB2	2:B:916:GLU:HA	1.97	0.46
3:C:488:PHE:O	3:C:492:ILE:HG12	2.15	0.46
3:C:814:SER:CA	3:C:901:SER:HB3	2.45	0.46
6:F:85:TYR:CE2	6:F:87:TYR:HB2	2.50	0.46
11:K:34:ASP:N	14:N:36:LYS:HA	2.31	0.46
16:P:28:PHE:CE2	16:P:74:VAL:HG21	2.50	0.46
16:P:79:HIS:CD2	16:P:93:ILE:HG22	2.51	0.46
1:A:39:LEU:HD11	2:B:964:GLU:O	2.15	0.46
1:A:177:LEU:HD13	1:A:239:TRP:HH2	1.81	0.46
1:A:1721:LYS:O	1:A:1725:GLY:N	2.45	0.46
2:B:104:VAL:O	2:B:108:VAL:HG22	2.16	0.46
2:B:207:ILE:HG23	2:B:211:LEU:HD23	1.97	0.46
2:B:883:ASN:ND2	2:B:972:ILE:HD13	2.31	0.46
3:C:434:PRO:O	3:C:438:THR:N	2.49	0.46
3:C:1060:GLU:O	3:C:1063:GLU:HG3	2.15	0.46
3:C:1105:ARG:NH2	3:C:1176:GLU:HB2	2.31	0.46
3:C:3744:ARG:O	3:C:3748:ARG:N	2.43	0.46
8:H:24:VAL:HG11	8:H:77:ILE:HD13	1.97	0.46
8:H:71:PHE:CD1	8:H:76:TYR:HB2	2.51	0.46
9:I:46:ILE:O	9:I:50:SER:HB3	2.16	0.46
1:A:7:TRP:CD1	1:A:315:VAL:HG13	2.51	0.46
1:A:2638:ALA:HB2	1:A:2875:ALA:HB1	1.97	0.46
2:B:160:GLN:HE22	2:B:243:LEU:HD13	1.80	0.46
3:C:269:LYS:CE	3:C:284:ARG:HD3	2.46	0.46
3:C:1058:ILE:O	3:C:1062:ILE:HG13	2.16	0.46
3:C:1182:LEU:CD1	3:C:1185:ARG:HE	2.28	0.46
8:H:42:ALA:HB2	8:H:61:VAL:HG22	1.98	0.46
10:J:28:GLN:HG3	10:J:49:PHE:CE2	2.51	0.46
11:K:40:ALA:O	11:K:44:THR:HG22	2.16	0.46
13:M:57:VAL:HG22	13:M:82:LEU:HD22	1.97	0.46
1:A:10:LEU:HD21	1:A:329:ASP:OD2	2.16	0.45
2:B:60:ASN:HD21	3:C:141:ARG:HE	1.64	0.45
2:B:155:ASN:N	2:B:180:LYS:HZ1	2.13	0.45
2:B:292:LEU:O	2:B:295:LEU:HG	2.16	0.45
2:B:437:ASN:O	2:B:441:LYS:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1246:PHE:CE2	2:B:1257:ILE:HG12	2.51	0.45
2:B:1268:TYR:HB3	2:B:1305:LEU:CD2	2.46	0.45
3:C:21:LEU:HD12	3:C:22:GLN:HB2	1.97	0.45
3:C:81:THR:HG22	3:C:126:ASN:H	1.81	0.45
3:C:1111:LEU:HG	3:C:1153:PHE:HB2	1.98	0.45
3:C:3355:GLN:O	3:C:3356:VAL:C	2.51	0.45
3:C:3378:ALA:C	3:C:3380:ILE:H	2.20	0.45
14:N:101:CYS:C	14:N:102:LEU:HD12	2.36	0.45
2:B:49:PHE:O	2:B:53:ILE:HG13	2.17	0.45
2:B:1102:LEU:HD12	2:B:1103:VAL:N	2.32	0.45
2:B:1189:GLN:HE21	2:B:1190:ILE:HG13	1.81	0.45
3:C:58:GLN:HB3	3:C:68:ILE:HG23	1.99	0.45
3:C:274:ARG:HH11	3:C:275:HIS:CD2	2.35	0.45
3:C:1142:ILE:O	3:C:1146:GLN:HG3	2.17	0.45
9:I:32:GLY:O	9:I:35:LEU:HB2	2.17	0.45
11:K:34:ASP:HB2	14:N:36:LYS:HB3	1.98	0.45
13:M:33:GLN:OE1	13:M:36:GLN:NE2	2.38	0.45
3:C:57:TYR:HD1	3:C:69:LYS:HE2	1.81	0.45
3:C:177:ARG:HH21	3:C:259:GLN:HG2	1.80	0.45
3:C:264:ASP:HA	3:C:267:ILE:HD12	1.98	0.45
3:C:821:LEU:HD23	3:C:922:ASN:HB3	1.98	0.45
3:C:1264:LYS:HD3	3:C:1264:LYS:HA	1.66	0.45
8:H:24:VAL:HA	8:H:49:PHE:CZ	2.52	0.45
17:T:103:SER:OG	17:T:107:LYS:HE3	2.15	0.45
2:B:159:ALA:O	2:B:162:TYR:HB3	2.16	0.45
2:B:392:ASP:OD1	2:B:393:ALA:N	2.49	0.45
2:B:591:TRP:CZ2	2:B:595:LEU:HD11	2.52	0.45
2:B:752:ILE:CD1	2:B:765:PHE:HB3	2.45	0.45
2:B:1320:PHE:HA	2:B:1323:ASN:HB2	1.98	0.45
3:C:151:ILE:O	3:C:152:GLN:NE2	2.50	0.45
3:C:253:ILE:HG22	3:C:311:LYS:HE2	1.99	0.45
3:C:3180:CYS:CB	3:C:3366:ALA:HB1	2.47	0.45
6:F:11:LEU:HD21	6:F:34:LYS:HE2	1.98	0.45
10:J:42:ILE:O	10:J:46:ILE:HG13	2.17	0.45
14:N:32:SER:HA	14:N:35:GLN:CB	2.39	0.45
17:T:31:PRO:HA	17:T:197:PHE:CZ	2.51	0.45
1:A:80:LEU:H	1:A:80:LEU:HD12	1.82	0.45
1:A:1338:GLU:O	1:A:1341:TRP:N	2.50	0.45
2:B:103:ASN:ND2	3:C:21:LEU:O	2.49	0.45
2:B:134:GLN:HB2	3:C:79:PHE:HZ	1.81	0.45
2:B:164:LEU:HD23	2:B:168:ILE:CG1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:TYR:HE2	2:B:412:LEU:HD13	1.81	0.45
2:B:756:ARG:HA	2:B:762:ILE:HD13	1.97	0.45
2:B:836:ILE:HA	2:B:839:LEU:HG	1.97	0.45
2:B:1147:ILE:HB	2:B:1214:LEU:CD1	2.47	0.45
3:C:55:ALA:O	3:C:93:VAL:HG12	2.16	0.45
3:C:58:GLN:HA	3:C:90:ASP:CG	2.36	0.45
3:C:177:ARG:NH2	3:C:255:ASN:O	2.50	0.45
3:C:807:GLU:O	3:C:811:LYS:HG2	2.17	0.45
3:C:1115:THR:HB	3:C:1186:ASN:HD22	1.80	0.45
3:C:2932:GLU:O	3:C:2935:LEU:N	2.42	0.45
6:F:67:LEU:HG	7:G:99:ILE:HG12	1.98	0.45
14:N:31:PRO:HB3	14:N:110:TYR:O	2.16	0.45
17:T:115:LYS:HG3	17:T:176:TYR:CZ	2.51	0.45
1:A:166:GLY:HA2	1:A:171:ARG:N	2.28	0.45
2:B:279:LYS:HB3	2:B:286:ASN:HB2	1.97	0.45
2:B:419:PHE:CD2	2:B:422:ARG:HD2	2.51	0.45
2:B:1227:ASP:O	2:B:1231:LYS:HG2	2.16	0.45
2:B:1345:LEU:O	2:B:1349:ILE:HG13	2.16	0.45
3:C:51:ASN:O	3:C:96:LEU:HD12	2.16	0.45
3:C:576:TYR:CG	3:C:624:PHE:HE1	2.35	0.45
3:C:792:GLU:HA	3:C:795:ILE:HD12	1.99	0.45
3:C:793:GLN:O	3:C:796:ILE:N	2.49	0.45
3:C:871:LEU:HD12	3:C:871:LEU:O	2.16	0.45
3:C:1055:PHE:CE1	3:C:1089:ALA:HB1	2.51	0.45
11:K:31:GLU:HA	14:N:32:SER:CB	2.47	0.45
1:A:175:ASN:HB3	1:A:198:ASP:C	2.36	0.45
1:A:287:PHE:C	1:A:318:PRO:HB3	2.36	0.45
1:A:1338:GLU:O	1:A:1342:GLN:N	2.45	0.45
1:A:1826:GLN:O	1:A:1829:SER:N	2.50	0.45
1:A:2920:GLN:O	1:A:2924:MET:N	2.41	0.45
1:A:3996:ASP:HA	1:A:4168:ASP:O	2.17	0.45
2:B:40:LYS:HA	2:B:43:VAL:HG22	1.98	0.45
2:B:230:GLU:OE2	2:B:346:GLU:HG3	2.17	0.45
2:B:236:ASN:HA	2:B:239:ASP:OD2	2.17	0.45
2:B:901:ASP:HB2	2:B:903:ARG:NH1	2.32	0.45
3:C:786:GLN:HB3	3:C:790:LYS:NZ	2.31	0.45
3:C:1018:SER:HA	3:C:1021:THR:HG23	1.99	0.45
3:C:1125:PRO:HG2	3:C:1128:ASP:HB2	1.97	0.45
10:J:59:HIS:CD2	10:J:92:LYS:HB3	2.52	0.45
11:K:47:ALA:HA	11:K:50:LYS:CE	2.47	0.45
2:B:1814:SER:O	2:B:1817:TRP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:535:ASN:CB	3:C:568:ARG:HH12	2.28	0.45
3:C:656:TYR:O	3:C:660:VAL:HG22	2.16	0.45
3:C:822:PRO:HG3	3:C:920:GLY:HA3	1.97	0.45
3:C:3343:HIS:C	3:C:3345:LYS:H	2.15	0.45
8:H:24:VAL:HG11	8:H:77:ILE:HG21	1.99	0.45
8:H:50:ARG:NH1	8:H:56:THR:HA	2.31	0.45
8:H:50:ARG:NH2	8:H:57:TRP:O	2.50	0.45
11:K:96:ILE:O	11:K:106:LEU:HD12	2.17	0.45
2:B:184:SER:HA	2:B:192:LYS:HE2	1.98	0.45
2:B:186:THR:HG22	2:B:188:PRO:HD2	1.99	0.45
2:B:553:GLN:NE2	2:B:557:GLN:HB2	2.32	0.45
2:B:914:ASP:HB2	2:B:915:PRO:HD3	1.98	0.45
2:B:1136:ASP:OD2	2:B:1218:GLU:HA	2.16	0.45
2:B:1146:VAL:HG12	2:B:1214:LEU:HD11	1.11	0.45
2:B:1282:ASN:HA	2:B:1285:GLU:OE1	2.16	0.45
2:B:1313:ASP:O	2:B:1317:LEU:HG	2.17	0.45
3:C:572:ILE:HG23	3:C:576:TYR:CE2	2.52	0.45
8:H:81:VAL:HG23	8:H:86:ILE:HD13	1.99	0.45
11:K:37:LEU:CB	14:N:36:LYS:HD2	2.45	0.45
12:L:61:VAL:HG13	12:L:67:PHE:CD2	2.52	0.45
14:N:112:SER:HB2	14:N:125:ILE:HG22	1.98	0.45
15:O:33:GLN:HB2	15:O:103:ILE:HG21	1.99	0.45
1:A:114:LEU:HA	1:A:120:GLN:O	2.16	0.45
1:A:222:PHE:HB2	2:B:952:PRO:CB	2.34	0.45
1:A:334:ARG:HA	1:A:354:VAL:HG23	1.97	0.45
2:B:154:PHE:CZ	3:C:161:GLN:HB3	2.52	0.45
2:B:517:ILE:HG13	2:B:518:TYR:N	2.32	0.45
2:B:583:PRO:HD3	2:B:682:LYS:NZ	2.32	0.45
2:B:1137:LYS:HB3	2:B:1215:GLN:HE21	1.81	0.45
3:C:21:LEU:HD12	3:C:22:GLN:N	2.32	0.45
3:C:231:ARG:HA	3:C:249:ARG:HH21	1.81	0.45
9:I:89:VAL:CG2	9:I:108:PHE:HB2	2.47	0.45
13:M:4:GLU:N	13:M:4:GLU:OE1	2.48	0.45
15:O:77:ASN:HB3	15:O:107:TYR:CZ	2.52	0.45
1:A:223:THR:HG22	2:B:955:PHE:HB3	1.98	0.44
1:A:290:ASP:OD1	1:A:291:SER:N	2.49	0.44
2:B:55:GLN:NE2	2:B:57:ASN:HB3	2.32	0.44
2:B:63:TRP:O	2:B:88:GLY:HA2	2.17	0.44
2:B:504:ALA:CB	2:B:539:GLU:HG3	2.47	0.44
2:B:1317:LEU:HD13	16:P:77:LEU:CB	2.35	0.44
2:B:2500:LEU:O	2:B:2504:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1178:ASP:O	3:C:1182:LEU:HB2	2.17	0.44
10:J:72:TYR:CD2	10:J:77:PHE:HB2	2.52	0.44
1:A:3437:ASP:O	1:A:3441:ILE:N	2.44	0.44
2:B:135:ASN:HA	2:B:138:ASN:HD22	1.82	0.44
2:B:853:GLN:HA	2:B:856:TRP:HD1	1.82	0.44
2:B:1046:ASN:HB2	2:B:1170:LYS:NZ	2.33	0.44
3:C:933:VAL:HG11	3:C:944:LEU:HD13	1.99	0.44
3:C:1234:GLY:HA3	3:C:1252:PHE:HE2	1.83	0.44
11:K:24:ALA:HB1	11:K:99:TYR:O	2.17	0.44
1:A:18:PRO:O	1:A:21:ARG:HB2	2.17	0.44
2:B:559:GLN:NE2	2:B:629:ILE:HG23	2.33	0.44
2:B:749:LYS:NZ	2:B:768:LYS:HE2	2.32	0.44
2:B:841:LYS:O	2:B:844:LEU:HB2	2.18	0.44
2:B:875:ILE:HB	2:B:962:PHE:HZ	1.81	0.44
2:B:1118:GLU:OE2	2:B:1200:ILE:HG13	2.18	0.44
3:C:744:ILE:HG21	3:C:756:ILE:HD11	1.99	0.44
6:F:23:TYR:O	6:F:35:ARG:HA	2.17	0.44
9:I:46:ILE:HD11	9:I:99:TYR:CE2	2.52	0.44
16:P:25:LEU:HB2	16:P:55:ILE:CD1	2.47	0.44
2:B:349:ASN:HA	2:B:352:ILE:HG22	1.99	0.44
2:B:1175:ASN:HA	2:B:1178:ILE:HD12	1.98	0.44
2:B:1214:LEU:HG	2:B:1215:GLN:H	1.83	0.44
3:C:32:PHE:O	3:C:38:LYS:HE2	2.17	0.44
3:C:80:PHE:O	3:C:88:ILE:HG13	2.18	0.44
3:C:429:LYS:HA	3:C:432:ASP:OD2	2.17	0.44
3:C:675:ILE:HD12	3:C:772:TRP:CH2	2.52	0.44
3:C:745:LYS:HZ1	3:C:756:ILE:HD13	1.82	0.44
11:K:79:PHE:HE1	11:K:108:TYR:HH	1.64	0.44
12:L:95:PHE:CD1	12:L:106:LEU:HB2	2.52	0.44
14:N:29:PHE:HE1	14:N:34:ILE:HG12	1.82	0.44
1:A:276:PHE:CE2	1:A:284:ASN:HB2	2.51	0.44
1:A:2525:ASN:O	1:A:2529:SER:CB	2.66	0.44
2:B:64:VAL:HG23	2:B:77:GLN:NE2	2.33	0.44
2:B:1149:ASP:H	2:B:1214:LEU:CD2	2.26	0.44
2:B:1271:LEU:HD21	2:B:1301:CYS:CB	2.45	0.44
3:C:55:ALA:HB3	3:C:93:VAL:CG1	2.48	0.44
3:C:139:TYR:HA	3:C:142:GLN:HG2	1.99	0.44
3:C:210:GLU:HG3	3:C:280:ASN:CG	2.37	0.44
3:C:853:VAL:HG23	3:C:854:GLU:N	2.33	0.44
3:C:2738:GLU:O	3:C:2742:ALA:N	2.49	0.44
7:G:63:THR:O	7:G:67:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:49:ASN:HB3	9:I:54:LEU:HB2	1.99	0.44
11:K:32:CYS:HB3	14:N:36:LYS:HE2	2.00	0.44
11:K:34:ASP:HA	11:K:37:LEU:HB3	1.99	0.44
1:A:79:PRO:HD2	1:A:121:TRP:CZ3	2.52	0.44
1:A:174:PHE:C	1:A:199:PRO:HA	2.38	0.44
2:B:52:PHE:HD1	2:B:58:SER:HB2	1.82	0.44
2:B:174:LEU:CD2	2:B:236:ASN:HB3	2.47	0.44
2:B:204:THR:HG22	2:B:208:LYS:HE3	2.00	0.44
2:B:368:ILE:O	2:B:372:GLU:N	2.51	0.44
2:B:436:PHE:CZ	2:B:499:LEU:HD13	2.53	0.44
2:B:440:GLU:OE1	2:B:441:LYS:NZ	2.50	0.44
3:C:56:TYR:CD1	3:C:80:PHE:HZ	2.36	0.44
3:C:794:LEU:O	3:C:798:VAL:HG23	2.18	0.44
3:C:981:ASP:OD1	3:C:982:LYS:N	2.48	0.44
3:C:3343:HIS:O	3:C:3345:LYS:CB	2.66	0.44
1:A:2044:TYR:HA	1:A:2085:PRO:HA	2.00	0.44
1:A:4114:PRO:O	1:A:4116:ASP:N	2.51	0.44
2:B:309:ASP:HA	2:B:358:PHE:HE2	1.81	0.44
2:B:789:LYS:HD3	2:B:842:GLU:OE1	2.17	0.44
2:B:962:PHE:HA	2:B:966:LYS:HE2	2.00	0.44
2:B:1146:VAL:CG1	2:B:1215:GLN:CG	2.91	0.44
2:B:1215:GLN:HB3	2:B:1218:GLU:CG	2.47	0.44
6:F:87:TYR:HH	6:F:98:LEU:HD13	1.82	0.44
7:G:118:ASP:HB3	7:G:120:THR:HG23	1.99	0.44
8:H:61:VAL:HG12	8:H:86:ILE:HG13	1.99	0.44
11:K:42:ARG:HG3	11:K:43:GLU:N	2.33	0.44
11:K:90:HIS:NE2	11:K:95:PHE:HB2	2.32	0.44
14:N:46:LEU:O	14:N:47:LYS:HG2	2.17	0.44
17:T:132:THR:OG1	17:T:133:ALA:N	2.50	0.44
1:A:2943:LYS:O	1:A:2947:ASN:N	2.43	0.44
2:B:134:GLN:O	2:B:137:LEU:HB2	2.18	0.44
2:B:729:LEU:HD22	2:B:737:VAL:HB	2.00	0.44
2:B:1259:ASN:OD1	2:B:1260:ALA:N	2.51	0.44
3:C:3354:ILE:O	3:C:3357:ALA:C	2.53	0.44
6:F:60:LYS:O	6:F:63:ILE:HG22	2.17	0.44
15:O:11:GLU:O	15:O:15:LYS:HG3	2.18	0.44
16:P:52:ASN:OD1	16:P:52:ASN:N	2.51	0.44
17:T:107:LYS:HD2	17:T:177:ARG:HG2	2.00	0.44
1:A:12:GLN:HE22	1:A:338:PHE:HE1	1.66	0.44
1:A:276:PHE:HB2	1:A:282:ARG:HB2	2.00	0.44
2:B:116:ASN:ND2	2:B:162:TYR:OH	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:GLU:HG3	3:C:51:ASN:HB2	1.99	0.44
2:B:380:LEU:HD21	2:B:427:LEU:HD12	2.00	0.44
2:B:561:ILE:HG12	2:B:566:LYS:HD3	2.00	0.44
2:B:813:ASP:CG	2:B:1075:TRP:NE1	2.72	0.44
2:B:876:GLN:OE1	2:B:966:LYS:HB3	2.18	0.44
2:B:1146:VAL:HG11	2:B:1215:GLN:CD	2.36	0.44
3:C:46:SER:HA	3:C:106:LYS:HZ1	1.83	0.44
3:C:239:PRO:O	3:C:243:LEU:HG	2.18	0.44
6:F:15:SER:HA	6:F:23:TYR:CE1	2.53	0.44
9:I:85:TYR:CE1	9:I:106:LEU:HD22	2.53	0.44
1:A:60:LEU:HD22	1:A:69:TRP:CZ2	2.53	0.43
1:A:212:PRO:HG2	1:A:235:GLU:OE2	2.18	0.43
1:A:341:TRP:CZ2	2:B:963:PHE:CG	3.06	0.43
1:A:343:ASN:HD21	2:B:931:ARG:NE	2.11	0.43
2:B:790:ILE:HD11	2:B:839:LEU:HB2	2.00	0.43
2:B:3748:ARG:O	2:B:3751:ALA:HB3	2.18	0.43
3:C:528:LEU:O	3:C:532:ILE:HG13	2.18	0.43
3:C:622:ASN:O	3:C:625:PRO:HD2	2.18	0.43
12:L:98:LEU:HG	12:L:100:PRO:HD2	2.00	0.43
16:P:83:TYR:CD1	16:P:88:VAL:HA	2.53	0.43
17:T:107:LYS:CB	17:T:177:ARG:HG2	2.48	0.43
1:A:1399:CYS:HA	1:A:1524:ARG:C	2.39	0.43
1:A:2434:LEU:O	1:A:2438:GLY:N	2.48	0.43
2:B:50:GLN:OE1	2:B:50:GLN:N	2.41	0.43
2:B:115:ASN:HB2	2:B:120:HIS:HB2	2.00	0.43
2:B:566:LYS:HG3	2:B:567:GLN:H	1.83	0.43
2:B:1127:ASN:HB2	2:B:1147:ILE:HD11	2.00	0.43
3:C:85:LEU:HG	3:C:87:LYS:N	2.32	0.43
3:C:557:LYS:HB2	3:C:557:LYS:HE3	1.77	0.43
3:C:591:LYS:HB2	3:C:609:TRP:CE3	2.53	0.43
12:L:61:VAL:HG13	12:L:67:PHE:CE2	2.53	0.43
1:A:51:ILE:HA	1:A:82:ARG:CG	2.47	0.43
2:B:99:LEU:HD12	2:B:99:LEU:HA	1.75	0.43
2:B:109:VAL:HG13	3:C:122:GLU:O	2.19	0.43
2:B:154:PHE:O	2:B:158:VAL:HG23	2.18	0.43
3:C:123:ILE:HD11	3:C:134:LEU:CD1	2.48	0.43
3:C:550:HIS:O	3:C:553:GLN:HG3	2.18	0.43
3:C:570:ASN:O	3:C:573:LEU:HG	2.17	0.43
8:H:50:ARG:HH12	8:H:56:THR:HG23	1.82	0.43
13:M:43:TYR:O	13:M:47:LYS:HD3	2.19	0.43
16:P:43:PHE:HE2	16:P:57:LYS:HG2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:HIS:CE1	1:A:201:GLY:HA3	2.53	0.43
1:A:222:PHE:O	1:A:222:PHE:CD1	2.70	0.43
1:A:4077:LEU:N	1:A:4102:HIS:O	2.51	0.43
2:B:358:PHE:HA	2:B:361:LYS:NZ	2.33	0.43
2:B:801:ILE:HG21	2:B:874:ALA:CB	2.47	0.43
2:B:1748:ASP:O	2:B:1751:GLY:N	2.46	0.43
3:C:132:ASN:ND2	3:C:169:SER:O	2.51	0.43
6:F:8:ASP:O	6:F:12:LYS:HG2	2.18	0.43
9:I:27:SER:OG	9:I:96:PHE:HB3	2.18	0.43
12:L:45:ASN:HD21	12:L:52:ASP:HB3	1.83	0.43
12:L:60:PHE:O	12:L:64:GLN:NE2	2.51	0.43
1:A:904:LEU:O	1:A:908:LEU:N	2.51	0.43
1:A:1399:CYS:HA	1:A:1524:ARG:O	2.19	0.43
2:B:200:ILE:HD11	2:B:256:ILE:HG21	2.00	0.43
2:B:434:VAL:O	2:B:438:LYS:HE2	2.18	0.43
2:B:872:SER:O	2:B:876:GLN:HG2	2.18	0.43
2:B:904:LEU:HD11	2:B:990:PHE:CE2	2.52	0.43
3:C:933:VAL:CG2	3:C:944:LEU:HB3	2.49	0.43
3:C:960:THR:O	3:C:964:ARG:HG2	2.19	0.43
3:C:992:ASP:O	3:C:996:VAL:HG22	2.17	0.43
3:C:3355:GLN:N	3:C:3358:ILE:CB	2.82	0.43
6:F:26:PHE:CD1	6:F:98:LEU:HD11	2.53	0.43
11:K:34:ASP:HB3	14:N:40:GLU:CB	2.37	0.43
1:A:154:PHE:C	1:A:156:GLY:H	2.21	0.43
1:A:397:PHE:O	1:A:405:GLU:HA	2.18	0.43
2:B:154:PHE:CE1	3:C:161:GLN:HB3	2.54	0.43
2:B:340:LEU:HD11	2:B:397:TYR:OH	2.18	0.43
2:B:367:LEU:HB2	2:B:372:GLU:HA	1.99	0.43
2:B:657:LYS:CB	2:B:748:VAL:HB	2.48	0.43
2:B:852:LYS:HB3	2:B:856:TRP:NE1	2.34	0.43
2:B:890:PHE:CE2	2:B:891:ILE:HG12	2.53	0.43
2:B:958:GLU:HB3	2:B:962:PHE:HE2	1.82	0.43
2:B:1138:LYS:O	2:B:1139:LEU:HD23	2.19	0.43
3:C:591:LYS:HG2	3:C:606:LYS:HA	2.00	0.43
3:C:675:ILE:HD12	3:C:772:TRP:HH2	1.84	0.43
9:I:90:GLN:O	9:I:93:THR:OG1	2.26	0.43
11:K:28:TRP:HA	11:K:29:PRO:HA	1.68	0.43
11:K:30:PRO:HG3	14:N:33:LYS:HZ3	1.82	0.43
16:P:12:LYS:HD2	16:P:12:LYS:C	2.39	0.43
17:T:140:LEU:HB3	17:T:145:TYR:HD2	1.83	0.43
2:B:15:ILE:HD11	2:B:33:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:PHE:CD1	2:B:302:LEU:HD12	2.50	0.43
2:B:385:ASP:O	2:B:389:LYS:HG2	2.19	0.43
2:B:428:HIS:CD2	2:B:428:HIS:N	2.86	0.43
2:B:875:ILE:HB	2:B:962:PHE:CE1	2.54	0.43
3:C:102:ALA:O	3:C:106:LYS:HG2	2.19	0.43
3:C:183:MET:HB3	3:C:216:TRP:CE2	2.54	0.43
3:C:269:LYS:HA	3:C:269:LYS:HD3	1.87	0.43
3:C:434:PRO:O	3:C:438:THR:HG23	2.17	0.43
3:C:686:VAL:HG11	3:C:689:ASP:HB2	2.00	0.43
3:C:1147:ALA:O	3:C:1151:MET:HG2	2.18	0.43
11:K:29:PRO:CG	14:N:30:TYR:H	2.29	0.43
11:K:48:LEU:HB2	11:K:49:LYS:HZ2	1.82	0.43
12:L:81:ASN:HB3	13:M:60:ASN:ND2	2.33	0.43
15:O:37:THR:HG22	15:O:38:TYR:H	1.84	0.43
15:O:37:THR:HG22	15:O:38:TYR:N	2.34	0.43
1:A:270:GLY:HA2	1:A:288:VAL:O	2.19	0.43
1:A:1758:LEU:N	1:A:1797:LEU:O	2.47	0.43
2:B:128:ILE:O	2:B:131:PRO:HD2	2.18	0.43
2:B:161:VAL:HG22	2:B:164:LEU:HD13	2.00	0.43
2:B:305:SER:OG	2:B:307:PRO:HD2	2.19	0.43
2:B:503:LEU:HD11	2:B:533:ARG:NH2	2.32	0.43
2:B:661:LEU:H	2:B:661:LEU:HD12	1.84	0.43
2:B:1057:LEU:HD22	2:B:1091:VAL:HG13	2.00	0.43
2:B:1270:LYS:HA	2:B:1270:LYS:HD2	1.67	0.43
2:B:1350:LYS:O	2:B:1357:ARG:NH2	2.47	0.43
2:B:2779:PHE:O	2:B:2783:PHE:N	2.50	0.43
3:C:80:PHE:CE1	3:C:87:LYS:HB3	2.54	0.43
3:C:339:LEU:HA	3:C:339:LEU:HD23	1.86	0.43
3:C:542:ILE:CG2	3:C:575:ASN:HB2	2.46	0.43
3:C:859:VAL:HA	3:C:975:GLN:NE2	2.29	0.43
3:C:3177:ASN:HA	3:C:3370:LEU:CB	2.49	0.43
6:F:14:LEU:O	6:F:17:LEU:HB2	2.18	0.43
8:H:64:ASN:OD1	8:H:64:ASN:N	2.51	0.43
9:I:60:CYS:HA	9:I:77:CYS:SG	2.59	0.43
11:K:30:PRO:HD3	14:N:33:LYS:HE2	2.00	0.43
16:P:58:VAL:CG2	16:P:65:LEU:HD11	2.48	0.43
17:T:49:LYS:HA	17:T:52:GLU:CD	2.39	0.43
1:A:48:ASP:HA	1:A:51:ILE:CG1	2.49	0.43
1:A:79:PRO:HD3	1:A:112:TYR:CZ	2.54	0.43
1:A:208:MET:CG	1:A:296:ILE:HG21	2.49	0.43
2:B:11:GLU:HB3	2:B:33:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:ASN:O	2:B:159:ALA:N	2.52	0.43
2:B:540:LEU:HB3	2:B:544:HIS:NE2	2.34	0.43
2:B:1308:LEU:HD23	2:B:1362:TYR:OH	2.19	0.43
2:B:1318:ILE:HG23	2:B:1345:LEU:CD1	2.49	0.43
3:C:252:LYS:HG2	3:C:256:TRP:CZ2	2.54	0.43
3:C:789:LYS:HB3	3:C:789:LYS:HE3	1.77	0.43
3:C:971:ASN:H	3:C:974:GLN:NE2	2.17	0.43
6:F:67:LEU:HD13	6:F:67:LEU:HA	1.90	0.43
7:G:63:THR:HA	7:G:66:ARG:NE	2.33	0.43
8:H:15:ASP:HB2	8:H:76:TYR:HB3	1.99	0.43
17:T:31:PRO:HA	17:T:197:PHE:HZ	1.83	0.43
1:A:89:ALA:N	1:A:96:LEU:O	2.46	0.43
2:B:110:VAL:HG12	3:C:122:GLU:CG	2.49	0.43
2:B:499:LEU:O	2:B:503:LEU:HG	2.18	0.43
2:B:802:ILE:HG12	2:B:877:THR:CG2	2.45	0.43
2:B:837:GLN:O	2:B:840:VAL:HG22	2.19	0.43
2:B:1136:ASP:HA	2:B:1218:GLU:HG2	1.39	0.43
2:B:1153:VAL:HG13	2:B:1157:ARG:NH1	2.34	0.43
2:B:1219:THR:HG23	2:B:1290:LEU:HD21	2.00	0.43
3:C:17:ILE:HD12	3:C:32:PHE:HZ	1.83	0.43
3:C:743:LYS:HZ2	3:C:795:ILE:HD13	1.84	0.43
3:C:1183:LEU:O	3:C:1187:TRP:CD1	2.72	0.43
6:F:38:LYS:HA	6:F:41:SER:O	2.18	0.43
10:J:28:GLN:HG3	10:J:49:PHE:CD2	2.54	0.43
11:K:33:ALA:CA	14:N:36:LYS:HD3	2.49	0.43
16:P:12:LYS:HD2	16:P:13:GLN:N	2.34	0.43
17:T:102:SER:HA	17:T:105:GLN:OE1	2.19	0.43
1:A:320:PRO:HG2	1:A:341:TRP:HB3	2.01	0.42
2:B:1115:ASP:HA	2:B:1118:GLU:HG2	2.02	0.42
2:B:2402:ILE:O	2:B:2405:ILE:N	2.52	0.42
3:C:86:GLU:OE2	3:C:87:LYS:HG2	2.19	0.42
3:C:531:PHE:HE2	3:C:538:ARG:HE	1.67	0.42
3:C:1226:PHE:HZ	3:C:1256:TYR:HB3	1.84	0.42
6:F:66:ASP:O	6:F:67:LEU:HD22	2.19	0.42
10:J:77:PHE:CZ	10:J:88:LEU:HD11	2.54	0.42
15:O:41:ASP:OD2	15:O:42:LYS:N	2.52	0.42
16:P:5:TYR:CD1	16:P:57:LYS:HE2	2.55	0.42
17:T:107:LYS:HD3	17:T:178:ARG:HA	2.01	0.42
2:B:380:LEU:CD2	2:B:427:LEU:HA	2.48	0.42
2:B:459:ILE:HG12	2:B:502:ARG:HD2	2.01	0.42
3:C:862:LEU:CD1	3:C:972:TRP:HE1	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:36:HIS:O	6:F:39:SER:OG	2.36	0.42
7:G:76:TYR:O	7:G:88:GLY:HA2	2.20	0.42
8:H:68:PHE:HD2	9:I:64:LYS:HE3	1.84	0.42
9:I:89:VAL:HG23	9:I:108:PHE:HB2	2.01	0.42
11:K:32:CYS:O	14:N:32:SER:OG	2.36	0.42
14:N:67:LEU:O	14:N:71:ILE:HD12	2.18	0.42
1:A:48:ASP:OD1	1:A:51:ILE:HD11	2.19	0.42
1:A:225:GLN:OE1	1:A:253:LEU:HG	2.19	0.42
1:A:276:PHE:HB2	1:A:282:ARG:CB	2.49	0.42
1:A:343:ASN:ND2	2:B:931:ARG:HE	2.13	0.42
2:B:26:LYS:HB3	2:B:28:LYS:HG2	2.01	0.42
2:B:348:CYS:HA	2:B:351:ILE:HD12	2.01	0.42
2:B:1121:LYS:HD3	2:B:1203:ARG:HG2	2.01	0.42
3:C:609:TRP:CZ2	3:C:613:LEU:HD11	2.54	0.42
3:C:819:VAL:CG1	3:C:909:MET:HG2	2.47	0.42
3:C:916:LYS:HB2	3:C:1073:ALA:HB1	2.02	0.42
3:C:951:ILE:HG21	3:C:1074:MET:HE1	2.02	0.42
7:G:127:ARG:CG	7:G:129:GLN:HE22	2.29	0.42
9:I:95:LEU:HD12	9:I:107:ILE:HD11	2.01	0.42
11:K:33:ALA:CB	14:N:39:LYS:HD3	2.49	0.42
11:K:49:LYS:HA	11:K:49:LYS:HD3	1.91	0.42
12:L:35:ILE:HD13	12:L:96:PHE:CE2	2.54	0.42
12:L:47:GLN:CD	12:L:48:GLY:H	2.22	0.42
17:T:186:LEU:HA	17:T:189:ARG:CG	2.49	0.42
1:A:3777:ASP:O	1:A:3781:TYR:N	2.46	0.42
2:B:337:PRO:N	2:B:338:PRO:HD2	2.34	0.42
2:B:349:ASN:O	2:B:352:ILE:HG22	2.20	0.42
2:B:391:LYS:HZ3	2:B:420:LEU:HD22	1.83	0.42
2:B:1034:ASN:HB2	2:B:1035:PRO:HD3	2.00	0.42
3:C:132:ASN:CB	3:C:169:SER:HB2	2.50	0.42
3:C:135:MET:HG3	3:C:165:PHE:CE2	2.54	0.42
3:C:315:LYS:HA	3:C:315:LYS:HD3	1.74	0.42
3:C:1185:ARG:HH12	3:C:1189:ILE:HD13	1.84	0.42
6:F:85:TYR:CD2	6:F:100:ILE:HG23	2.55	0.42
7:G:132:LEU:H	7:G:132:LEU:HD23	1.85	0.42
9:I:37:GLU:HB3	9:I:70:LYS:NZ	2.34	0.42
13:M:12:MET:SD	13:M:16:MET:HG3	2.59	0.42
16:P:25:LEU:HD22	16:P:103:MET:SD	2.59	0.42
1:A:2360:GLY:N	1:A:2490:PHE:O	2.50	0.42
2:B:123:SER:CB	3:C:96:LEU:HD21	2.49	0.42
2:B:853:GLN:HA	2:B:856:TRP:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:986:PHE:HD1	2:B:989:ARG:HH21	1.67	0.42
2:B:1536:GLU:O	2:B:1539:ARG:N	2.53	0.42
3:C:362:MET:HE3	3:C:365:LEU:HB3	2.00	0.42
3:C:628:VAL:O	3:C:628:VAL:HG12	2.20	0.42
3:C:1160:TYR:CZ	3:C:1176:GLU:HG2	2.55	0.42
3:C:1183:LEU:O	3:C:1187:TRP:HD1	2.02	0.42
3:C:3726:VAL:O	3:C:3730:LEU:N	2.44	0.42
14:N:61:GLU:O	14:N:65:LEU:HD23	2.19	0.42
15:O:30:ASP:C	15:O:33:GLN:HE21	2.22	0.42
16:P:28:PHE:CG	16:P:74:VAL:HG11	2.54	0.42
18:V:221:UNK:O	18:V:222:UNK:C	2.68	0.42
2:B:389:LYS:HA	2:B:392:ASP:OD2	2.19	0.42
2:B:504:ALA:HB1	2:B:539:GLU:HG3	2.02	0.42
2:B:813:ASP:OD1	2:B:1075:TRP:CD1	2.73	0.42
2:B:1179:THR:HA	2:B:1183:THR:HG22	2.00	0.42
2:B:1229:PHE:HA	2:B:1232:GLU:HG2	2.01	0.42
3:C:409:LEU:HD11	3:C:461:ILE:HA	2.00	0.42
3:C:568:ARG:HD2	3:C:568:ARG:O	2.19	0.42
3:C:3503:TRP:O	3:C:3506:GLN:N	2.52	0.42
12:L:27:ALA:HB3	12:L:30:LEU:HD13	2.00	0.42
14:N:29:PHE:CE1	14:N:34:ILE:HG12	2.54	0.42
15:O:25:PHE:CD2	15:O:50:ILE:HD11	2.54	0.42
1:A:52:ALA:HB3	1:A:53:PRO:HD3	2.02	0.42
1:A:145:PRO:HD2	1:A:171:ARG:HH12	1.85	0.42
2:B:64:VAL:HG22	2:B:83:LYS:NZ	2.33	0.42
2:B:164:LEU:HG	2:B:175:PRO:HA	2.02	0.42
2:B:394:TYR:CE2	2:B:412:LEU:HD13	2.55	0.42
3:C:132:ASN:HB3	3:C:169:SER:HB2	2.02	0.42
3:C:278:HIS:HB2	3:C:282:ARG:CD	2.49	0.42
3:C:315:LYS:HA	3:C:318:THR:HG23	2.02	0.42
3:C:812:THR:O	3:C:816:VAL:HG23	2.20	0.42
10:J:47:LYS:NZ	10:J:58:TRP:O	2.53	0.42
1:A:35:MET:HB3	1:A:58:PHE:HB2	2.01	0.42
1:A:2203:ALA:HB2	1:A:3956:ALA:HA	2.02	0.42
2:B:1137:LYS:HD3	2:B:1144:MET:HG2	2.00	0.42
2:B:1494:VAL:O	2:B:1498:TYR:N	2.53	0.42
3:C:327:LEU:HA	3:C:376:ASN:OD1	2.20	0.42
3:C:677:ARG:HA	3:C:723:PHE:HE1	1.83	0.42
3:C:745:LYS:HA	3:C:745:LYS:HD3	1.72	0.42
3:C:1105:ARG:HH22	3:C:1176:GLU:HB2	1.84	0.42
3:C:3540:TRP:O	3:C:3544:LYS:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:23:TYR:HD1	6:F:36:HIS:CG	2.38	0.42
9:I:41:VAL:O	9:I:62:TYR:HE2	2.02	0.42
9:I:43:GLN:HA	9:I:46:ILE:HD12	2.00	0.42
1:A:63:THR:O	1:A:66:ASN:HB2	2.20	0.42
1:A:288:VAL:CG1	1:A:290:ASP:H	2.31	0.42
2:B:248:LEU:HD23	2:B:280:LYS:HZ3	1.83	0.42
2:B:376:ALA:O	2:B:380:LEU:CB	2.68	0.42
2:B:418:SER:HA	2:B:421:GLU:OE1	2.20	0.42
3:C:23:LEU:HD23	3:C:24:LYS:O	2.18	0.42
3:C:679:ASP:OD1	3:C:679:ASP:N	2.51	0.42
3:C:910:LYS:HE3	3:C:998:VAL:HB	2.01	0.42
3:C:1116:LYS:HA	3:C:1116:LYS:HD2	1.64	0.42
7:G:99:ILE:HD13	7:G:99:ILE:HA	1.87	0.42
10:J:13:PRO:HD2	10:J:79:PHE:O	2.20	0.42
10:J:92:LYS:HD2	10:J:92:LYS:HA	1.88	0.42
13:M:24:ALA:HA	13:M:41:ILE:HD11	2.02	0.42
1:A:46:TYR:OH	1:A:104:SER:HB3	2.19	0.42
1:A:53:PRO:C	1:A:82:ARG:HB3	2.40	0.42
2:B:36:GLN:HB3	2:B:39:ASP:HB2	2.02	0.42
2:B:352:ILE:HA	2:B:352:ILE:HD12	1.78	0.42
2:B:796:ASN:HA	2:B:799:VAL:HG22	2.01	0.42
2:B:1208:LYS:O	2:B:1212:ILE:HG13	2.19	0.42
3:C:431:ALA:O	3:C:434:PRO:HD2	2.19	0.42
3:C:928:LYS:N	3:C:929:PRO:HD2	2.35	0.42
3:C:3353:ARG:C	3:C:3354:ILE:O	2.53	0.42
8:H:39:LYS:HB2	8:H:39:LYS:HE2	1.88	0.42
1:A:952:LYS:O	1:A:956:GLU:N	2.35	0.41
2:B:169:LYS:HZ1	3:C:150:LYS:HD2	1.84	0.41
2:B:651:SER:OG	2:B:673:PHE:HB3	2.20	0.41
2:B:1045:PRO:HG2	2:B:1050:PHE:CE1	2.55	0.41
2:B:1308:LEU:HD21	2:B:1359:PHE:CE2	2.55	0.41
3:C:572:ILE:HG23	3:C:576:TYR:HE2	1.85	0.41
3:C:804:ASN:OD1	3:C:808:ASN:ND2	2.52	0.41
3:C:871:LEU:HB2	3:C:873:PRO:O	2.19	0.41
3:C:3232:ILE:O	3:C:3233:ILE:C	2.59	0.41
11:K:87:GLN:O	11:K:88:ALA:HB2	2.20	0.41
1:A:1226:LEU:O	1:A:1230:ALA:HB2	2.20	0.41
2:B:801:ILE:HD13	2:B:874:ALA:C	2.40	0.41
2:B:835:GLN:OE1	2:B:838:LYS:HB3	2.20	0.41
2:B:875:ILE:HD12	2:B:962:PHE:HZ	1.84	0.41
2:B:880:LEU:HA	2:B:883:ASN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3652:GLY:O	2:B:3655:GLU:N	2.53	0.41
3:C:89:GLN:OE1	3:C:126:ASN:ND2	2.52	0.41
3:C:1035:ILE:H	3:C:1035:ILE:HG13	1.66	0.41
8:H:73:ARG:O	8:H:75:TYR:HD1	2.03	0.41
11:K:56:GLU:HB2	11:K:59:LYS:HD3	2.02	0.41
1:A:60:LEU:HD11	1:A:67:CYS:CB	2.39	0.41
1:A:3629:LEU:O	1:A:3631:GLN:N	2.53	0.41
2:B:156:ASN:C	2:B:159:ALA:H	2.23	0.41
2:B:324:ILE:HG23	2:B:397:TYR:CE1	2.55	0.41
2:B:387:CYS:HB3	2:B:391:LYS:HZ3	1.85	0.41
2:B:422:ARG:CD	2:B:478:MET:HA	2.50	0.41
2:B:618:GLU:O	2:B:622:VAL:HG23	2.20	0.41
2:B:1314:ALA:HA	16:P:76:SER:HA	2.00	0.41
2:B:2563:LYS:N	2:B:2601:ILE:O	2.52	0.41
3:C:31:SER:OG	3:C:69:LYS:O	2.34	0.41
3:C:451:ASP:O	3:C:455:ARG:HG2	2.20	0.41
3:C:621:ILE:HG22	3:C:641:TYR:HD2	1.85	0.41
3:C:744:ILE:HD11	3:C:795:ILE:HD11	2.02	0.41
8:H:11:ILE:HA	8:H:79:LEU:HB2	2.02	0.41
12:L:16:LEU:HD13	12:L:19:HIS:CE1	2.56	0.41
13:M:15:ASP:OD1	13:M:16:MET:N	2.52	0.41
14:N:100:LYS:HD3	15:O:89:GLN:NE2	2.35	0.41
17:T:115:LYS:HE3	17:T:115:LYS:HB3	1.90	0.41
2:B:160:GLN:NE2	2:B:243:LEU:HD13	2.35	0.41
2:B:1065:SER:HA	2:B:1084:LYS:HE3	2.02	0.41
2:B:1340:ASP:OD1	2:B:1343:LYS:HB3	2.19	0.41
2:B:3466:ALA:O	2:B:3469:ARG:N	2.53	0.41
3:C:26:MET:O	3:C:26:MET:HE3	2.20	0.41
3:C:1213:LYS:O	3:C:1217:LYS:HG2	2.20	0.41
3:C:3784:GLU:O	3:C:3787:ASP:N	2.53	0.41
9:I:41:VAL:HG12	9:I:63:ILE:HD12	2.02	0.41
14:N:100:LYS:HD3	15:O:89:GLN:HE22	1.85	0.41
15:O:85:ILE:HG13	15:O:98:ILE:CG2	2.50	0.41
1:A:154:PHE:CZ	1:A:234:ILE:HD11	2.56	0.41
1:A:257:MET:HE3	1:A:267:PHE:H	1.85	0.41
1:A:288:VAL:N	1:A:318:PRO:HB3	2.36	0.41
2:B:40:LYS:HB3	2:B:45:ASN:O	2.21	0.41
2:B:173:MET:HG2	2:B:173:MET:O	2.21	0.41
2:B:217:GLN:O	2:B:220:LYS:HG2	2.20	0.41
2:B:687:PHE:HD1	2:B:692:LEU:HB2	1.85	0.41
2:B:832:ASN:O	2:B:836:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1360:LYS:HD2	2:B:1363:ASN:CB	2.46	0.41
3:C:106:LYS:HA	3:C:106:LYS:HD3	1.86	0.41
3:C:250:MET:O	3:C:254:THR:OG1	2.28	0.41
3:C:694:GLN:O	3:C:698:GLU:HG3	2.20	0.41
3:C:798:VAL:HG13	3:C:802:ILE:HD12	2.03	0.41
3:C:3740:ILE:O	3:C:3744:ARG:N	2.46	0.41
8:H:63:ARG:HA	8:H:63:ARG:NE	2.35	0.41
11:K:34:ASP:OD1	11:K:37:LEU:HB3	2.20	0.41
12:L:41:LEU:HD11	12:L:56:ASN:CB	2.51	0.41
16:P:16:ASP:OD2	16:P:16:ASP:C	2.58	0.41
1:A:93:ASP:OD1	1:A:94:LYS:HG3	2.21	0.41
2:B:558:VAL:HG13	2:B:595:LEU:HD22	2.03	0.41
2:B:585:ILE:HG21	2:B:644:TRP:HB2	2.02	0.41
2:B:800:LYS:O	2:B:803:GLU:HG3	2.21	0.41
2:B:868:ILE:HG21	2:B:957:GLN:HB3	2.03	0.41
2:B:931:ARG:O	2:B:931:ARG:NH1	2.52	0.41
2:B:1126:LYS:HE3	2:B:1126:LYS:HB3	1.92	0.41
3:C:9:ARG:HE	3:C:45:LEU:HD13	1.86	0.41
3:C:80:PHE:CD1	3:C:80:PHE:N	2.87	0.41
3:C:881:GLU:O	3:C:884:LYS:HG2	2.20	0.41
8:H:73:ARG:NH1	8:H:73:ARG:HG2	2.36	0.41
9:I:37:GLU:HB3	9:I:70:LYS:HZ2	1.85	0.41
14:N:69:GLU:O	14:N:72:LYS:HB2	2.20	0.41
1:A:102:TYR:HD2	1:A:107:ARG:HB2	1.86	0.41
2:B:12:ASP:HA	2:B:15:ILE:HD12	2.03	0.41
2:B:63:TRP:HE3	2:B:89:ILE:O	2.04	0.41
2:B:136:PRO:O	2:B:140:GLN:HB2	2.21	0.41
2:B:266:THR:O	2:B:270:PRO:HD2	2.19	0.41
2:B:721:ASN:HB3	2:B:777:PHE:CE2	2.56	0.41
3:C:140:SER:HA	3:C:162:VAL:HG11	2.03	0.41
3:C:183:MET:HG3	3:C:216:TRP:CG	2.56	0.41
3:C:214:ASN:O	3:C:218:ASN:ND2	2.53	0.41
3:C:354:ARG:HD2	3:C:355:PHE:N	2.36	0.41
3:C:548:LEU:HD12	3:C:548:LEU:HA	1.82	0.41
3:C:984:THR:HA	3:C:987:ASP:OD2	2.21	0.41
1:A:53:PRO:HD2	1:A:82:ARG:HB2	2.01	0.41
1:A:154:PHE:O	1:A:156:GLY:N	2.53	0.41
1:A:170:GLN:OE1	2:B:861:ASP:HB3	2.20	0.41
1:A:268:ILE:O	1:A:291:SER:OG	2.34	0.41
1:A:283:THR:CB	2:B:939:ASN:HB3	2.51	0.41
1:A:283:THR:CG2	2:B:939:ASN:HB3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:GLU:OE1	2:B:542:LYS:HD3	2.20	0.41
2:B:1363:ASN:HA	2:B:1366:VAL:HB	2.03	0.41
3:C:335:ILE:O	3:C:338:THR:HB	2.21	0.41
3:C:405:LEU:HD23	3:C:468:GLN:NE2	2.34	0.41
7:G:73:VAL:HA	7:G:149:GLN:HA	2.02	0.41
8:H:73:ARG:HA	8:H:73:ARG:NE	2.36	0.41
13:M:16:MET:SD	13:M:19:ARG:NH2	2.94	0.41
1:A:21:ARG:HA	1:A:39:LEU:O	2.21	0.41
1:A:146:ARG:HH22	1:A:176:ASP:CG	2.22	0.41
1:A:341:TRP:HH2	2:B:967:GLN:NE2	2.17	0.41
1:A:941:GLU:O	1:A:945:ASP:CB	2.69	0.41
2:B:122:ASN:HB2	2:B:159:ALA:CB	2.51	0.41
2:B:152:GLU:O	2:B:180:LYS:HD2	2.21	0.41
2:B:317:PHE:CE1	2:B:351:ILE:HG12	2.56	0.41
2:B:435:GLN:HA	2:B:438:LYS:CE	2.50	0.41
2:B:444:LEU:HD11	2:B:456:ILE:HD11	2.03	0.41
2:B:715:LEU:HB2	2:B:766:ILE:HD11	2.02	0.41
2:B:765:PHE:CE2	2:B:766:ILE:HG13	2.56	0.41
2:B:931:ARG:HH11	2:B:934:ILE:HB	1.86	0.41
2:B:1044:ILE:O	2:B:1044:ILE:HG22	2.21	0.41
2:B:1113:LEU:HD13	2:B:1164:MET:HE1	2.02	0.41
2:B:1317:LEU:CD2	16:P:32:TRP:HZ3	2.31	0.41
2:B:2385:HIS:O	2:B:2388:ASN:N	2.54	0.41
3:C:151:ILE:H	3:C:151:ILE:HD12	1.85	0.41
3:C:324:ILE:O	3:C:328:TYR:HD2	2.03	0.41
3:C:467:ILE:HG12	3:C:488:PHE:HZ	1.86	0.41
3:C:491:ILE:O	3:C:495:PHE:HB2	2.20	0.41
3:C:875:VAL:HG12	3:C:877:PRO:HD2	2.03	0.41
3:C:1035:ILE:HD13	3:C:1095:GLN:HG2	2.03	0.41
3:C:1062:ILE:O	3:C:1065:ILE:HG23	2.21	0.41
3:C:1084:SER:O	3:C:1088:TRP:CD1	2.74	0.41
8:H:27:VAL:HG21	8:H:52:ARG:HH12	1.85	0.41
8:H:52:ARG:HG3	8:H:53:TYR:CD2	2.56	0.41
8:H:89:PHE:HD2	8:H:91:THR:HG23	1.86	0.41
10:J:41:LYS:HD2	10:J:41:LYS:HA	1.91	0.41
10:J:77:PHE:CE1	10:J:88:LEU:HD11	2.56	0.41
11:K:34:ASP:OD1	11:K:38:GLU:HG2	2.20	0.41
12:L:41:LEU:O	12:L:44:GLU:HG3	2.20	0.41
12:L:52:ASP:O	12:L:56:ASN:ND2	2.54	0.41
12:L:64:GLN:HB3	12:L:66:GLU:HG2	2.02	0.41
13:M:28:VAL:HG21	13:M:77:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:43:PHE:CZ	16:P:55:ILE:HG23	2.55	0.41
17:T:49:LYS:NZ	17:T:184:THR:HG23	2.36	0.41
1:A:220:TRP:CG	1:A:221:SER:N	2.89	0.41
1:A:2495:ASP:O	1:A:2497:ARG:N	2.54	0.41
2:B:89:ILE:HD12	2:B:112:GLU:HG2	2.02	0.41
2:B:929:THR:HG22	2:B:930:ILE:N	2.34	0.41
2:B:1214:LEU:HG	2:B:1215:GLN:N	2.36	0.41
2:B:1215:GLN:HB3	2:B:1218:GLU:CB	2.48	0.41
2:B:1240:PHE:HD1	2:B:1243:LYS:HZ1	1.69	0.41
2:B:1243:LYS:HA	2:B:1248:TYR:HE1	1.86	0.41
3:C:56:TYR:HD1	3:C:80:PHE:CZ	2.39	0.41
3:C:989:ILE:HG23	3:C:994:GLU:OE2	2.20	0.41
3:C:1008:GLY:O	3:C:1012:LYS:HG3	2.21	0.41
3:C:1014:ASN:HA	3:C:1017:LEU:HB2	2.03	0.41
3:C:1099:ASP:HA	3:C:1102:LYS:HG2	2.02	0.41
6:F:74:ILE:HG22	6:F:91:GLN:HG2	2.03	0.41
6:F:77:ILE:HG22	6:F:79:LEU:CD2	2.51	0.41
7:G:77:LEU:HD12	7:G:90:PHE:CE2	2.56	0.41
13:M:77:ILE:HG13	13:M:80:LEU:HB2	2.02	0.41
17:T:187:GLU:HB2	17:T:188:PRO:CD	2.51	0.41
1:A:45:ASN:OD1	1:A:48:ASP:N	2.49	0.40
2:B:848:LYS:HD3	2:B:848:LYS:HA	1.83	0.40
2:B:1054:ILE:HD13	2:B:1054:ILE:HA	1.84	0.40
2:B:1108:THR:O	2:B:1111:LYS:HG2	2.21	0.40
2:B:1138:LYS:HE3	2:B:1145:LYS:CD	2.51	0.40
2:B:1353:PRO:HG2	2:B:1356:ILE:HG12	2.03	0.40
3:C:186:GLY:HA2	3:C:212:LYS:NZ	2.36	0.40
3:C:327:LEU:HD21	3:C:372:GLN:HG3	2.03	0.40
3:C:917:LYS:HA	3:C:917:LYS:HD2	1.89	0.40
3:C:1037:LYS:HE3	3:C:1037:LYS:HB3	1.77	0.40
7:G:79:VAL:HG12	7:G:85:VAL:HA	2.04	0.40
15:O:37:THR:O	15:O:39:ASN:ND2	2.54	0.40
16:P:60:ILE:HB	16:P:77:LEU:HD13	2.03	0.40
1:A:195:ASN:N	1:A:196:PRO:CD	2.85	0.40
1:A:252:ASN:HA	1:A:272:SER:O	2.22	0.40
1:A:253:LEU:O	1:A:272:SER:N	2.54	0.40
1:A:3742:GLY:O	1:A:3746:TRP:N	2.51	0.40
2:B:277:GLU:HG2	2:B:285:ALA:HB3	2.04	0.40
2:B:347:ILE:O	2:B:351:ILE:HG13	2.21	0.40
2:B:586:ALA:HB1	2:B:686:TYR:CE2	2.56	0.40
2:B:1057:LEU:HA	2:B:1060:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:THR:HG22	3:C:126:ASN:N	2.35	0.40
3:C:343:MET:O	3:C:346:ILE:HG22	2.21	0.40
3:C:521:ILE:HD12	3:C:521:ILE:HA	1.95	0.40
3:C:569:TYR:HA	3:C:572:ILE:HD12	2.03	0.40
3:C:601:PRO:CG	3:C:697:ARG:HB3	2.52	0.40
3:C:753:LEU:HB2	3:C:754:PRO:HD3	2.03	0.40
12:L:23:PHE:HE2	12:L:93:LEU:HD23	1.86	0.40
14:N:33:LYS:HA	14:N:36:LYS:HG3	2.03	0.40
1:A:7:TRP:HD1	1:A:315:VAL:HG22	1.85	0.40
1:A:60:LEU:HA	1:A:60:LEU:HD12	1.88	0.40
1:A:287:PHE:CG	1:A:320:PRO:HD3	2.55	0.40
2:B:90:ALA:HB3	2:B:111:VAL:CG2	2.51	0.40
2:B:376:ALA:O	2:B:380:LEU:HB2	2.21	0.40
2:B:653:GLN:HG2	2:B:671:VAL:HG22	2.04	0.40
2:B:788:GLN:HA	2:B:791:HIS:NE2	2.36	0.40
2:B:956:LEU:HD23	2:B:959:ILE:HD12	2.02	0.40
2:B:1264:ILE:HD13	2:B:1264:ILE:HG21	1.87	0.40
3:C:139:TYR:O	3:C:142:GLN:HG2	2.20	0.40
3:C:398:TRP:HB2	3:C:496:LYS:HB2	2.03	0.40
3:C:402:PRO:CA	3:C:468:GLN:HE22	2.35	0.40
3:C:425:ASP:O	3:C:429:LYS:HG2	2.21	0.40
3:C:818:LEU:H	3:C:909:MET:CE	2.34	0.40
3:C:948:LEU:HD21	3:C:1006:ILE:HG23	2.03	0.40
3:C:995:ILE:O	3:C:999:ILE:HG13	2.22	0.40
7:G:108:LYS:HA	7:G:111:ARG:NE	2.36	0.40
8:H:56:THR:N	8:H:92:GLY:O	2.49	0.40
10:J:17:GLU:HB3	10:J:18:MET:SD	2.61	0.40
2:B:314:TYR:CE1	2:B:389:LYS:HB3	2.57	0.40
2:B:444:LEU:HB2	2:B:452:LEU:HD22	2.02	0.40
2:B:444:LEU:CD2	2:B:456:ILE:HG12	2.50	0.40
2:B:477:ILE:HB	2:B:484:LYS:CB	2.52	0.40
2:B:599:ILE:O	2:B:602:PRO:HD2	2.22	0.40
2:B:836:ILE:O	2:B:840:VAL:HG13	2.22	0.40
2:B:851:LYS:CD	2:B:854:ASN:HB3	2.52	0.40
2:B:898:PRO:CG	2:B:1074:SER:HB3	2.43	0.40
2:B:1305:LEU:HA	2:B:1305:LEU:HD23	1.92	0.40
2:B:1311:MET:C	2:B:1362:TYR:CE1	2.95	0.40
3:C:221:SER:OG	3:C:287:GLU:OE1	2.38	0.40
3:C:715:ILE:HG12	18:V:221:UNK:C	2.52	0.40
3:C:1036:LYS:O	3:C:1040:LYS:HG3	2.22	0.40
3:C:1150:ASP:HA	3:C:1153:PHE:HB3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:29:ASP:O	9:I:92:ASN:HA	2.20	0.40
12:L:22:ARG:HD2	12:L:95:PHE:HE2	1.84	0.40
12:L:37:GLN:HG3	12:L:60:PHE:CE2	2.56	0.40
15:O:34:VAL:HG22	15:O:104:ASN:CG	2.42	0.40
15:O:51:ILE:HD11	15:O:71:ALA:HB2	2.03	0.40
15:O:101:TYR:CZ	15:O:103:ILE:HD11	2.57	0.40
16:P:69:VAL:HG12	16:P:74:VAL:O	2.21	0.40
17:T:175:MET:SD	17:T:176:TYR:N	2.94	0.40
2:B:11:GLU:HB3	2:B:33:LEU:CD1	2.51	0.40
2:B:429:LEU:HD13	2:B:470:PHE:CD2	2.57	0.40
2:B:875:ILE:HD12	2:B:962:PHE:CZ	2.57	0.40
3:C:36:LYS:HA	3:C:39:ASN:HD22	1.87	0.40
3:C:215:GLU:HA	3:C:218:ASN:HD22	1.87	0.40
3:C:420:LYS:HD3	3:C:421:LYS:HZ2	1.86	0.40
3:C:663:ILE:O	3:C:667:LYS:HG3	2.21	0.40
3:C:715:ILE:HD12	3:C:715:ILE:HA	1.75	0.40
3:C:1262:MET:HE3	3:C:1262:MET:O	2.21	0.40
7:G:105:LEU:HA	7:G:108:LYS:HE2	2.04	0.40
8:H:48:ASP:O	8:H:52:ARG:HG2	2.21	0.40
13:M:77:ILE:HG13	13:M:77:ILE:O	2.22	0.40
16:P:30:ALA:HB2	16:P:77:LEU:HD12	2.03	0.40
16:P:39:LEU:HD11	16:P:96:GLN:C	2.41	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	3371/4168 (81%)	2907 (86%)	454 (14%)	10 (0%)	41	77
2	B	4229/4595 (92%)	3790 (90%)	429 (10%)	10 (0%)	47	81
3	C	4232/4620 (92%)	3885 (92%)	337 (8%)	10 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	d	445/667 (67%)	400 (90%)	45 (10%)	0	100 100
5	e	529/670 (79%)	459 (87%)	69 (13%)	1 (0%)	47 81
6	F	96/133 (72%)	82 (85%)	14 (15%)	0	100 100
7	G	93/159 (58%)	81 (87%)	12 (13%)	0	100 100
8	H	83/92 (90%)	81 (98%)	2 (2%)	0	100 100
9	I	87/110 (79%)	79 (91%)	8 (9%)	0	100 100
10	J	82/93 (88%)	77 (94%)	5 (6%)	0	100 100
11	K	93/111 (84%)	81 (87%)	12 (13%)	0	100 100
12	L	95/111 (86%)	90 (95%)	5 (5%)	0	100 100
13	M	84/87 (97%)	82 (98%)	2 (2%)	0	100 100
14	N	107/132 (81%)	99 (92%)	8 (8%)	0	100 100
15	O	109/117 (93%)	103 (94%)	6 (6%)	0	100 100
16	P	101/110 (92%)	94 (93%)	7 (7%)	0	100 100
17	T	127/309 (41%)	109 (86%)	16 (13%)	2 (2%)	9 44
All	All	13963/16284 (86%)	12499 (90%)	1431 (10%)	33 (0%)	50 81

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	THR
1	A	1823	VAL
2	B	1651	ASN
2	B	1652	PRO
2	B	2557	PRO
2	B	3703	PRO
2	B	4008	PRO
2	B	4432	PRO
3	C	2978	PRO
3	C	2979	PRO
3	C	3203	PRO
3	C	3379	GLN
3	C	4182	PRO
3	C	4188	PRO
3	C	4546	PRO
5	e	142	VAL
1	A	1351	ASP
1	A	4084	ILE

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Mol	Chain	Res	Type
2	B	4556	THR
3	C	3204	ALA
2	B	3923	PRO
3	C	3378	ALA
17	T	188	PRO
1	A	982	ILE
1	A	3108	ASN
17	T	129	ASP
2	B	4557	TYR
1	A	1040	VAL
1	A	3665	PRO
2	B	3922	MET
3	C	4121	VAL
1	A	1824	GLY
1	A	3593	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	291/3691 (8%)	288 (99%)	3 (1%)	76 86
2	B	1215/4145 (29%)	1208 (99%)	7 (1%)	86 92
3	C	1094/4196 (26%)	1091 (100%)	3 (0%)	92 95
4	d	386/609 (63%)	385 (100%)	1 (0%)	92 95
5	e	364/597 (61%)	363 (100%)	1 (0%)	92 95
6	F	87/109 (80%)	85 (98%)	2 (2%)	50 70
7	G	86/149 (58%)	85 (99%)	1 (1%)	71 83
8	H	76/83 (92%)	75 (99%)	1 (1%)	69 81
9	I	76/95 (80%)	76 (100%)	0	100 100
10	J	74/82 (90%)	74 (100%)	0	100 100
11	K	81/97 (84%)	81 (100%)	0	100 100
12	L	86/99 (87%)	86 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	77/78 (99%)	77 (100%)	0	100 100
14	N	96/119 (81%)	96 (100%)	0	100 100
15	O	98/104 (94%)	96 (98%)	2 (2%)	55 74
16	P	97/104 (93%)	96 (99%)	1 (1%)	76 86
17	T	118/271 (44%)	118 (100%)	0	100 100
All	All	4402/14628 (30%)	4380 (100%)	22 (0%)	89 93

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LYS
1	A	189	ARG
1	A	282	ARG
2	B	171	LYS
2	B	296	LYS
2	B	450	LYS
2	B	461	LYS
2	B	851	LYS
2	B	1093	ARG
2	B	1126	LYS
3	C	97	ARG
3	C	107	LYS
3	C	1184	ARG
4	d	124	LYS
5	e	1123	SER
6	F	78	ARG
6	F	80	ARG
7	G	91	LYS
8	H	22	LYS
15	O	60	LYS
15	O	90	ASP
16	P	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	44	ASN
1	A	55	ASN

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Mol	Chain	Res	Type
1	A	184	ASN
1	A	284	ASN
1	A	343	ASN
2	B	45	ASN
2	B	54	GLN
2	B	55	GLN
2	B	60	ASN
2	B	77	GLN
2	B	134	GLN
2	B	138	ASN
2	B	156	ASN
2	B	160	GLN
2	B	167	GLN
2	B	223	ASN
2	B	236	ASN
2	B	322	HIS
2	B	335	ASN
2	B	404	ASN
2	B	437	ASN
2	B	553	GLN
2	B	666	ASN
2	B	724	HIS
2	B	876	GLN
2	B	894	ASN
2	B	922	ASN
2	B	935	ASN
2	B	1034	ASN
2	B	1104	ASN
2	B	1112	ASN
2	B	1175	ASN
2	B	1189	GLN
2	B	1258	ASN
2	B	1321	GLN
2	B	1323	ASN
2	B	1332	GLN
3	C	39	ASN
3	C	51	ASN
3	C	62	GLN
3	C	74	GLN
3	C	89	GLN
3	C	111	GLN
3	C	126	ASN

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Mol	Chain	Res	Type
3	C	152	GLN
3	C	218	ASN
3	C	278	HIS
3	C	350	HIS
3	C	357	ASN
3	C	424	ASN
3	C	468	GLN
3	C	575	ASN
3	C	678	HIS
3	C	741	ASN
3	C	809	ASN
3	C	864	GLN
3	C	971	ASN
3	C	974	GLN
3	C	975	GLN
3	C	1098	GLN
3	C	1186	ASN
3	C	1214	GLN
4	d	164	ASN
4	d	1202	GLN
5	e	52	ASN
5	e	874	ASN
5	e	1141	ASN
5	e	1168	GLN
5	e	1188	ASN
6	F	72	ASN
7	G	70	HIS
7	G	98	ASN
7	G	129	GLN
8	H	36	ASN
9	I	26	ASN
9	I	48	ASN
9	I	76	GLN
10	J	23	ASN
10	J	40	ASN
10	J	59	HIS
10	J	65	HIS
11	K	91	ASN
11	K	93	ASN
12	L	28	GLN
12	L	81	ASN
13	M	26	ASN

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Mol	Chain	Res	Type
13	M	54	ASN
13	M	60	ASN
14	N	55	ASN
14	N	57	ASN
15	O	39	ASN
15	O	44	ASN
15	O	48	GLN
15	O	78	HIS
16	P	79	HIS
17	T	165	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
19	ADP	C	4702	-	24,29,29	0.92	1 (4%)	29,45,45	1.55	4 (13%)
20	ATP	C	4704	-	26,33,33	0.88	1 (3%)	31,52,52	1.68	5 (16%)
19	ADP	C	4701	-	24,29,29	0.91	1 (4%)	29,45,45	1.50	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	ADP	C	4703	-	24,29,29	0.96	1 (4%)	29,45,45	1.51	3 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	ADP	C	4702	-	-	4/12/32/32	0/3/3/3
20	ATP	C	4704	-	-	4/18/38/38	0/3/3/3
19	ADP	C	4701	-	-	3/12/32/32	0/3/3/3
19	ADP	C	4703	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	C	4701	ADP	C5-C4	2.20	1.46	1.40
19	C	4702	ADP	C5-C4	2.14	1.46	1.40
19	C	4703	ADP	C5-C4	2.14	1.46	1.40
20	C	4704	ATP	C5-C4	2.06	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	C	4704	ATP	PA-O3A-PB	-5.12	115.24	132.83
19	C	4703	ADP	PA-O3A-PB	-4.58	117.12	132.83
19	C	4701	ADP	PA-O3A-PB	-4.21	118.36	132.83
20	C	4704	ATP	PB-O3B-PG	-4.15	118.57	132.83
19	C	4702	ADP	PA-O3A-PB	-4.13	118.66	132.83
19	C	4702	ADP	N3-C2-N1	-3.58	123.08	128.68
20	C	4704	ATP	N3-C2-N1	-3.58	123.08	128.68
19	C	4701	ADP	N3-C2-N1	-3.55	123.13	128.68
19	C	4703	ADP	N3-C2-N1	-3.21	123.66	128.68
19	C	4702	ADP	C3'-C2'-C1'	3.18	105.77	100.98
19	C	4703	ADP	C4-C5-N7	-2.92	106.36	109.40
19	C	4701	ADP	C3'-C2'-C1'	2.77	105.15	100.98
19	C	4701	ADP	C4-C5-N7	-2.56	106.73	109.40
20	C	4704	ATP	C4-C5-N7	-2.17	107.14	109.40
19	C	4702	ADP	C4-C5-N7	-2.16	107.14	109.40
20	C	4704	ATP	N6-C6-N1	2.15	123.04	118.57
19	C	4701	ADP	O3B-PB-O2B	2.09	115.64	107.64

There are no chirality outliers.

All (12) torsion outliers are listed below:

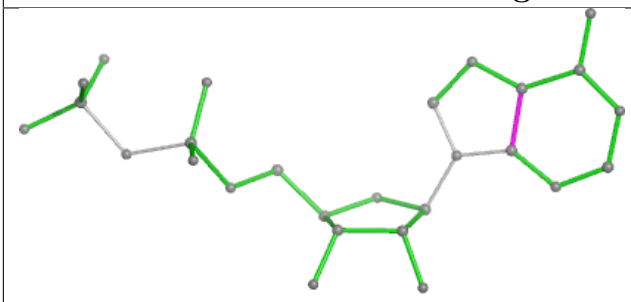
Mol	Chain	Res	Type	Atoms
19	C	4701	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	C5'-O5'-PA-O2A
20	C	4704	ATP	C5'-O5'-PA-O1A
20	C	4704	ATP	C5'-O5'-PA-O3A
20	C	4704	ATP	C3'-C4'-C5'-O5'
20	C	4704	ATP	O4'-C4'-C5'-O5'
19	C	4701	ADP	C5'-O5'-PA-O3A
19	C	4701	ADP	C5'-O5'-PA-O2A
19	C	4702	ADP	C5'-O5'-PA-O3A
19	C	4703	ADP	C5'-O5'-PA-O1A
19	C	4702	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

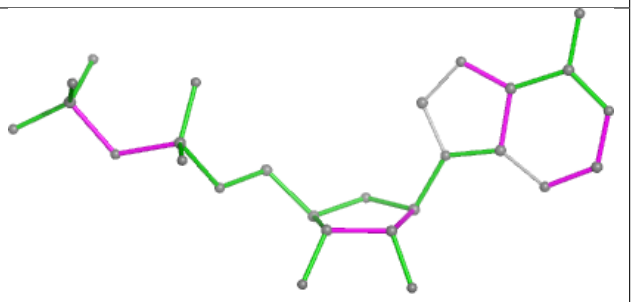
No monomer is involved in short contacts.

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

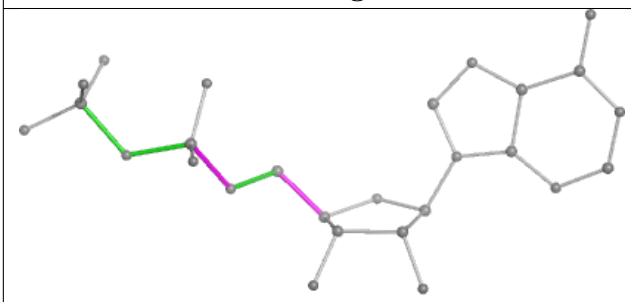
Ligand ADP C 4702



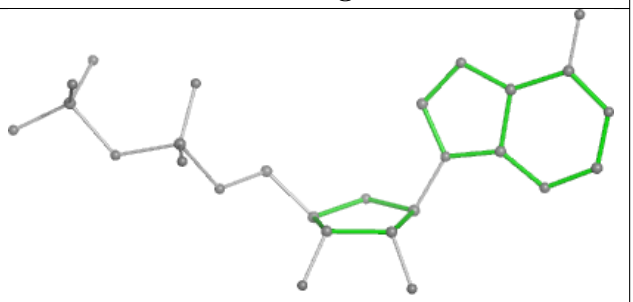
Bond lengths



Bond angles

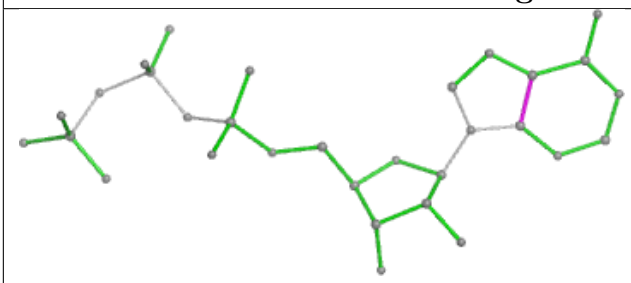


Torsions

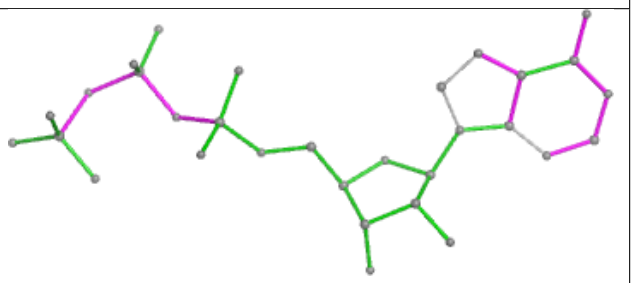


Rings

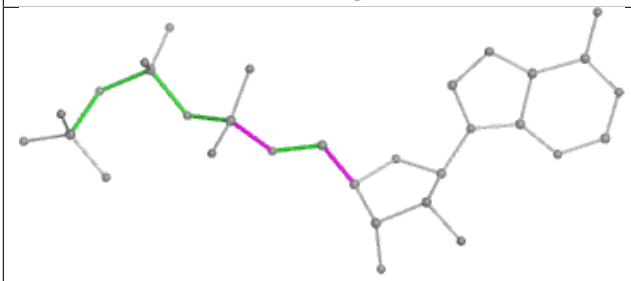
Ligand ATP C 4704



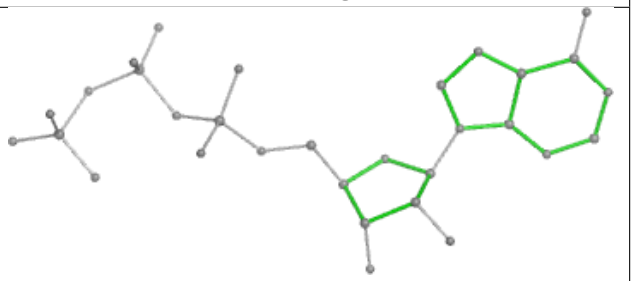
Bond lengths



Bond angles

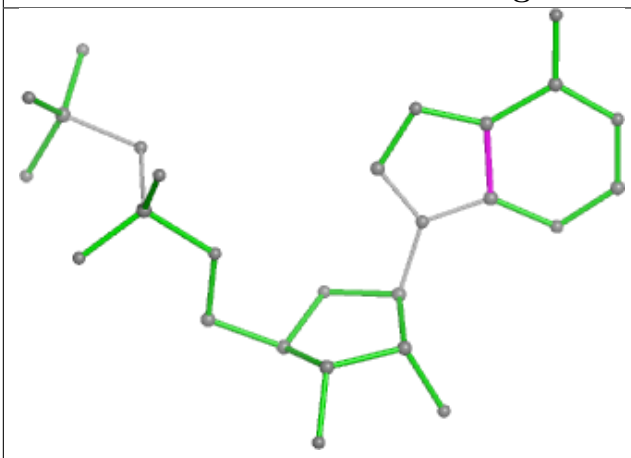


Torsions

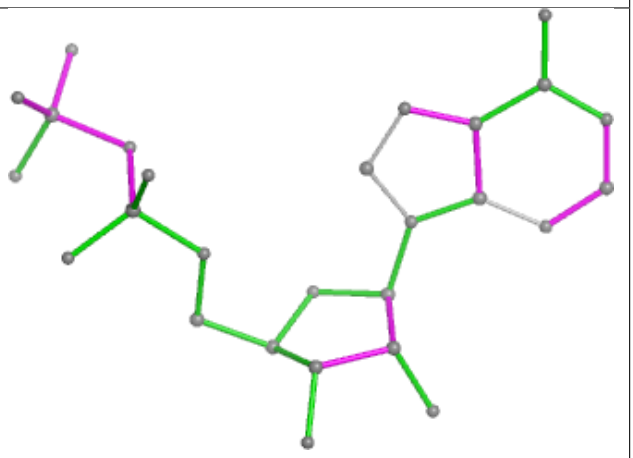


Rings

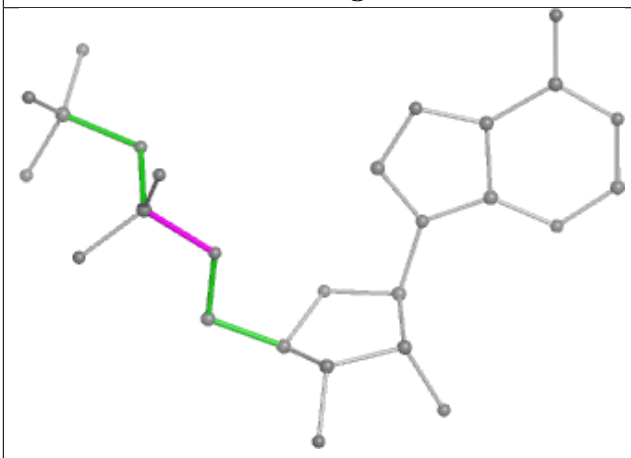
Ligand ADP C 4701



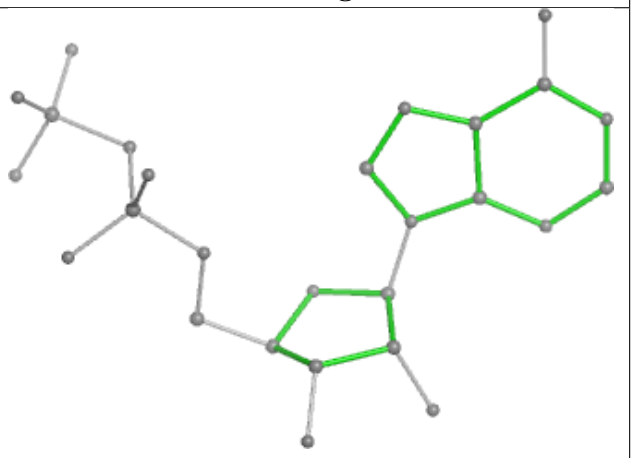
Bond lengths



Bond angles

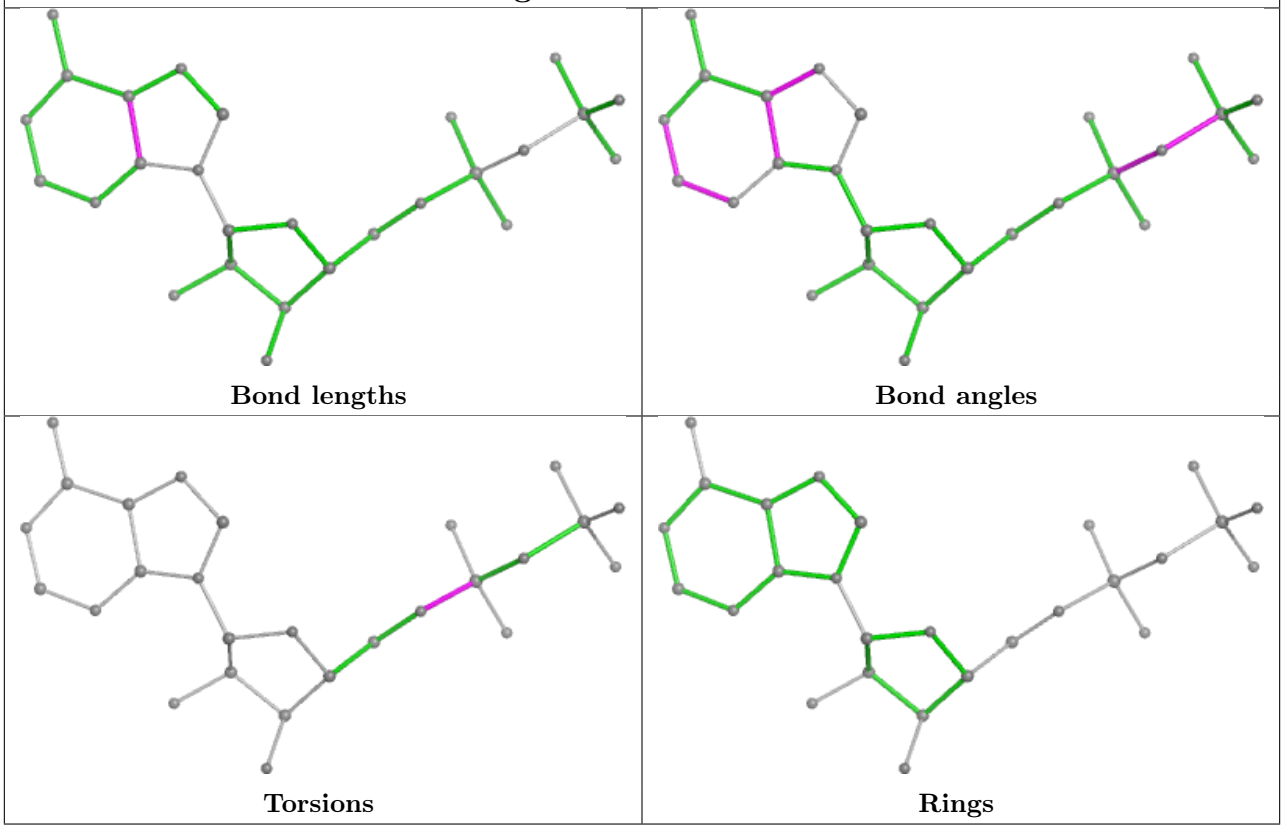


Torsions



Rings

Ligand ADP C 4703



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	22
2	B	13
3	C	9
5	e	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	389:ASP	C	390:THR	N	29.62
1	e	1233:LEU	C	1234:ALA	N	29.14
1	e	1201:ARG	C	1202:GLN	N	19.87
1	A	1299:VAL	C	1300:GLN	N	17.01

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	1251:GLU	C	1252:LYS	N	15.83
1	A	2300:SER	C	2301:ASP	N	13.90
1	A	2232:GLU	C	2233:PRO	N	13.47
1	B	4440:MET	C	4441:ILE	N	12.83
1	A	1507:PRO	C	1508:GLY	N	12.62
1	B	2495:LYS	C	2496:VAL	N	12.29
1	A	2533:PRO	C	2534:VAL	N	10.44
1	A	4018:CYS	C	4019:ILE	N	10.38
1	B	2583:MET	C	2584:VAL	N	9.42
1	A	2296:ALA	C	2297:GLY	N	9.01
1	A	4109:ASN	C	4110:ALA	N	8.24
1	A	2058:THR	C	2059:LEU	N	8.10
1	A	2897:GLN	C	2898:ARG	N	6.96
1	A	1972:PHE	C	1973:ASP	N	6.76
1	B	1775:VAL	C	1776:ARG	N	6.38
1	A	2132:ALA	C	2133:GLY	N	5.82
1	A	3472:THR	C	3473:ILE	N	5.79
1	A	3921:LYS	C	3922:THR	N	5.38
1	B	2658:SER	C	2659:GLY	N	5.09
1	A	2630:GLU	C	2631:ALA	N	4.86
1	B	2091:ARG	C	2092:GLY	N	4.86
1	B	3793:ASP	C	3794:GLU	N	4.34
1	A	1725:GLY	C	1726:TYR	N	4.16
1	A	2000:LEU	C	2001:MET	N	3.91
1	A	2612:GLU	C	2613:THR	N	3.44
1	B	4123:ASP	C	4124:PRO	N	3.30
1	B	2229:LYS	C	2230:THR	N	3.20
1	B	3552:ASN	C	3553:LEU	N	3.19
1	A	2495:ASP	C	2496:MET	N	3.16
1	B	2702:LYS	C	2703:ALA	N	3.15
1	B	2006:PRO	C	2007:GLY	N	3.09
1	A	1592:ARG	C	1593:SER	N	3.08
1	A	2176:THR	C	2177:ILE	N	3.05
1	B	1212:ILE	C	1213:PRO	N	2.70
1	C	3218:LYS	C	3219:ASP	N	1.19
1	C	3227:LYS	C	3228:LYS	N	1.19
1	C	3311:ASN	C	3312:GLN	N	1.19
1	C	3216:GLU	C	3217:SER	N	1.18
1	C	3225:ALA	C	3226:ASN	N	1.18
1	C	3234:LYS	C	3235:TYR	N	1.18
1	C	3272:SER	C	3273:TYR	N	1.18
1	C	3304:GLU	C	3305:LEU	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3334:LYS	C	3335:TRP	N	1.18

6 Map visualisation

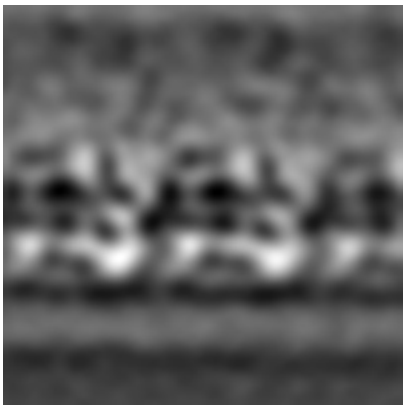
This section contains visualisations of the EMDB entry EMD-16304. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

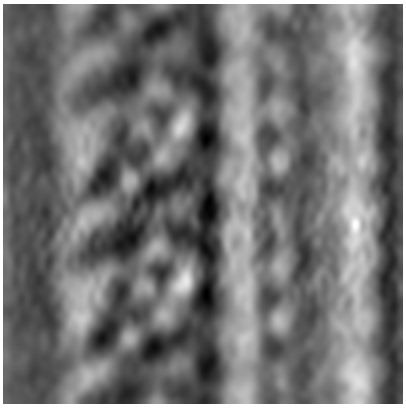
X



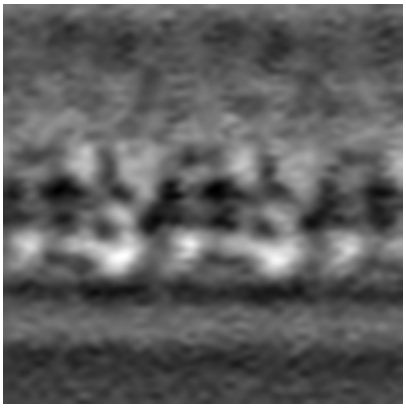
Y

Z

6.1.2 Raw map



X



Y

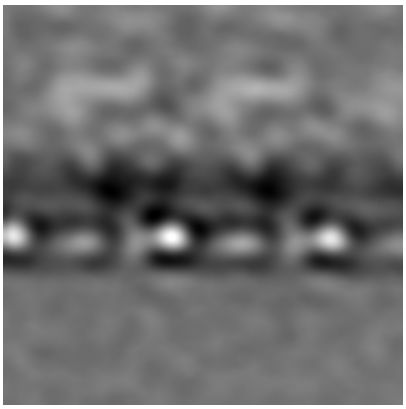
Z

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

6.2 Central slices (i)

6.2.1 Primary map

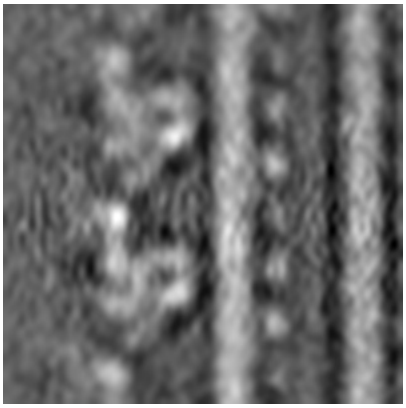
X Index: 37



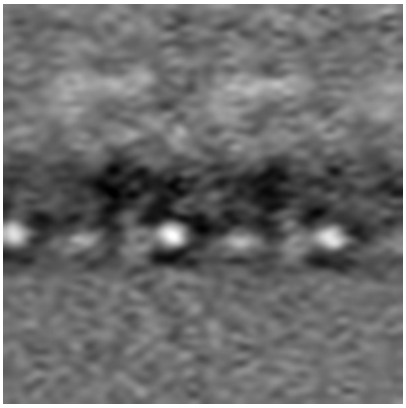
Y Index: 37

Z Index: 37

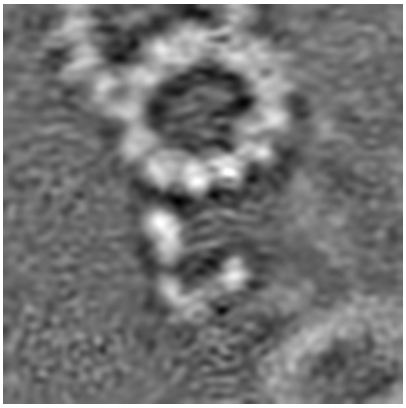
6.2.2 Raw map



X Index: 37



Y Index: 37



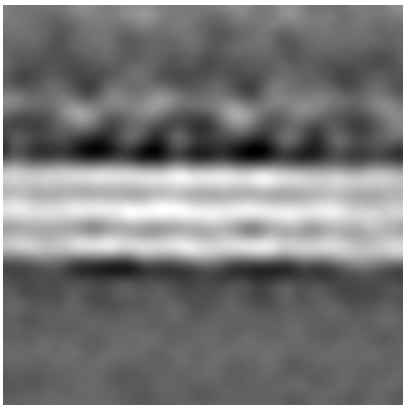
Z Index: 37

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

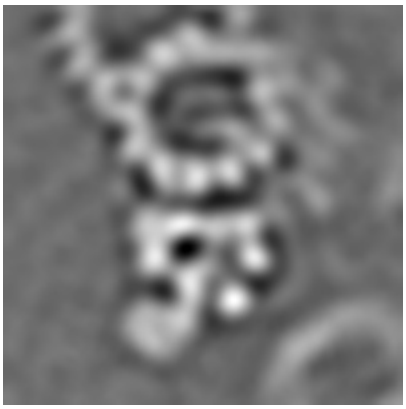
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 29

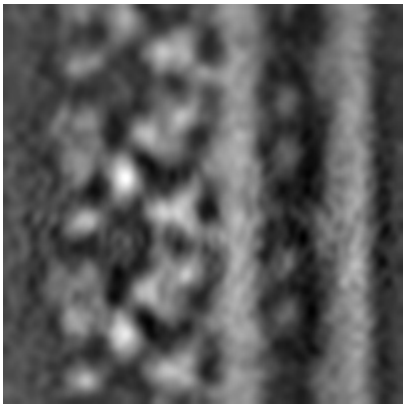


Y Index: 42

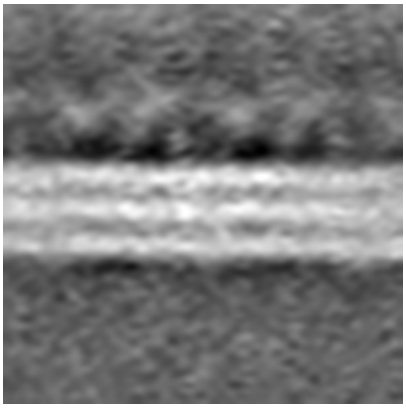


Z Index: 22

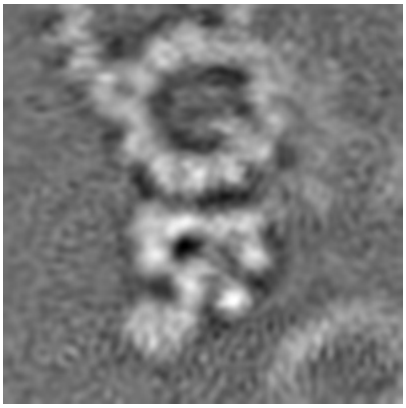
6.3.2 Raw map



X Index: 29



Y Index: 42

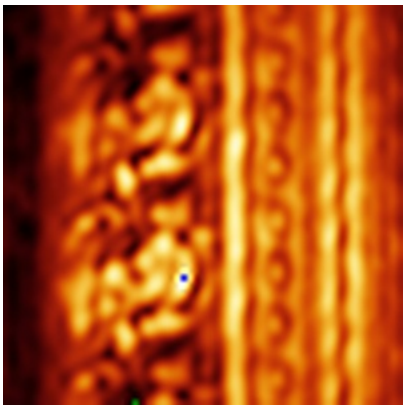


Z Index: 22

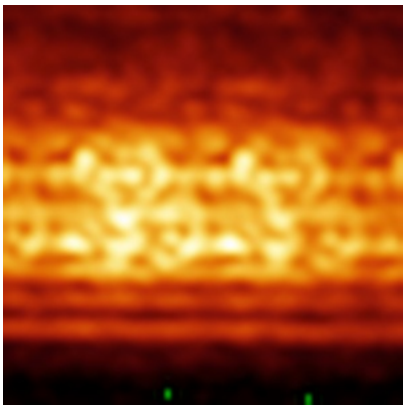
The images above show the largest variance slices of the map in three orthogonal directions.

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

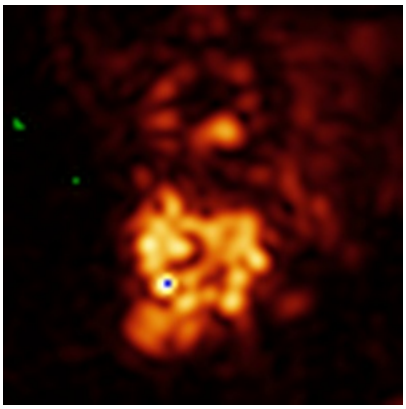
6.4.1 Primary map



X

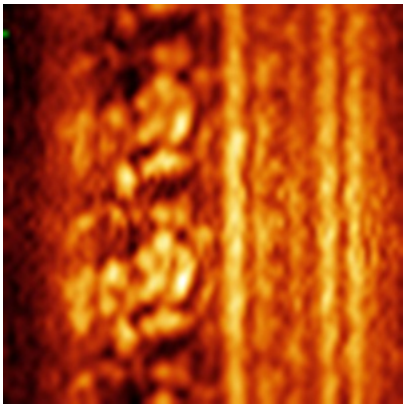


Y

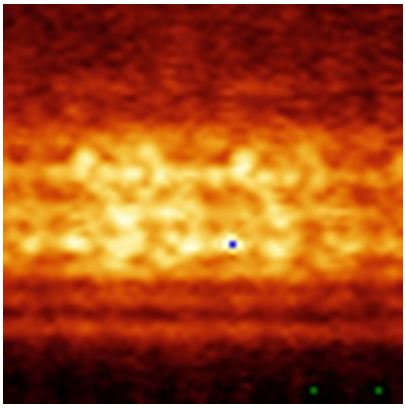


Z

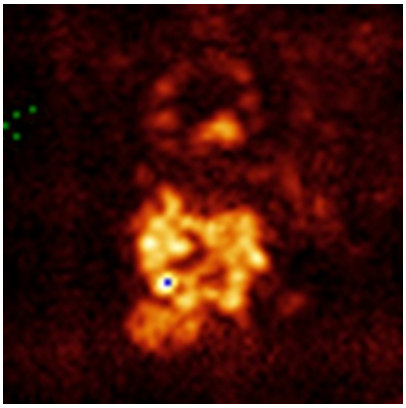
6.4.2 Raw map



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 0.07. 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.

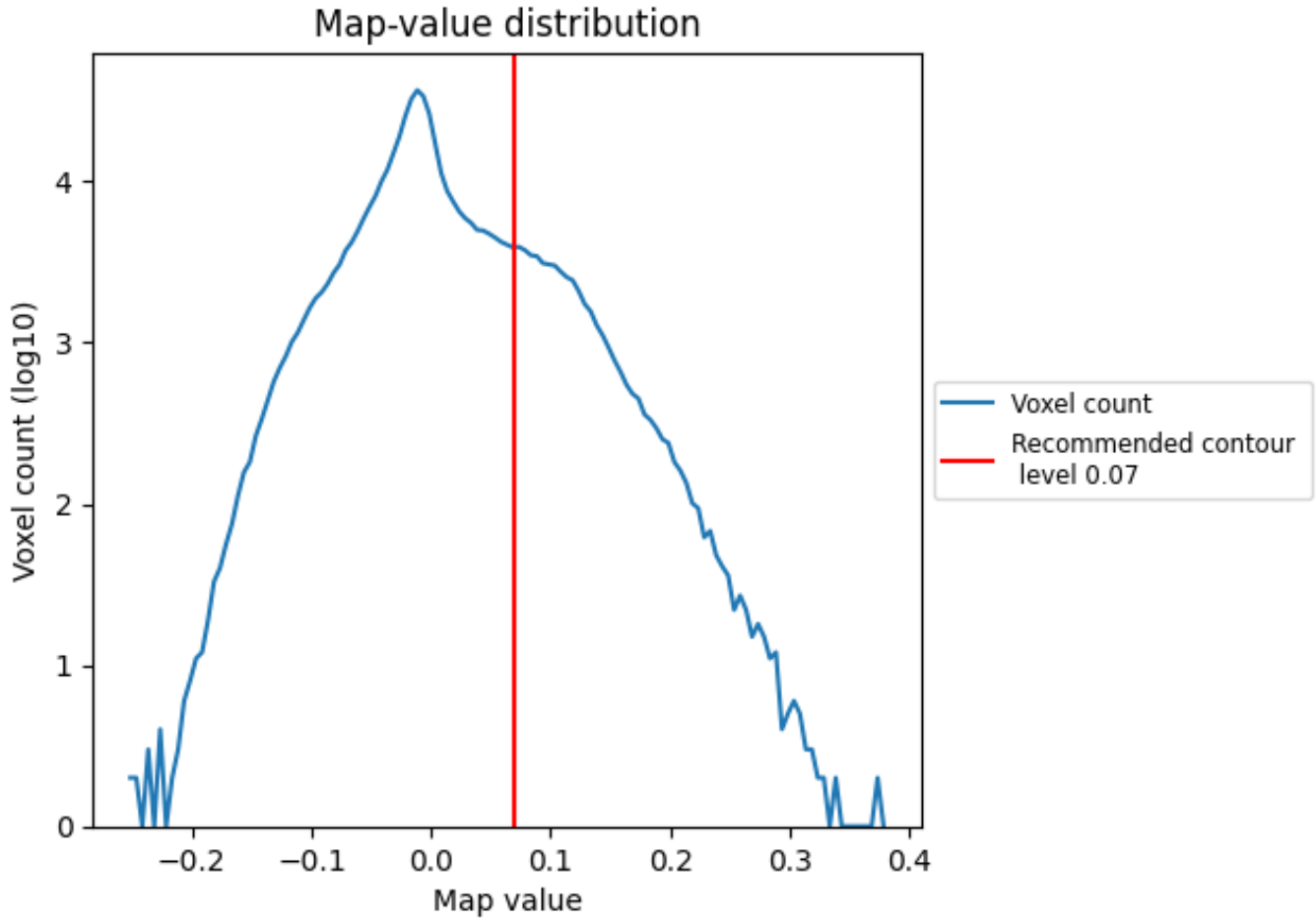
6.6 Mask visualisation (i)

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

7 Map analysis

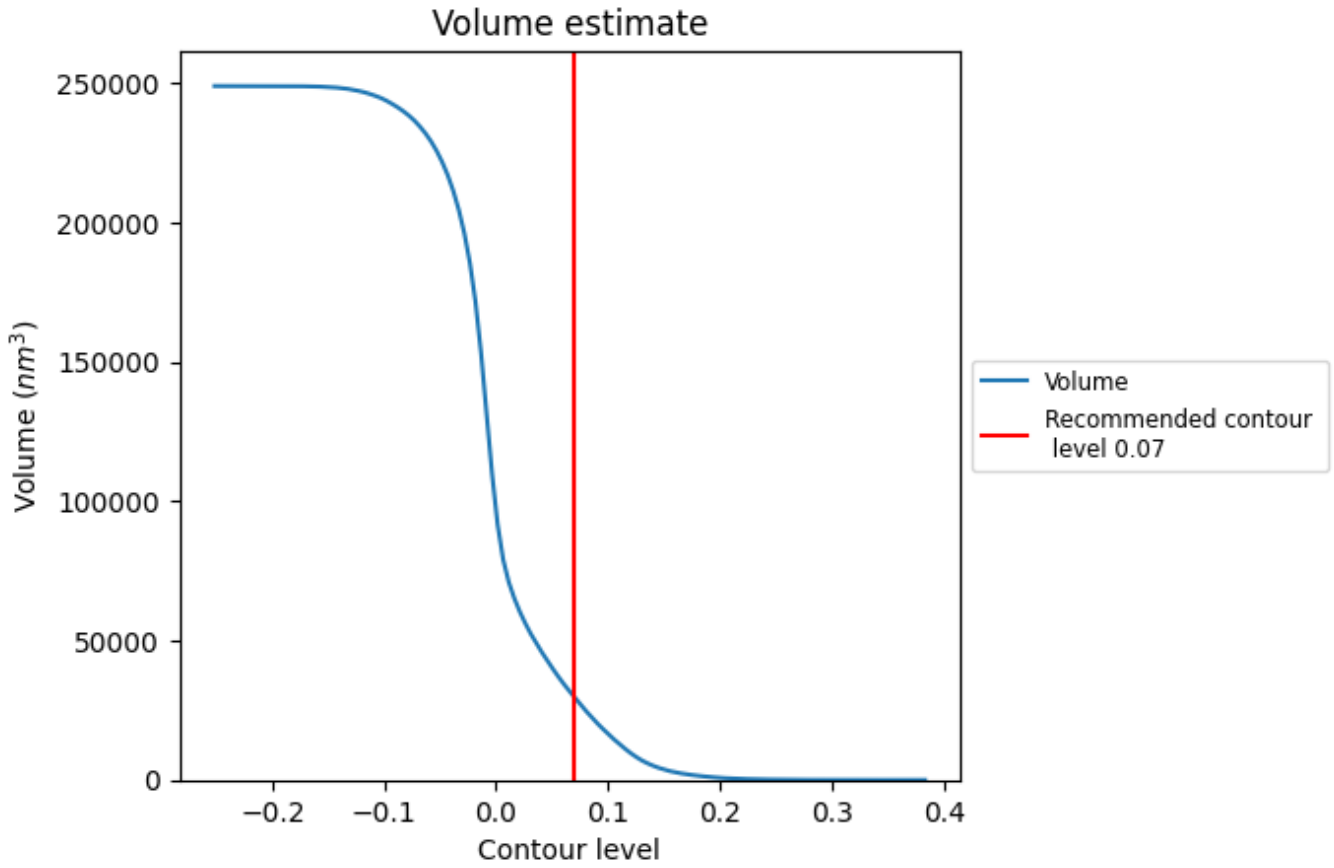
This section contains the results of statistical analysis of the map.

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.

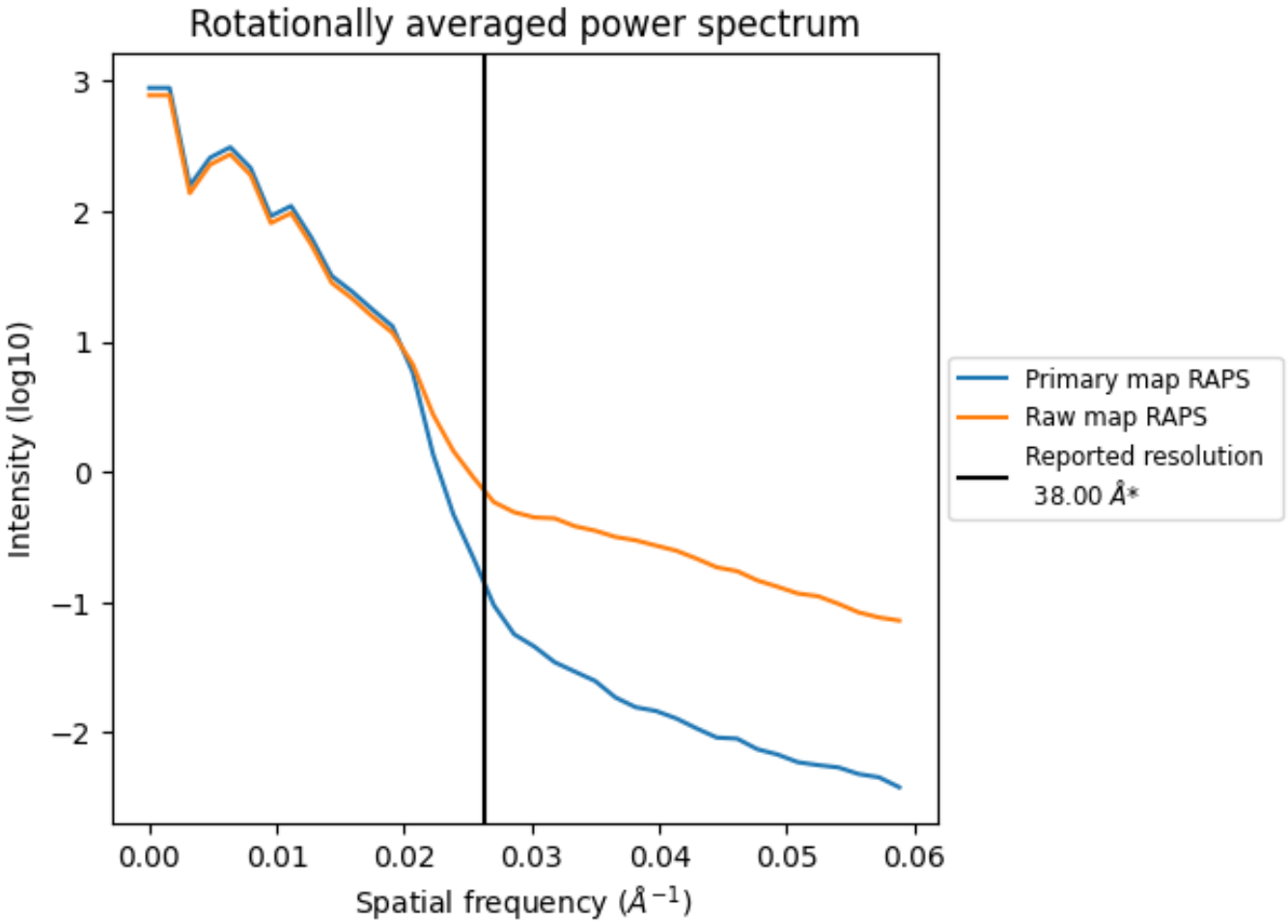
7.2 Volume estimate



The volume at the recommended contour level is 29745 nm^3; this corresponds to an approximate mass of 26870 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)

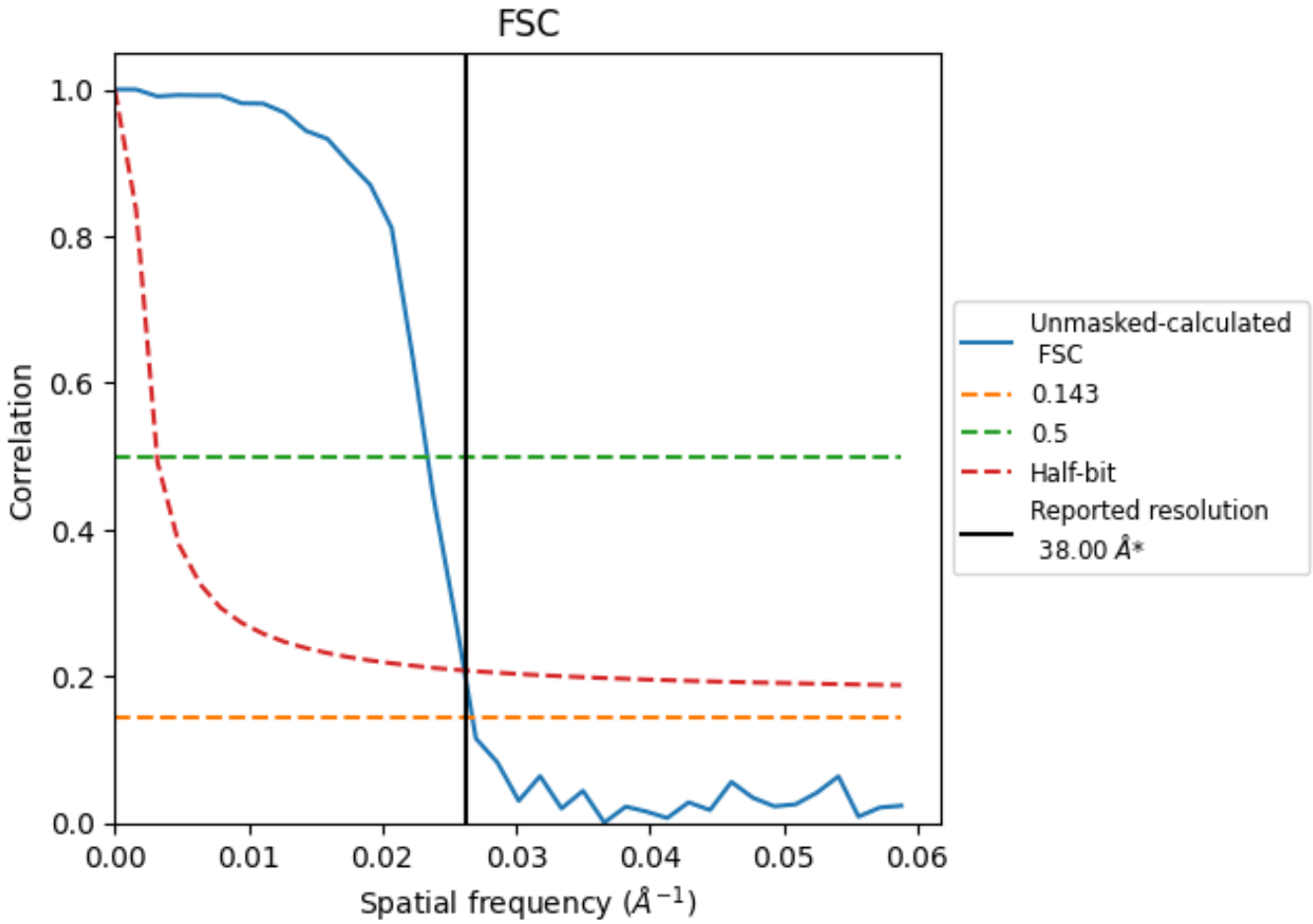


*Reported resolution corresponds to spatial frequency of 0.026 Å^{-1}

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 0.026 Å^{-1}

8.2 Resolution estimates (i)

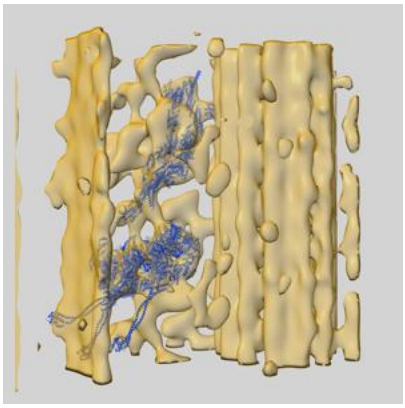
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	38.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	37.31	42.74	38.17

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

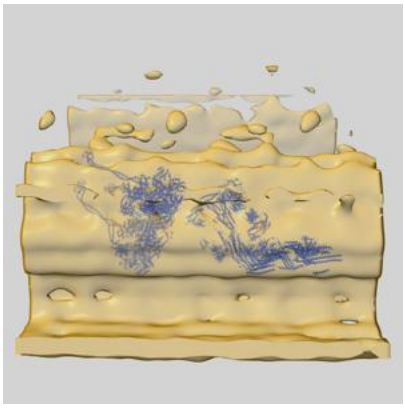
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16304 and PDB model 8BWY. Per-residue inclusion information can be found in section 3 on page 9.

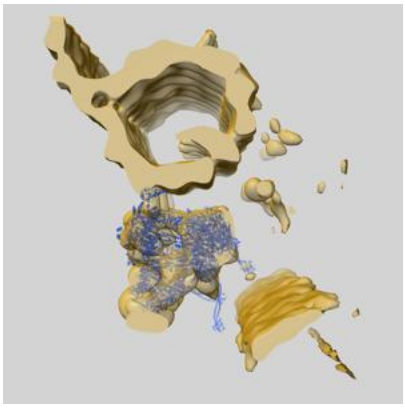
9.1 Map-model overlay



X



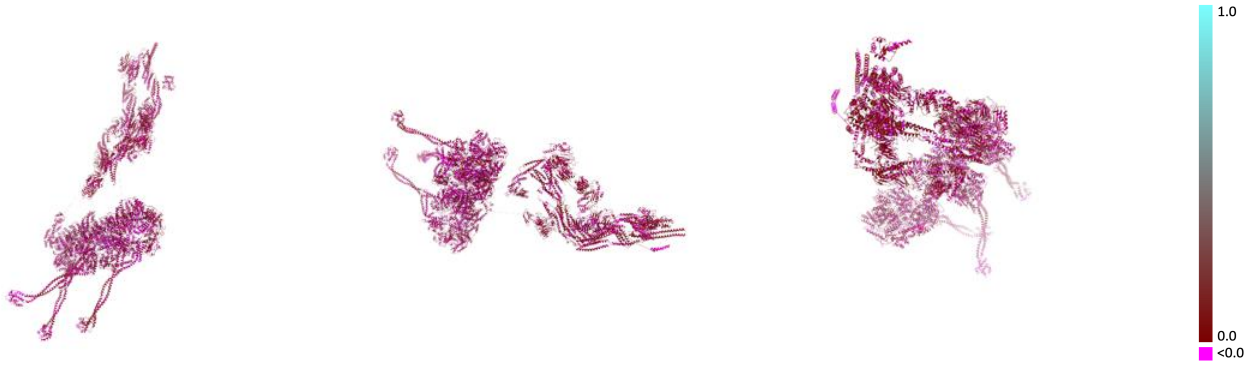
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

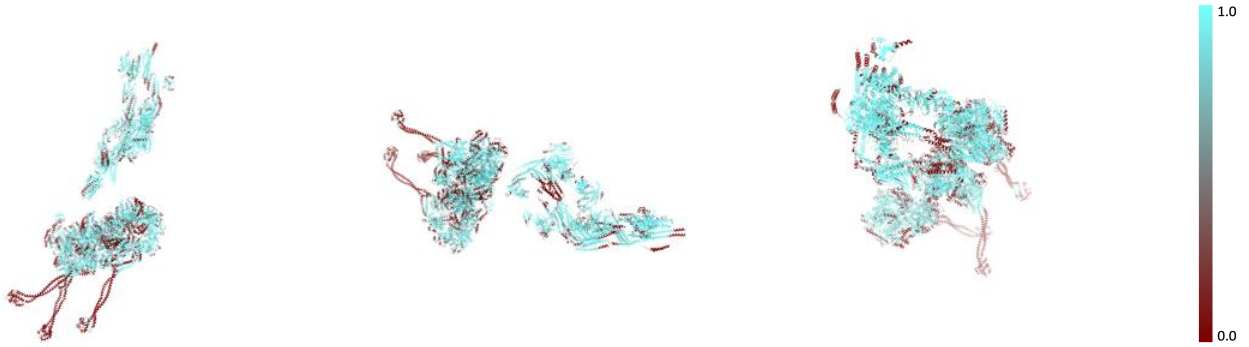
9.2 Q-score mapped to coordinate model (i)



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.

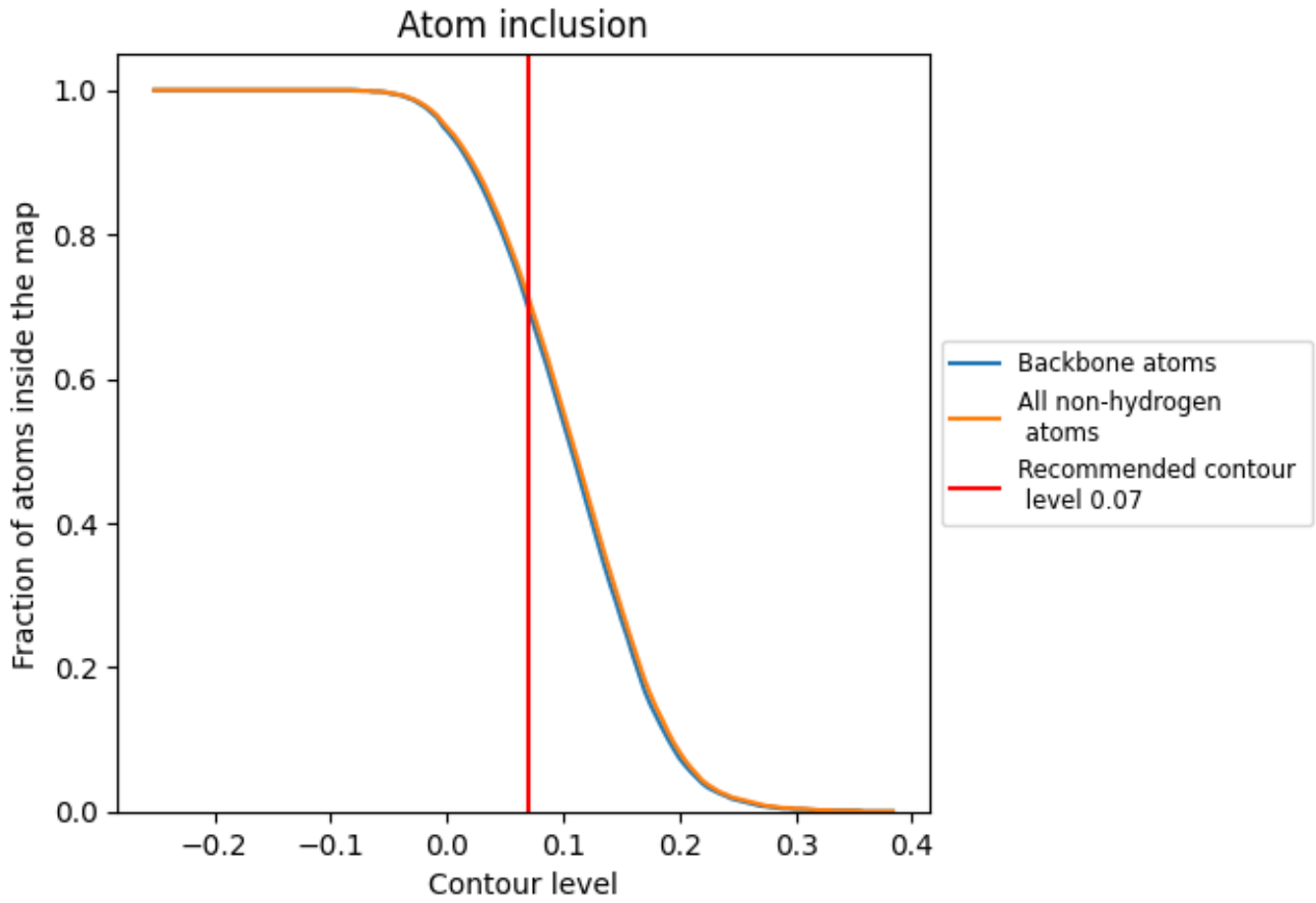
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 71% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7120	0.0390
A	0.6750	0.0370
B	0.6630	0.0380
C	0.7000	0.0390
F	0.8470	0.0450
G	0.8310	0.0380
H	0.9050	0.0530
I	0.8240	0.0560
J	0.9210	0.0690
K	0.7370	0.0400
L	0.7260	0.0150
M	0.9820	0.0700
N	0.9300	0.0450
O	0.8320	0.0260
P	0.9330	0.0590
T	0.6940	0.0350
V	0.7880	0.0600
d	0.9190	0.0420
e	0.7580	0.0260
x	0.6910	0.0510