Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 03:29 AM EST

PDB ID	:	7UA4
EMDB ID	:	EMD-26414
Title	:	Structure of PKA phosphorylated human RyR2-R2474S in the open state in the presence of Calmodulin
Authors	:	Miotto, M.C.; Marks, A.R.
Deposited on	:	2022-03-11
Resolution	:	2.93 Å(reported)
Based on initial model	:	7UA3

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

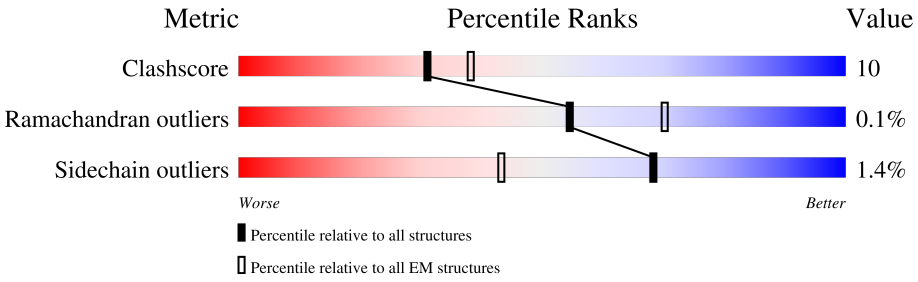
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.93 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	4967	6% 69% 18% • 12%
1	B	4967	6% 69% 18% • 12%
1	C	4967	7% 69% 19% 12%
1	D	4967	6% 69% 18% • 12%
2	E	108	77% 20% •••
2	F	108	77% 20% •••
2	G	108	75% 22% •••
2	H	108	77% 20% •••

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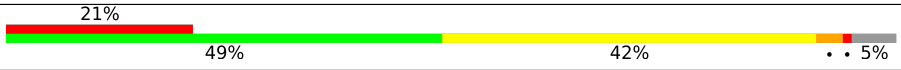
Mol	Chain	Length	Quality of chain
3	I	149	
3	J	149	
3	K	149	
3	L	149	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 147856 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
1	B	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
1	C	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		
1	D	4369	Total	C	N	O	S	2	0
			34959	22247	5957	6525	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	G	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

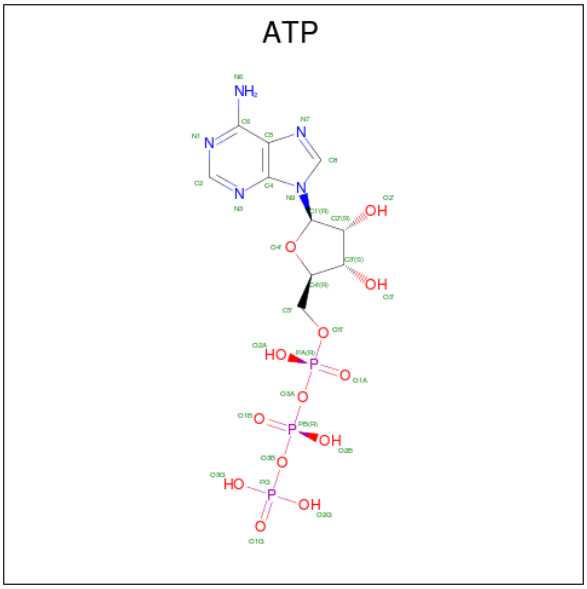
- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	J	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	K	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		
3	L	142	Total	C	N	O	S	0	0
			1112	687	181	234	10		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	

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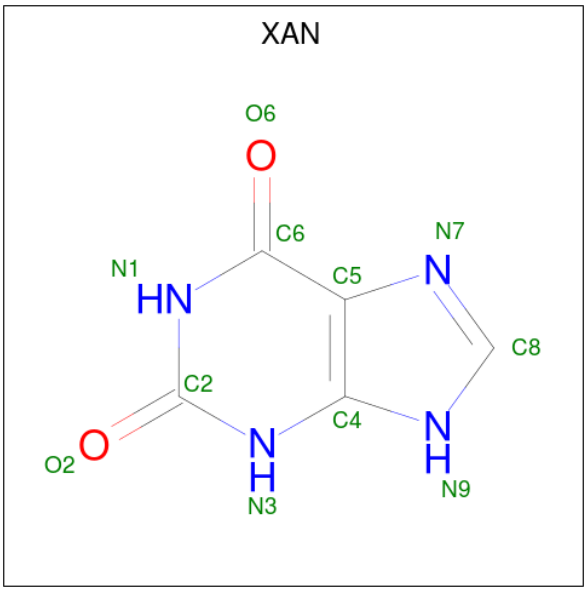
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	B	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	C	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	D	1	Total	C	N	O	P	0
			62	20	10	26	6	
5	D	1	Total	C	N	O	P	0
			62	20	10	26	6	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	
6	C	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	

- Molecule 7 is XANTHINE (three-letter code: XAN) (formula: $C_5H_4N_4O_2$) (labeled as "Ligand of Interest" by depositor).



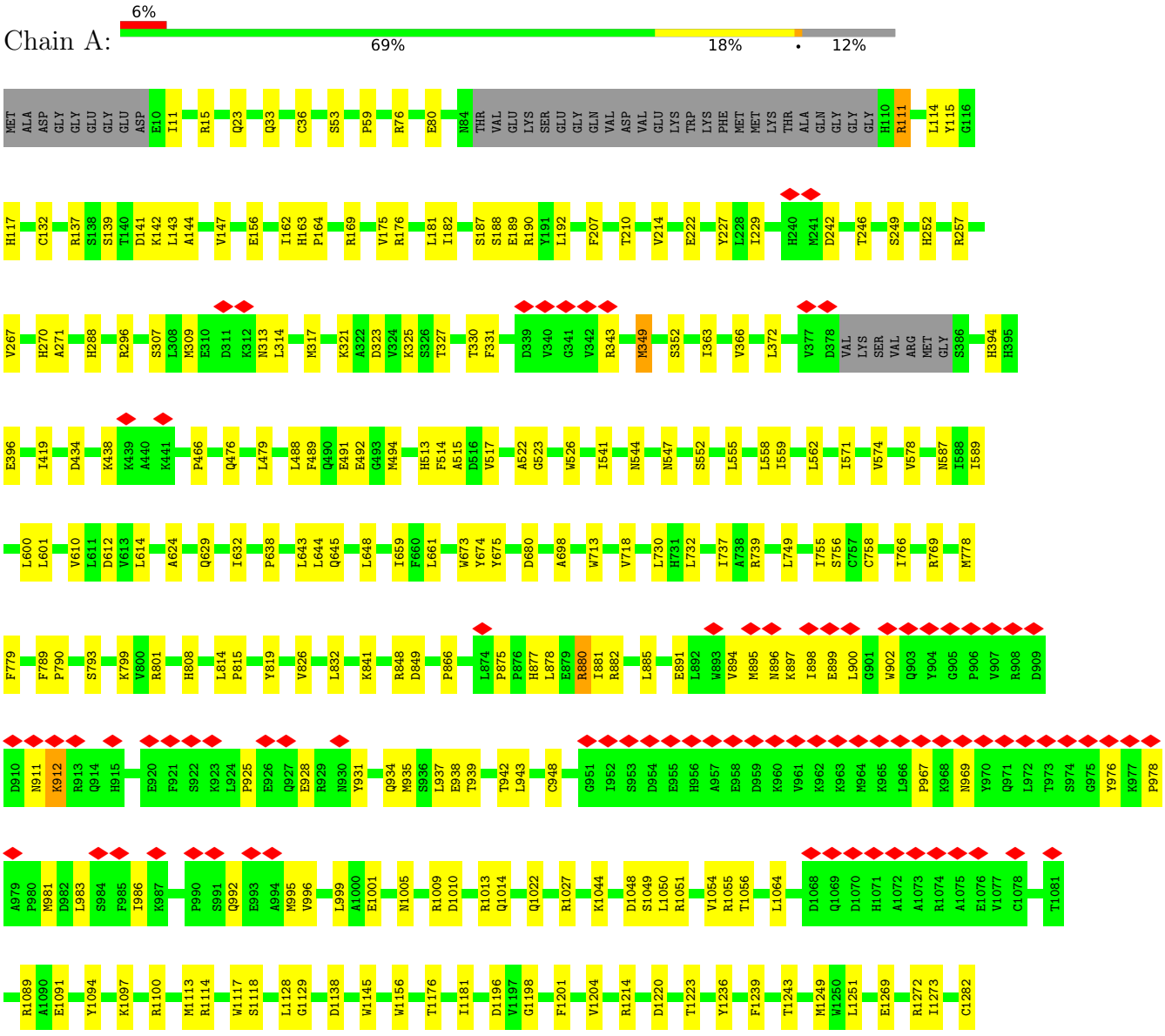
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 11 5 4 2	0
7	B	1	Total C N O 11 5 4 2	0
7	C	1	Total C N O 11 5 4 2	0
7	D	1	Total C N O 11 5 4 2	0

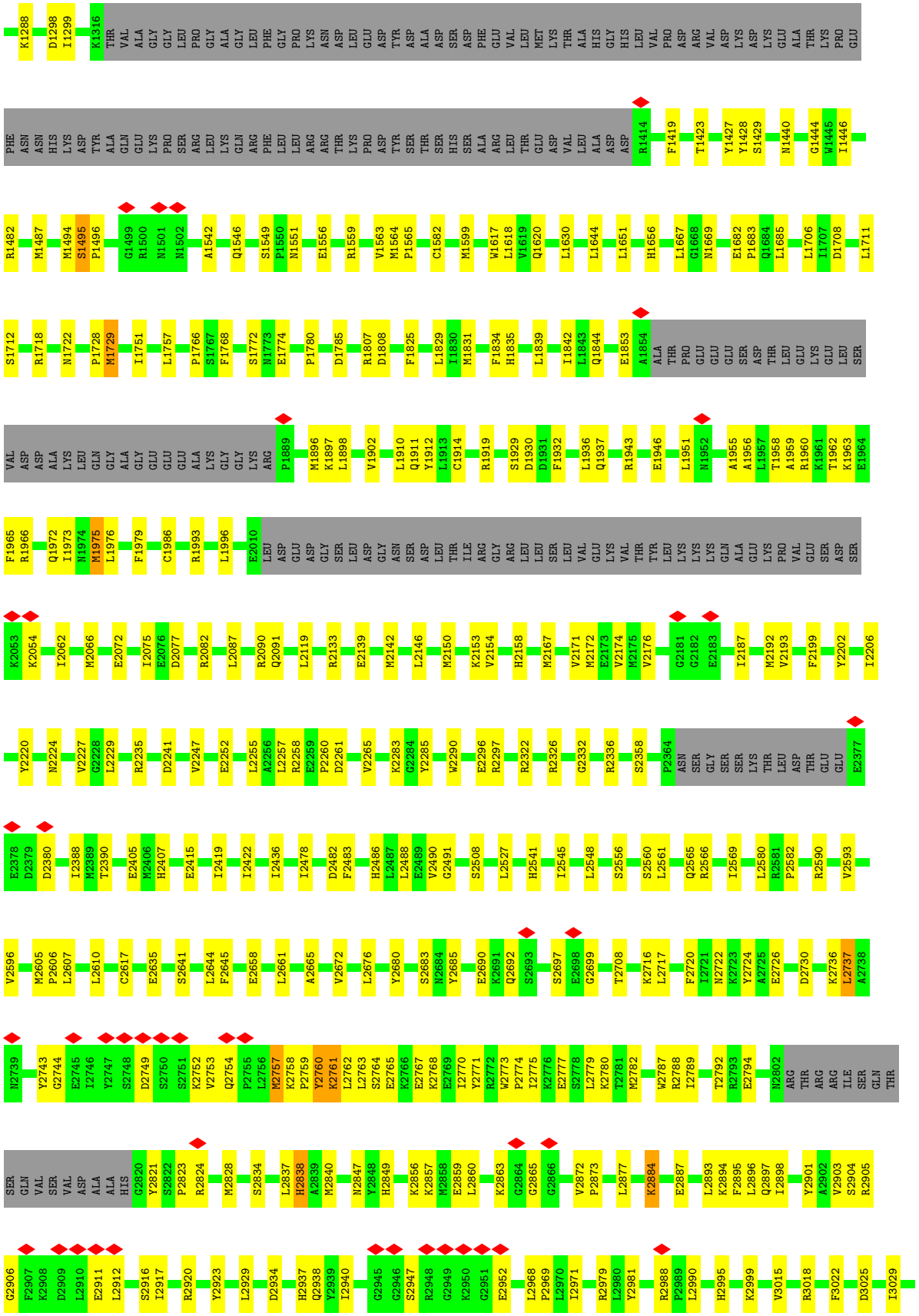
3 Residue-property plots (i)

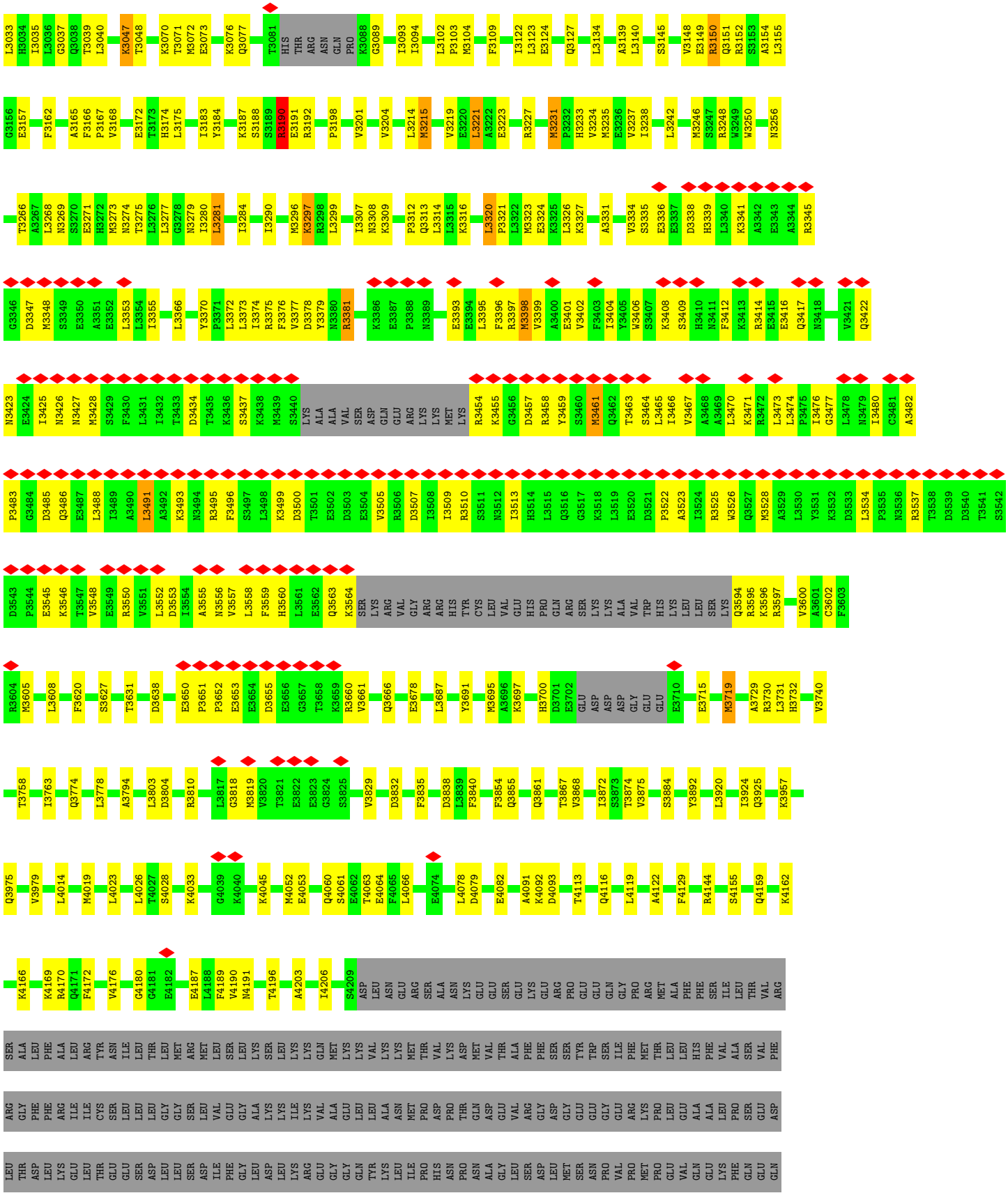
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ryanodine receptor 2

Chain A:




K1288 D1298 I1299 K1316
PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP R1414 F1419 T1423 Y1427 Y1428 S1429 N1440 G1444 W1445 I1446
R1482 M1487 M1494 S1495 P1496 G1499 R1500 N1501 N1502 A1542 Q1546 S1549 P1550 N1551 E1556 R1559 V1563 M1564 P1565 C1582 M1599 W1617 L1618 V1619 Q1620 L1630 L1644 L1651 H1656 L1667 G1668 N1669 E1682 P1683 Q1684 L1685 L1706 I1707 D1708 L1711
S1712 R1718 N1722 P1728 M1729 I1751 L1757 P1766 S1767 F1768 S1772 N1773 E1774 P1780 D1785 R1807 D1808 F1825 L1829 I1830 M1831 F1834 H1835 L1839 I1842 L1843 Q1844 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR LEU GLU LYS GLU LEU SER
VAL ASP ASP ALA LYS LEU GLN GLY GLU GLY GLU GLU ALA LYS GLY GLY LYS ARG P1889 M1896 K1897 L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 R1919 S1929 D1930 D1931 F1932 L1936 Q1937 R1943 E1946 L1951 N1952 A1955 A1956 L1957 T1958 A1959 R1960 K1961 T1962 K1963 E1964
F1965 R1966 Q1972 I1973 N1974 M1975 L1976 F1979 C1986 R1993 L1996 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL GLU SER ASP SER
K2053 K2054 I2062 M2066 E2072 I2075 E2076 D2077 R2082 L2087 R2090 Q2091 L2119 R2133 E2139 M2142 L2146 M2150 K2153 V2154 H2158 M2167 V2171 M2172 E2173 V2174 M2175 V2176 G2181 G2182 E2183 I2187 M2192 V2193 F2199 Y2202 I2206
Y2220 N2224 V2227 G2228 L2229 R2235 D2241 V2247 E2252 L2255 A2256 L2257 R2258 E2259 P2260 D2261 V2265 K2283 G2284 Y2285 W2290 E2296 R2297 R2322 R2326 G2332 R2336 S2358 P2364 ASN SER GLY SER SER LYS THR LEU ASP THR GLU GLU E2377
E2378 D2379 D2380 I2388 M2389 T2390 E2405 M2406 H2407 E2415 I2419 I2422 I2436 I2478 D2482 F2483 H2486 L2487 L2488 E2489 V2490 G2491 S2508 L2527 H2541 I2545 L2548 S2556 S2560 L2561 Q2565 R2566 I2569 L2580 R2581 P2582 R2590 V2593
V2596 M2605 P2606 L2607 L2610 C2617 E2635 S2641 L2644 F2645 E2658 L2661 A2665 V2672 L2676 Y2680 S2683 N2684 Y2685 E2690 K2691 Q2692 S2693 S2697 E2698 G2699 T2708 K2716 L2717 F2720 I2721 N2722 K2723 Y2724 A2725 E2726 D2730 K2736 L2737 A2738
N2739 Y2743 G2744 E2745 I2746 Y2747 S2748 D2749 S2750 S2751 K2752 V2753 Q2754 P2755 L2756 M2757 K2758 P2759 Y2760 K2761 L2762 L2763 S2764 E2765 K2766 E2767 K2768 E2769 I2770 Y2771 R2772 W2773 P2774 I2775 K2776 E2777 S2778 L2779 K2780 T2781 M2782 W2787 R2788 I2789 T2792 R2793 E2794 N2802 ARG THR ARG ARG ILE SER GLN THR
SER GLN VAL SER VAL ASP ALA ALA HIS G2820 Y2821 S2822 P2823 R2824 M2828 S2834 L2837 H2838 A2839 M2840 N2847 Y2848 H2849 K2856 K2857 M2858 E2859 L2860 K2863 G2864 G2865 G2866 V2872 P2873 L2877 K2884 E2887 L2893 K2894 F2895 L2896 Q2897 I2898 Y2901 A2902 V2903 S2904 R2905
G2906 F2907 K2908 D2909 L2910 E2911 L2912 S2916 I2917 R2920 Y2923 L2929 D2934 H2937 Q2938 Y2939 I2940 G2945 G2946 S2947 R2948 G2949 K2950 G2951 E2952 L2968 P2969 L2970 I2971 R2979 L2980 Y2981 R2988 P2989 L2990 H2995 K2999 V3015 R3018 F3022 D3025 I3029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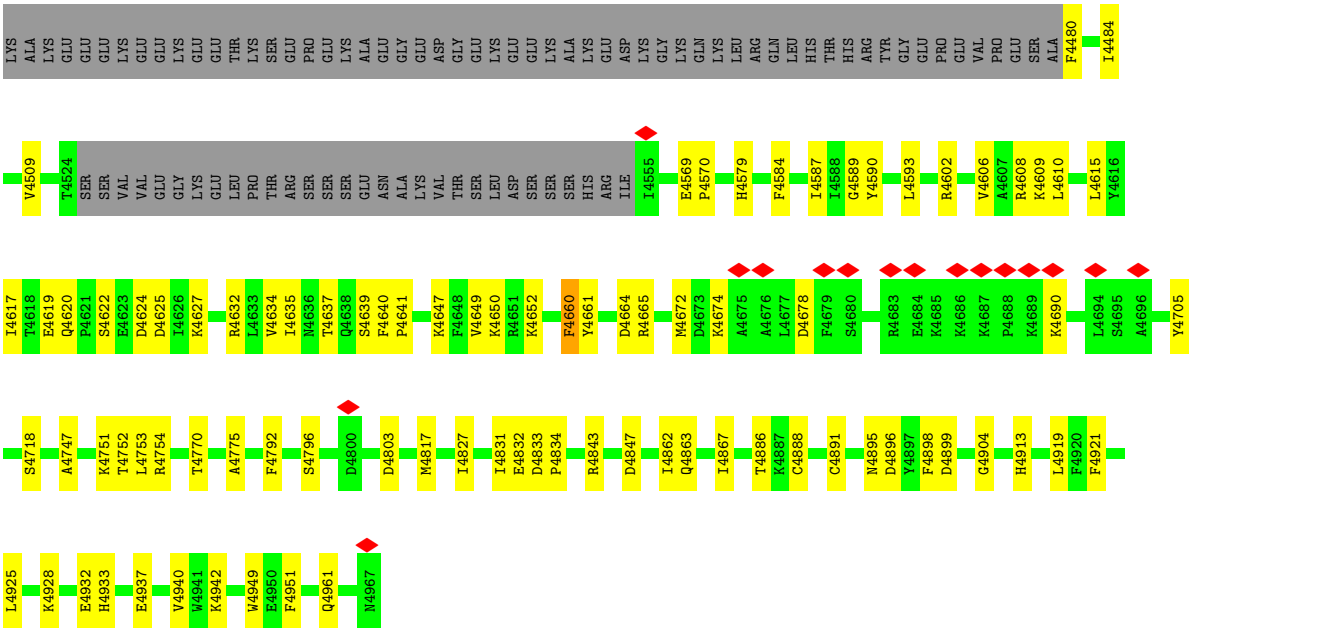
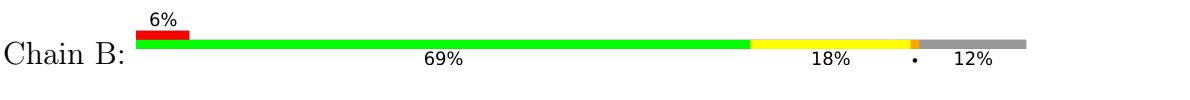
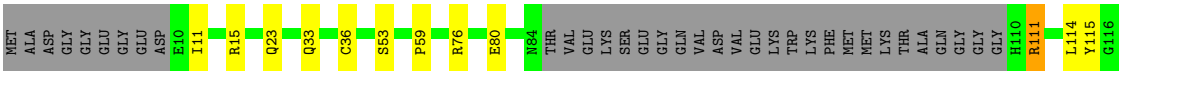
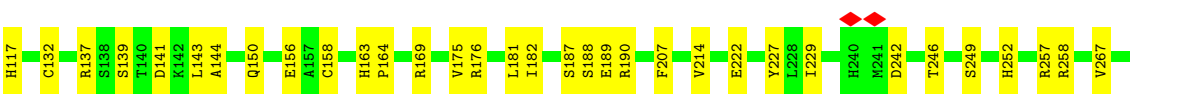
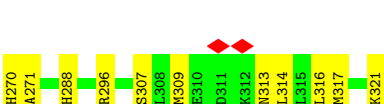
G3156 E3157 F3162 A3165 F3166 P3167 V3168 E3172 T3173 H3174 L3175 I3183 Y3184 K3187 S3188 S3189 R3190 E3191 R3192 P3198 V3201 V3204 L3214 M3215 V3219 E3220 L3221 A3222 E3223 R3227 M3231 P3232 H3233 V3234 M3235 E3236 V3237 I3238 L3242 M3246 S3247 R3248 W3249 W3250 N3256
T3266 A3267 L3268 N3269 S3270 E3271 H3272 M3273 N3274 T3275 L3276 L3277 G3278 N3279 I3280 L3281 I3284 I3290 M3296 K3297 R3298 L3299 I3307 N3308 K3309 P3312 Q3313 L3314 L3315 K3316 L3320 P3321 L3322 M3323 E3324 K3325 L3326 K3327 A3331 V3334 S3335 E3336 E3337 D3338 H3339 L3340 K3341 A3342 E3343 A3344 R3345
G3346 D3347 M3348 S3349 E3350 A3351 E3352 L3353 L3354 I3355 L3366 Y3370 P3371 L3372 L3373 I3374 R3375 F3376 V3377 D3378 Y3379 N3380 R3381 K3386 E3387 P3388 N3389 E3393 E3394 L3395 F3396 R3397 M3398 V3399 A3400 E3401 V3402 F3403 I3404 Y3405 W3406 S3407 K3408 S3409 H3410 N3411 F3412 K3413 R3414 E3415 E3416 Q3417 N3418 V3421 Q3422
N3423 E3424 I3425 N3426 N3427 M3428 S3429 F3430 L3431 I3432 T3433 D3434 T3435 K3436 S3437 K3438 M3439 S3440 LYS ALA ALA VAL SER ASP GLN GLU ARG LYS LYS MET LYS R3454 K3455 G3456 D3457 R3458 Y3459 S3460 M3461 Q3462 T3463 S3464 L3465 I3466 V3467 A3468 A3469 L3470 K3471 R3472 L3473 L3474 P3475 I3476 G3477 L3478 N3479 I3480 C3481 A3482
P3483 G3484 D3485 Q3486 E3487 L3488 I3489 A3490 L3491 A3492 K3493 N3494 R3495 F3496 S3497 L3498 K3499 D3500 T3501 E3502 D3503 E3504 V3505 R3506 D3507 I3508 I3509 R3510 S3511 N3512 I3513 H3514 L3515 Q3516 G3517 K3518 L3519 E3520 D3521 P3522 A3523 I3524 R3525 W3526 Q3527 M3528 A3529 L3530 Y3531 K3532 D3533 L3534 P3535 N3536 R3537 T3538 D3539 D3540 T3541 S3542
D3543 P3544 E3545 K3546 T3547 V3548 E3549 R3550 V3551 L3552 D3553 I3554 A3555 N3556 V3557 L3558 F3559 H3560 L3561 E3562 Q3563 K3564 SER LYS ARG VAL GLY ARG ARG HIS TYR CYS LEU VAL GLU HIS PRO GLN ARG SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS Q3594 R3595 K3596 R3597 V3600 A3601 C3602 F3603
R3604 M3605 L3608 F3620 S3627 T3631 D3638 E3650 P3651 P3652 E3653 E3654 D3655 E3656 G3657 T3658 K3659 R3660 V3661 Q3666 E3678 L3687 Y3691 M3695 A3696 K3697 H3700 D3701 E3702 GLU ASP ASP ASP GLY GLU GLU E3710 E3715 M3719 A3729 R3730 L3731 H3732 V3740
T3758 I3763 Q3774 L3778 A3794 L3803 D3804 R3810 L3817 G3818 M3819 V3820 T3821 E3822 E3823 G3824 S3825 V3829 D3832 F3835 D3838 L3839 F3840 F3854 Q3855 Q3861 T3867 V3868 I3872 S3873 T3874 V3875 S3884 Y3892 L3920 I3924 Q3925 K3957
Q3975 V3979 L4014 M4019 L4023 L4026 T4027 S4028 K4033 G4039 K4040 K4045 M4052 E4053 Q4060 S4061 E4062 T4063 E4064 F4065 L4066 E4074 L4078 D4079 E4082 A4091 K4092 D4093 T4113 Q4116 L4119 A4122 F4129 R4144 S4155 Q4159 K4162
K4166 K4169 R4170 Q4171 F4172 V4176 G4180 G4181 E4182 E4187 L4188 F4189 V4190 N4191 T4196 A4203 I4206 S4209 ASP LEU ASN GLU ARG SER ALA ASN LYS GLU GLU SER GLU LYS GLU ARG PRO GLU GLU GLN GLY PRO ARG MET ALA PHE PHE SER ILE LEU THR VAL ARG
SER ALA LEU PHE ALA LEU ARG TYR ASN ILE LEU THR LEU MET ARG MET LEU SER LEU LYS SER LEU LYS LYS GLN MET LYS LYS VAL LYS LYS MET THR VAL LYS ASP MET VAL THR ALA PHE PHE SER SER TYR TRP SER ILE PHE MET THR LEU LEU LEU HIS PHE VAL ALA SER VAL PHE
ARG GLY PHE PHE ARG ILE ILE CYS SER LEU LEU LEU GLY GLY SER LEU VAL GLU GLY ALA LYS LYS ILE LYS VAL ALA GLU LEU LEU GLU ALA ASN MET PRO ASP PRO THR GLN ASP GLU VAL ARG GLY ASP GLY GLU GLU GLU GLY GLU ARG LYS PRO LEU GLU GLU ALA ALA LEU PRO SER GLU GLU ASP
LEU THR ASP LEU LYS GLU LEU THR GLU SER GLU GLU SER ASP ILE PHE GLY LEU ASP LEU LYS ARG GLU GLY GLY GLN TYR LYS LEU ILE PRO HIS ASN PRO ASN ALA GLY LEU SER ASP LEU MET SER ASN PRO VAL PRO MET PRO GLU VAL GLN GLU LYS PHE GLN GLU GLN





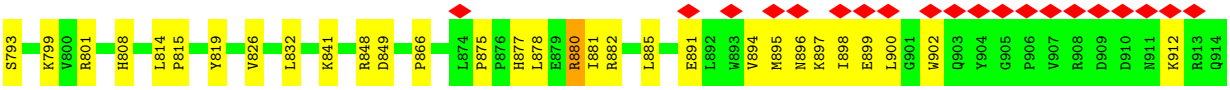


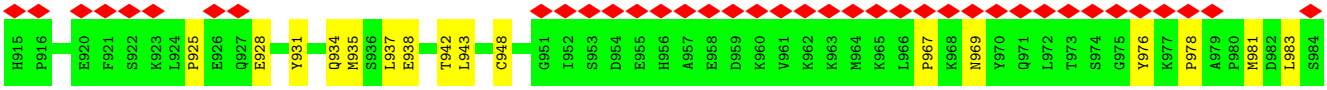


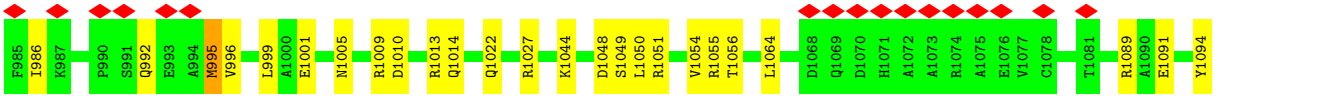


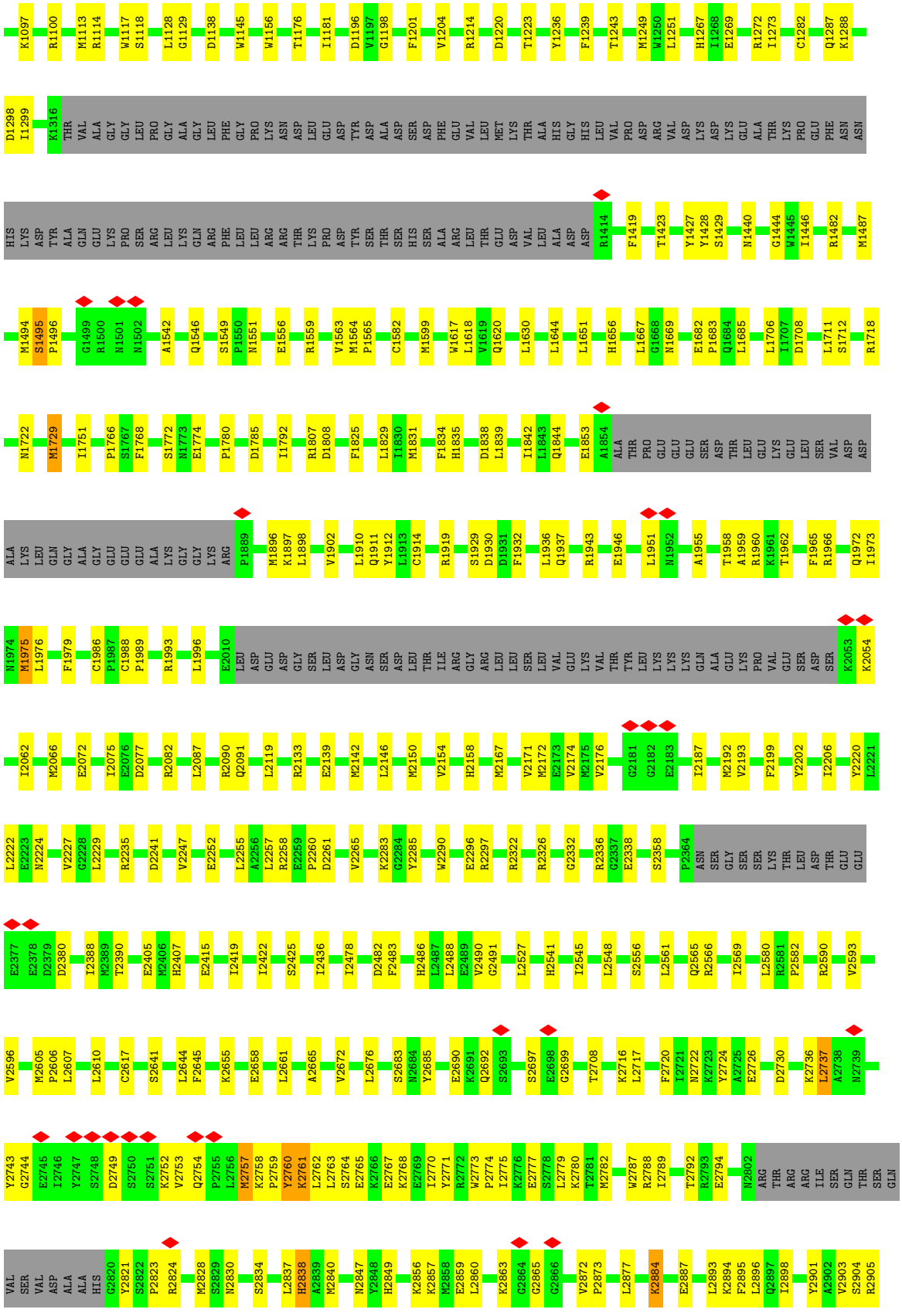
• Molecule 1: Ryanodine receptor 2

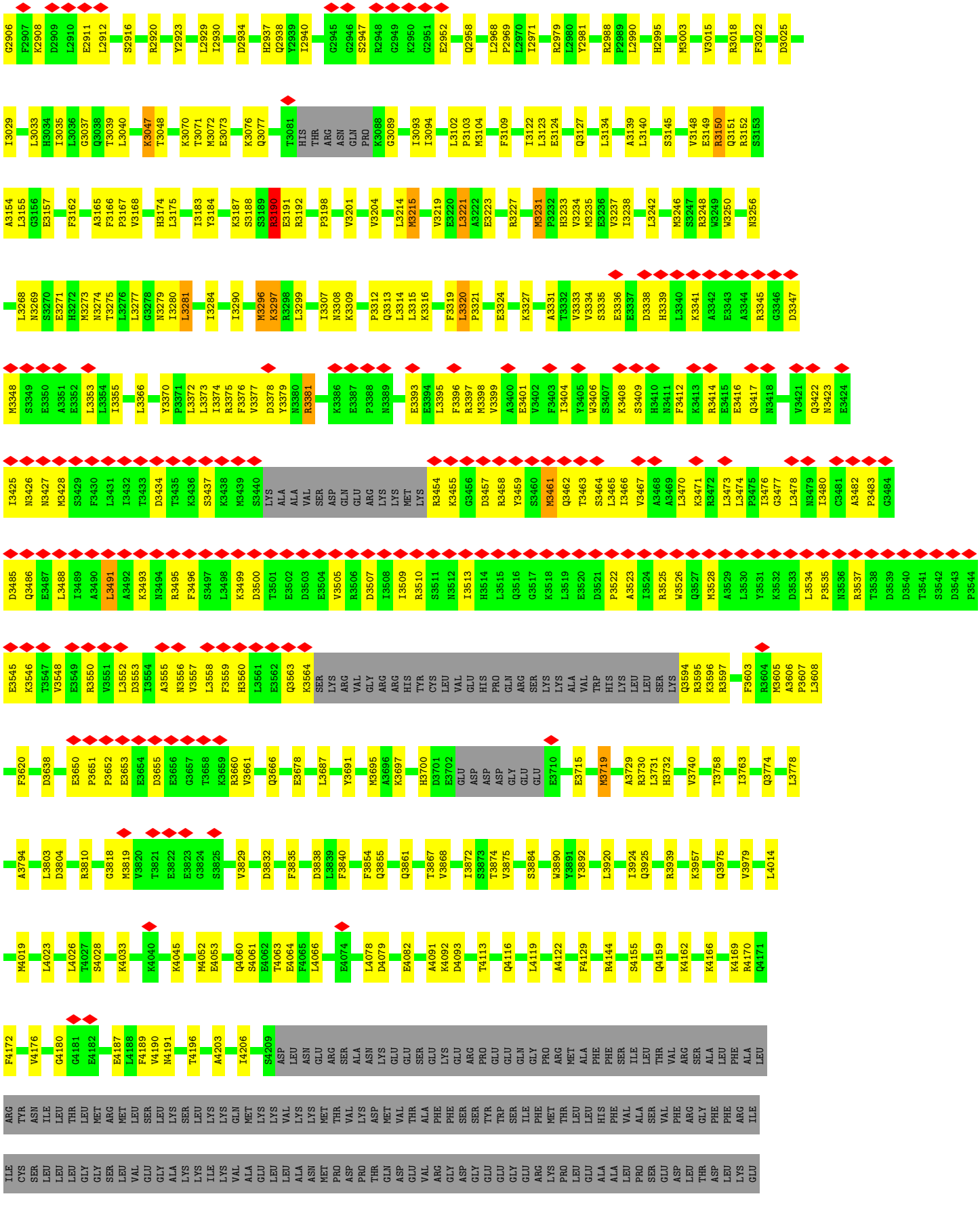
Chain B:

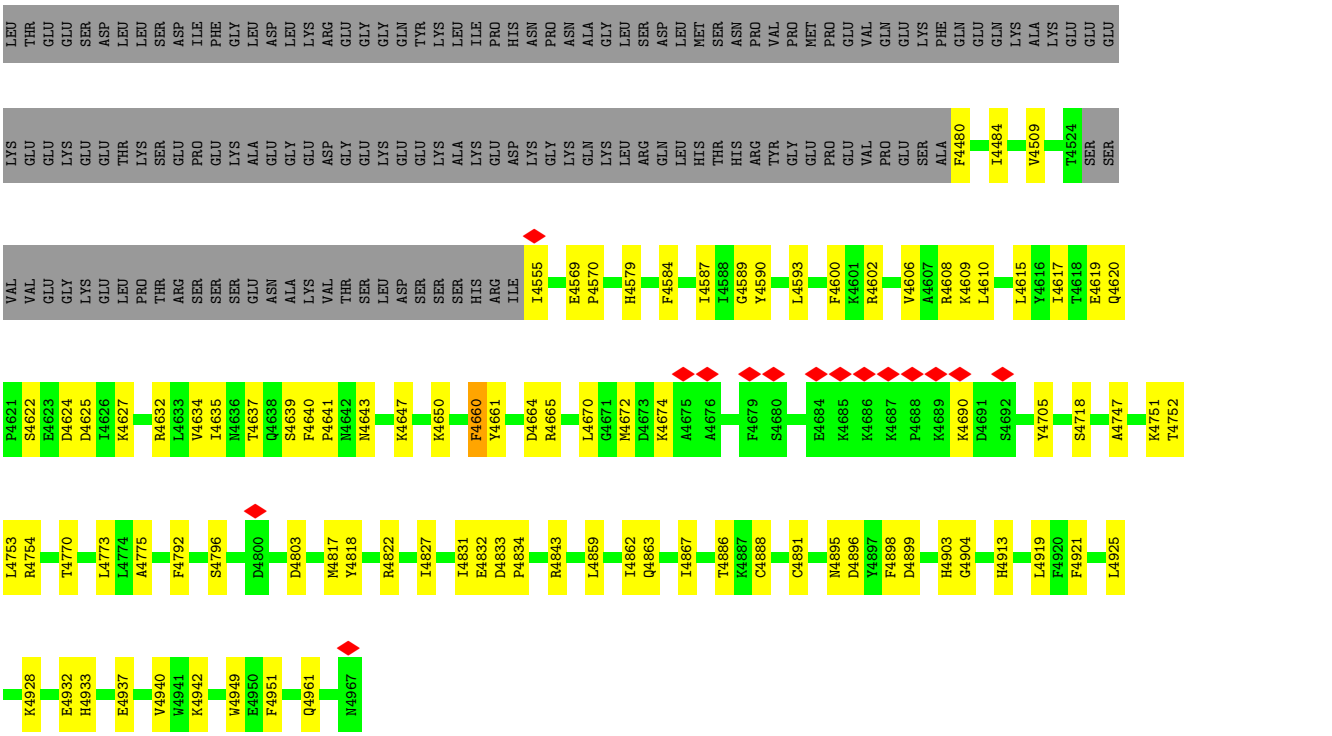






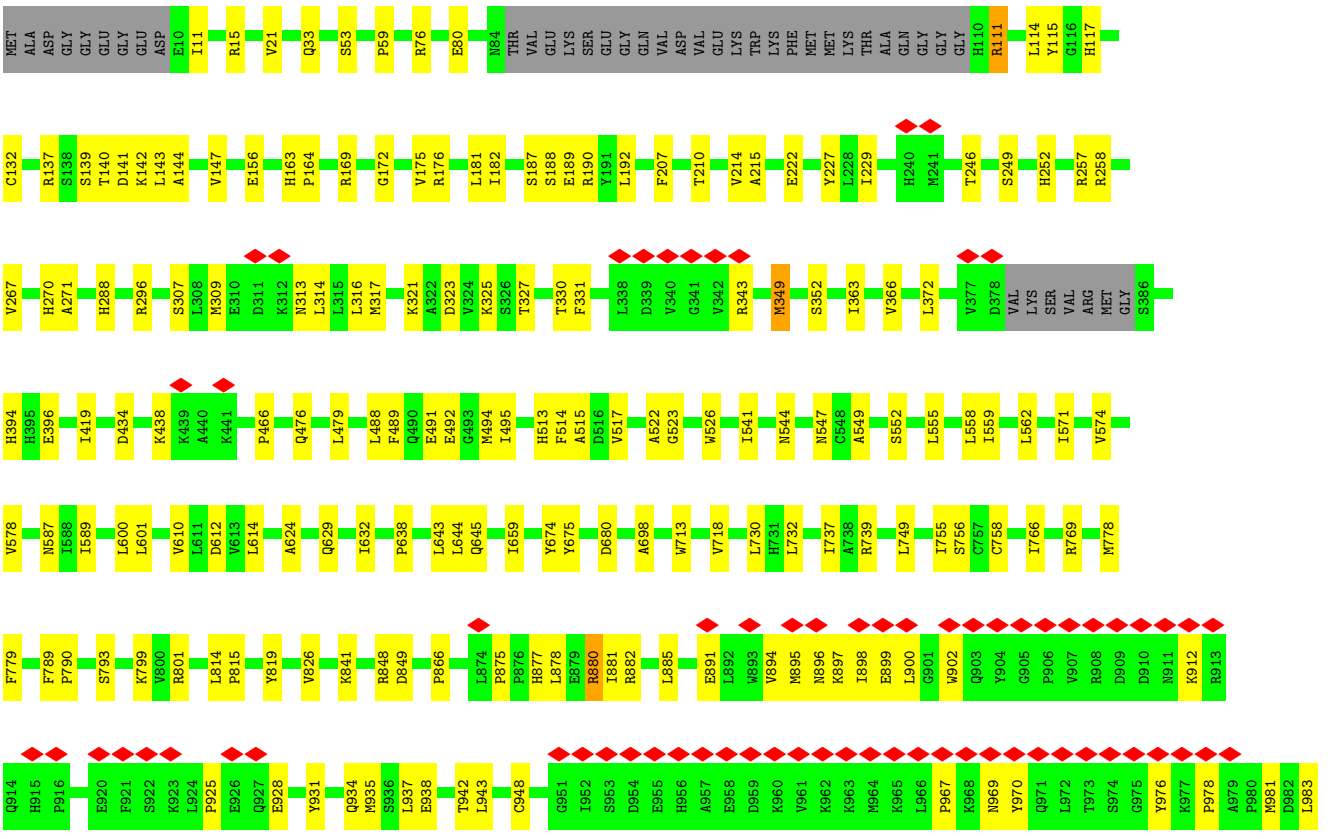


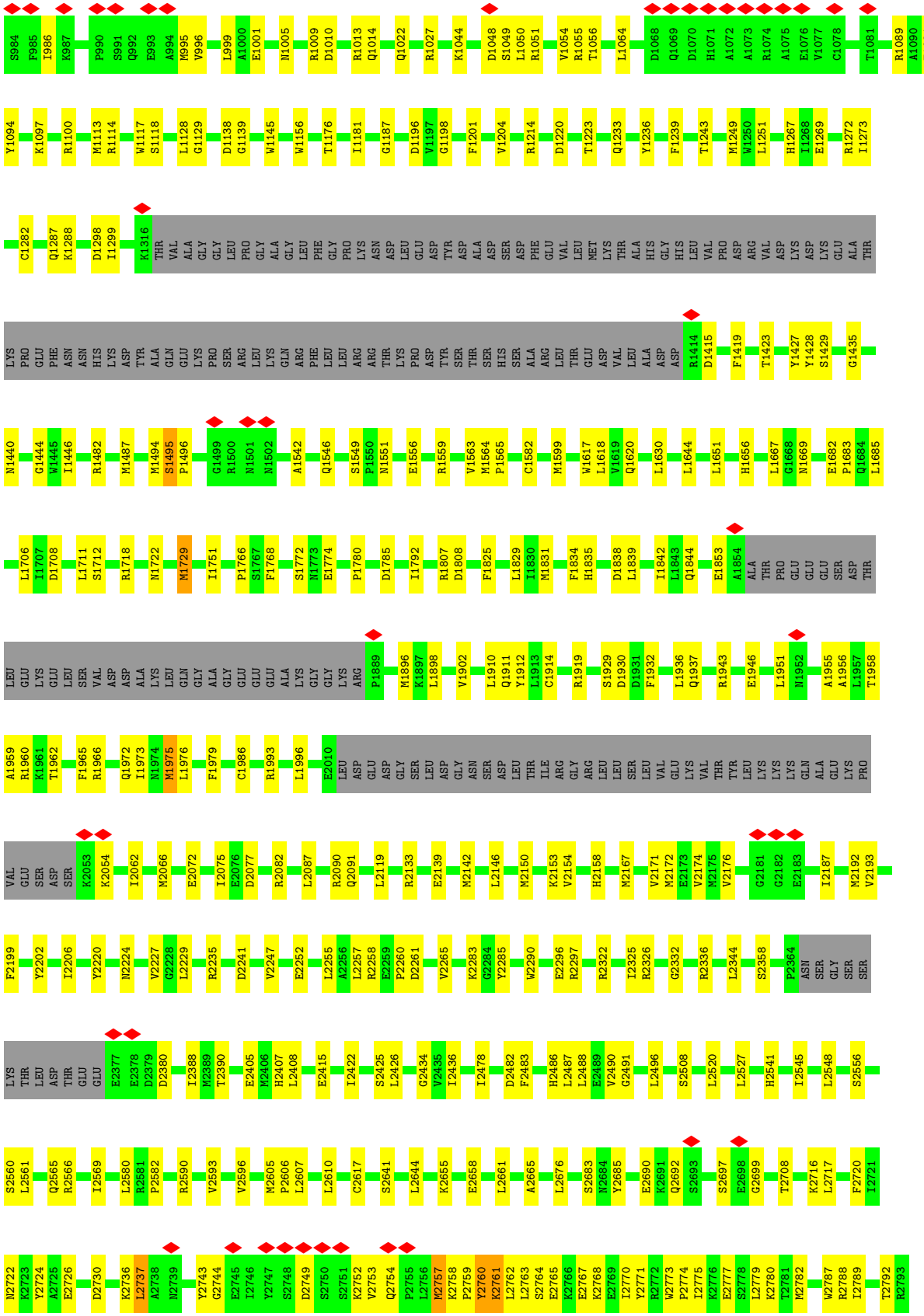




• Molecule 1: Ryanodine receptor 2

Chain C:

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Y1094 K1097 R1100 M1113 R1114 W1117 S1118 L1128 G1129 D1138 G1139 W1145 W1156 T1176 I1181 G1187 D1196 Y1197 G1198 F1201 V1204 R1214 D1220 T1223 Q1233 Y1236 F1239 T1243 M1249 W1250 L1251 H1267 I1268 E1269 R1272 I1273
C1282 Q1287 K1288 D1298 I1299 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR
LYS PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 D1415 F1419 T1423 Y1427 Y1428 S1429 G1435
N1440 G1444 W1445 I1446 R1482 M1487 M1494 S1495 P1496 G1499 R1500 N1501 M1502 A1542 Q1546 S1549 P1550 N1551 E1556 R1559 V1563 M1564 P1565 C1582 M1599 W1617 L1618 V1619 Q1620 L1630 L1644 L1651 H1656 L1667 G1668 N1669 E1682 P1683 Q1684 L1685
L1706 I1707 D1708 L1711 S1712 R1718 N1722 M1729 I1751 P1766 S1767 F1768 S1772 N1773 E1774 P1780 D1785 I1792 R1807 D1808 F1825 L1829 I1830 M1831 F1834 H1835 D1838 L1839 I1842 L1843 Q1844 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP THR
LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 M1896 K1897 L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 R1919 S1929 D1930 D1931 F1932 L1936 Q1937 R1943 E1946 L1951 N1952 A1955 A1956 L1957 T1958
A1959 R1960 K1961 T1962 F1965 R1966 Q1972 I1973 N1974 M1975 L1976 F1979 C1986 R1993 L1996 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO
VAL GLU SER ASP SER K2053 K2054 I2062 M2066 E2072 I2075 E2076 D2077 R2082 L2087 R2090 Q2091 L2119 R2133 E2139 M2142 L2146 M2150 K2153 V2154 H2158 M2167 V2171 M2172 E2173 V2174 M2175 V2176 G2181 G2182 E2183 I2187 M2192 V2193
F2199 Y2202 I2206 Y2220 N2224 V2227 G2228 L2229 R2235 D2241 V2247 E2252 L2255 A2256 L2257 R2258 E2259 P2260 D2261 V2265 K2283 G2284 Y2285 W2290 E2296 R2297 R2322 I2325 R2326 G2332 R2336 L2344 S2358 P2364 ASN SER GLY SER SER
LYS THR LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 I2388 M2389 T2390 E2405 M2406 H2407 L2408 E2415 I2422 S2425 L2426 G2434 V2435 I2436 I2478 D2482 F2483 H2486 L2487 L2488 E2489 V2490 G2491 L2496 S2508 L2520 L2527 H2541 I2545 L2548 S2556
S2560 L2561 Q2565 R2566 I2569 L2580 R2581 P2582 R2590 V2593 V2596 M2605 P2606 L2607 L2610 C2617 S2641 L2644 K2655 E2658 L2661 A2665 L2676 S2683 N2684 Y2685 E2690 K2691 Q2692 S2693 S2697 E2698 G2699 T2708 K2716 L2717 F2720 I2721
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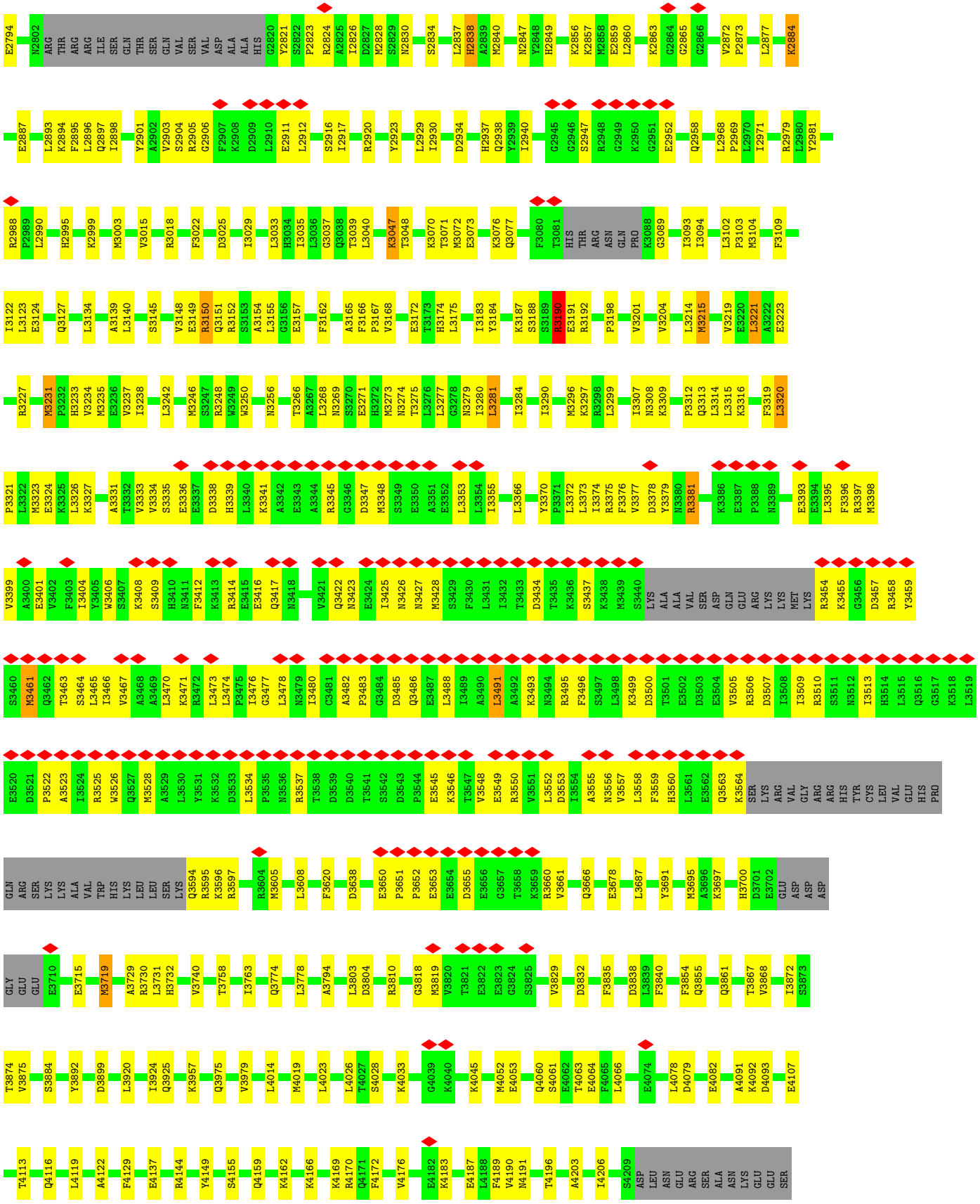
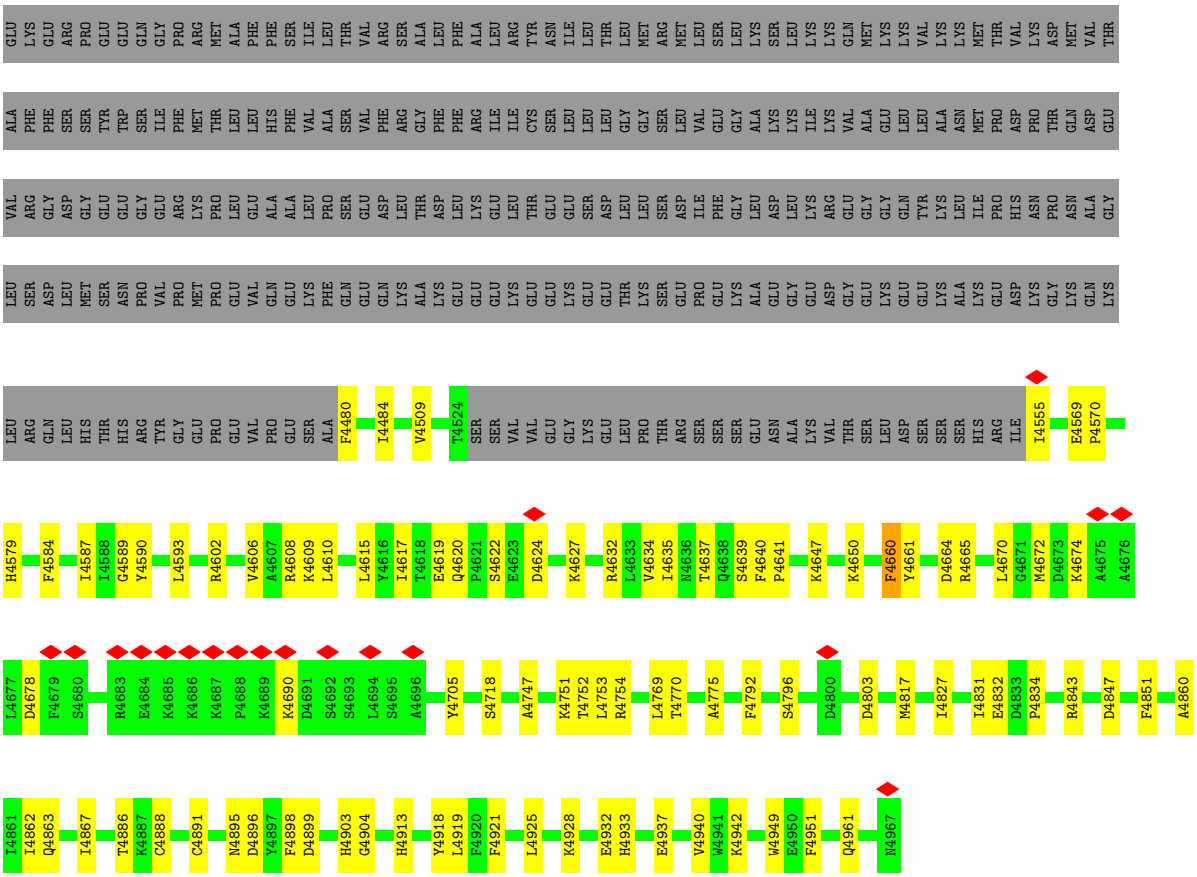
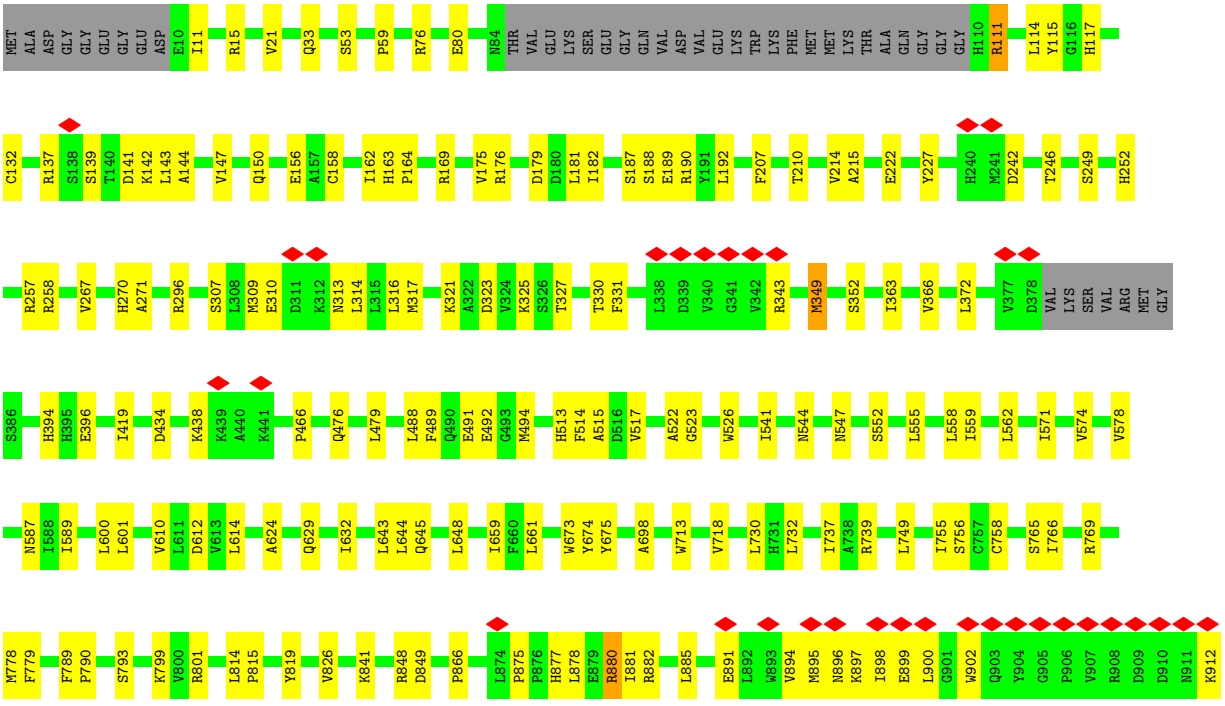
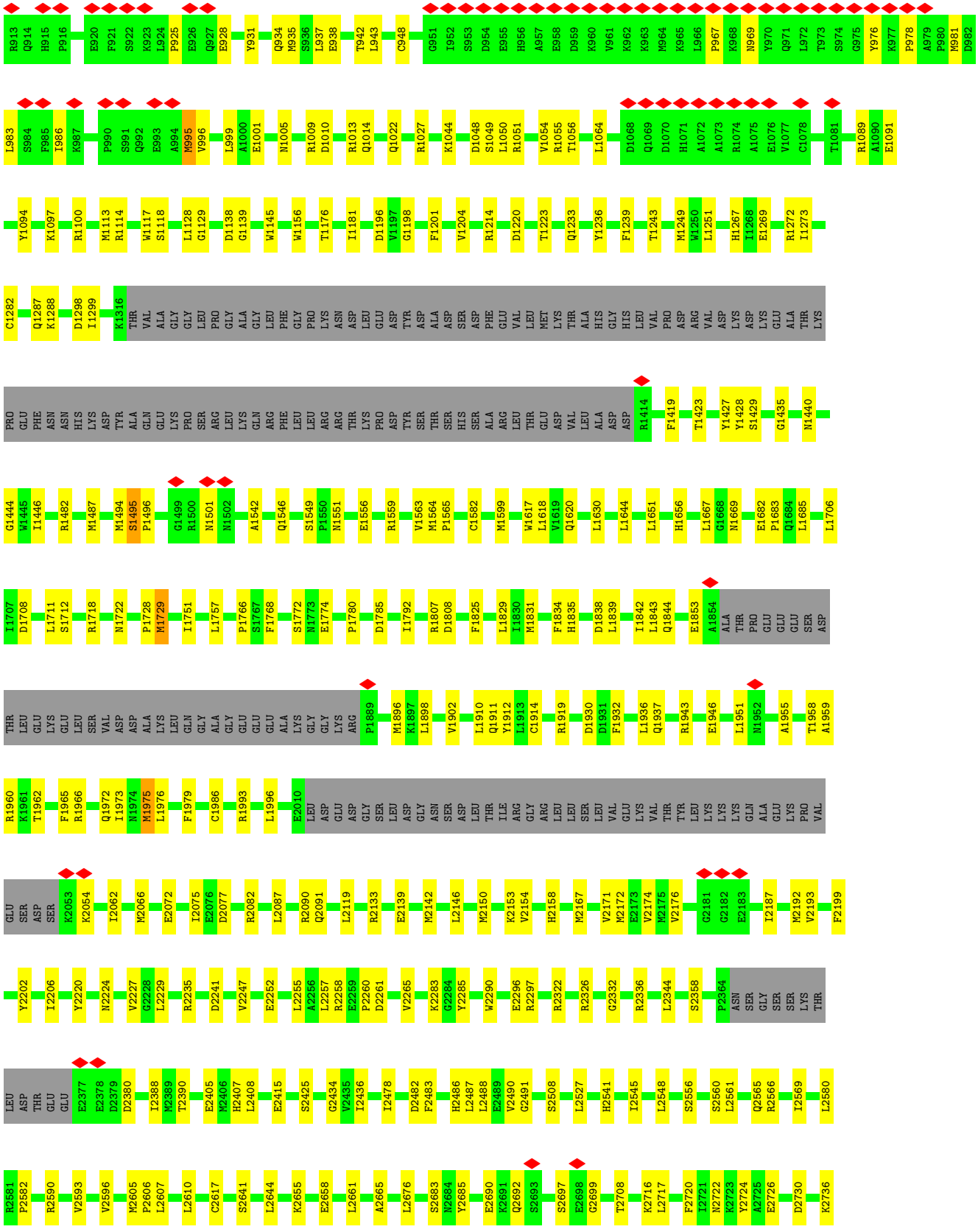




• Molecule 1: Ryanodine receptor 2

Chain D:

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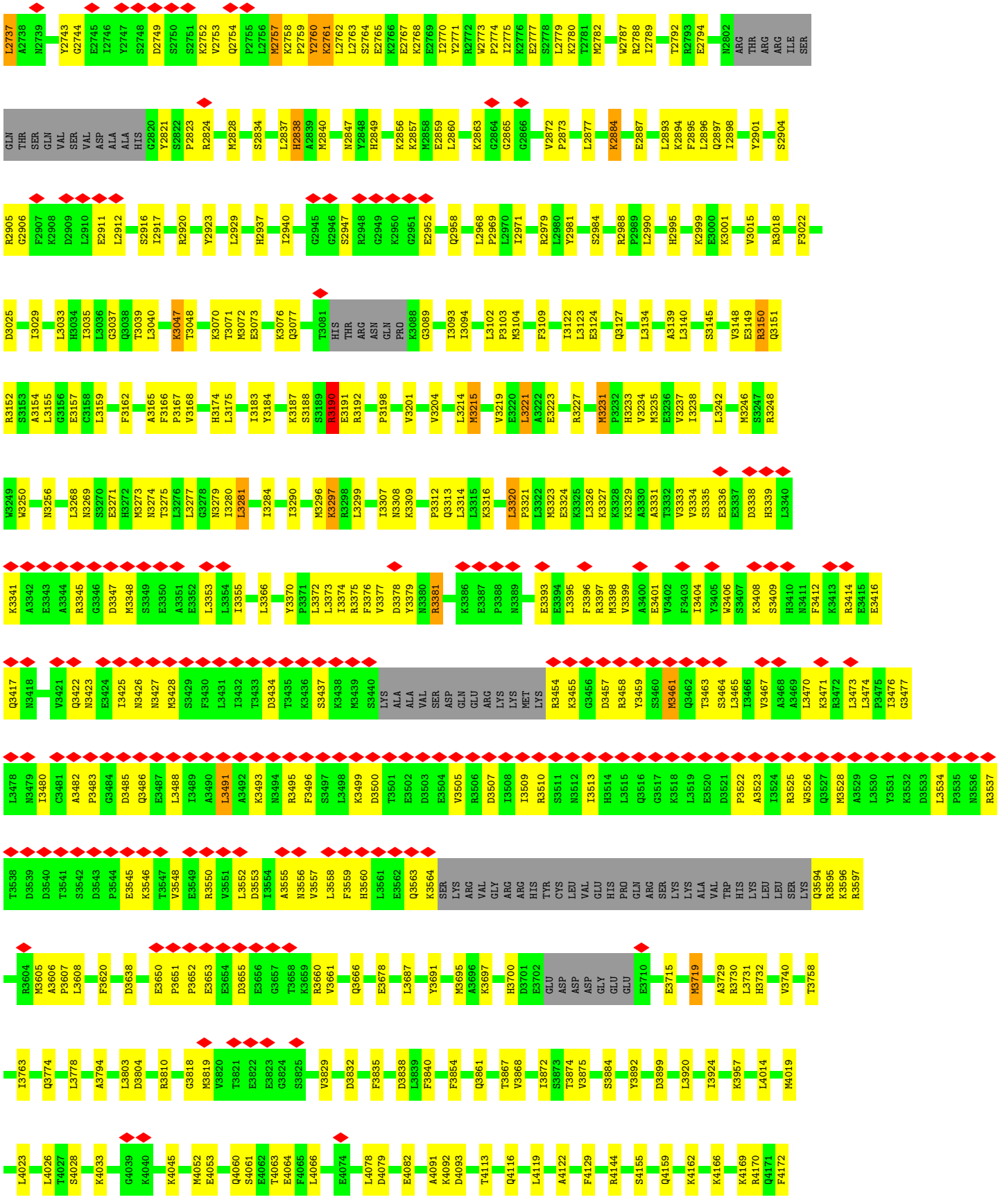
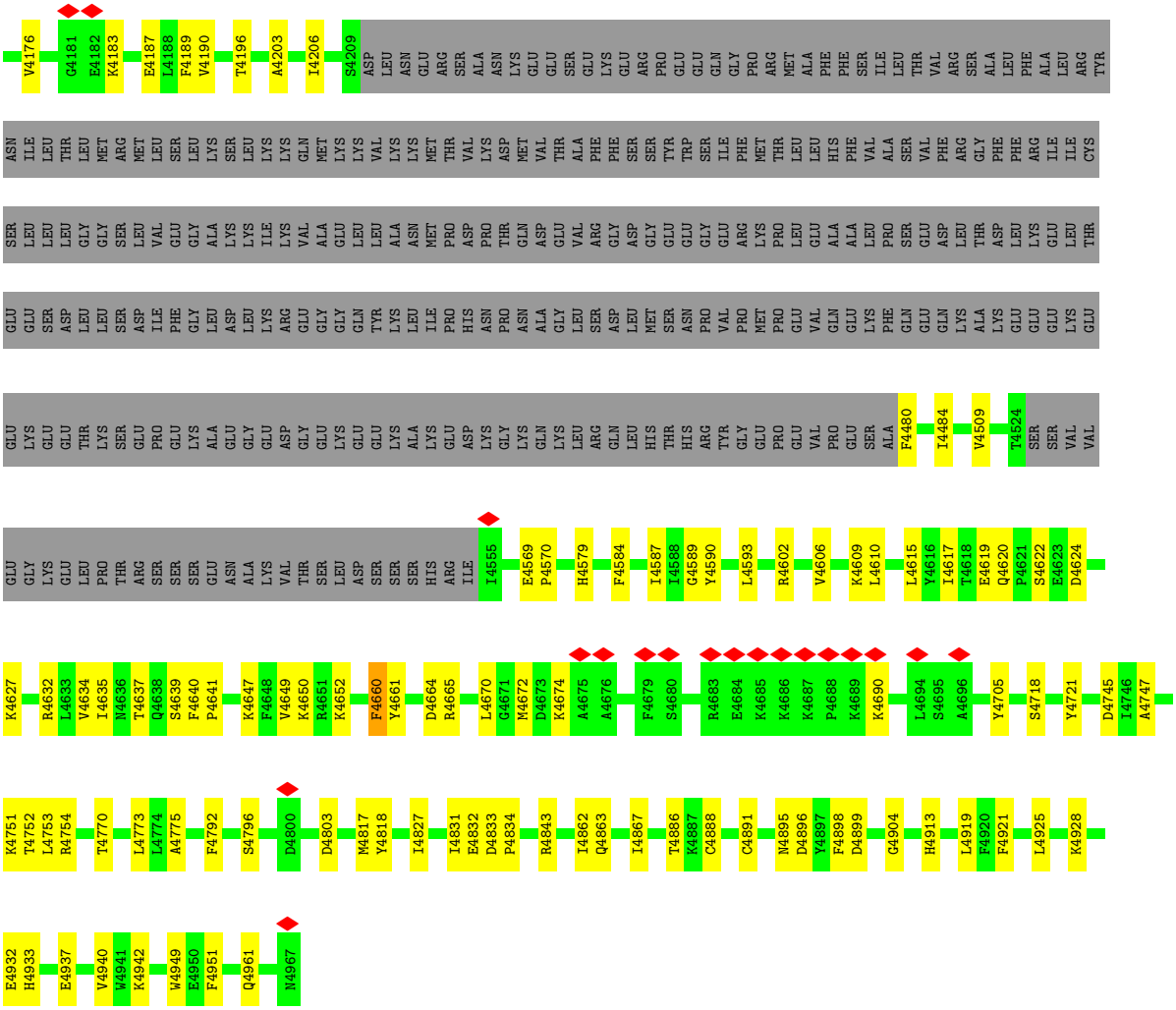
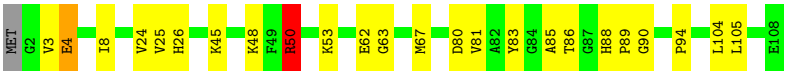
L983 S984 F985 I986 K987 P990 S991 Q992 E993 A994 M995 V996 L999 A1000 E1001 N1005 R1009 D1010 R1013 Q1014 Q1022 R1027 K1044 D1048 S1049 L1050 R1051 V1054 R1055 T1056 L1064 D1068 Q1069 D1070 H1071 A1072 A1073 R1074 A1075 E1076 V1077 C1078 T1081 R1089 A1090 E1091
Y1094 K1097 R1100 M1113 R1114 W1117 S1118 L1128 G1129 D1138 G1139 W1145 W1156 T1176 I1181 D1196 V1197 G1198 F1201 V1204 R1214 D1220 T1223 Q1233 Y1236 F1239 T1243 M1249 W1250 L1251 H1267 I1268 E1269 R1272 I1273
C1282 Q1287 K1288 D1298 I1299 K1316 THR VAL ALA GLY GLY LEU PRO GLY ALA GLY LEU PHE GLY PRO LYS ASN ASP LEU GLU ASP TYR ASP ALA ASP SER ASP PHE GLU VAL LEU MET LYS THR ALA HIS GLY HIS LEU VAL PRO ASP ARG VAL ASP LYS ASP LYS GLU ALA THR LYS
PRO GLU PHE ASN ASN HIS LYS ASP TYR ALA GLN GLU LYS PRO SER ARG LEU LYS GLN ARG PHE LEU LEU ARG ARG THR LYS PRO ASP TYR SER THR SER HIS SER ALA ARG LEU THR GLU ASP VAL LEU ALA ASP ASP R1414 F1419 T1423 Y1427 Y1428 S1429 G1435 N1440
G1444 W1445 I1446 R1482 M1487 M1494 S1495 P1496 G1499 R1500 N1501 N1502 A1542 Q1546 S1549 P1550 N1551 E1556 R1559 V1563 M1564 P1565 C1582 M1599 W1617 L1618 V1619 Q1620 L1630 L1644 L1651 H1656 L1667 G1668 N1669 E1682 P1683 Q1694 L1685 L1706
I1707 D1708 L1711 S1712 R1718 N1722 P1728 M1729 I1751 L1757 P1766 S1767 F1768 S1772 N1773 E1774 P1780 D1785 I1792 R1807 D1808 F1825 L1829 I1830 M1831 F1834 H1835 D1838 L1839 I1842 L1843 Q1844 E1853 A1854 ALA THR PRO GLU GLU GLU SER ASP
THR LEU GLU LYS GLU LEU SER VAL ASP ASP ALA LYS LEU GLN GLY ALA GLY GLU GLU GLU ALA LYS GLY GLY LYS ARG P1889 M1896 K1897 L1898 V1902 L1910 Q1911 Y1912 L1913 C1914 R1919 D1930 D1931 F1932 L1936 Q1937 R1943 E1946 L1951 N1952 A1955 T1958 A1959
R1960 K1961 T1962 F1965 R1966 Q1972 I1973 N1974 M1975 L1976 F1979 C1986 R1993 L1996 E2010 LEU ASP GLU ASP GLY SER LEU ASP GLY ASN SER ASP LEU THR ILE ARG GLY ARG LEU LEU SER LEU VAL GLU LYS VAL THR TYR LEU LYS LYS LYS GLN ALA GLU LYS PRO VAL
GLU SER ASP SER K2053 K2054 I2062 M2066 E2072 I2075 E2076 D2077 R2082 L2087 R2090 Q2091 L2119 R2133 E2139 M2142 L2146 M2150 K2153 V2154 H2158 M2167 V2171 M2172 E2173 V2174 M2175 V2176 G2181 G2182 E2183 I2187 M2192 V2193 F2199
Y2202 I2206 Y2220 N2224 V2227 G2228 L2229 R2235 D2241 V2247 E2252 L2255 A2256 L2257 R2258 E2259 P2260 D2261 V2265 K2283 G2284 Y2285 W2290 E2296 R2297 R2322 R2326 G2332 R2336 L2344 S2358 P2364 ASN SER GLY SER SER LYS THR
LEU ASP THR GLU GLU E2377 E2378 D2379 D2380 I2388 M2389 T2390 E2405 M2406 H2407 L2408 E2415 S2425 G2434 V2435 I2436 I2478 D2482 F2483 H2486 L2487 L2488 E2489 V2490 G2491 S2508 L2527 H2541 I2545 L2548 S2556 S2560 L2561 Q2565 R2566 I2569 L2580
R2581 P2582 R2590 V2593 V2596 M2605 P2606 L2607 L2610 C2617 S2641 L2644 K2655 E2658 L2661 A2665 L2676 S2683 N2684 Y2685 E2690 K2691 Q2692 S2693 S2697 E2698 G2699 T2708 K2716 L2717 F2720 I2721 N2722 K2723 Y2724 A2725 E2726 D2730 K2736





• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

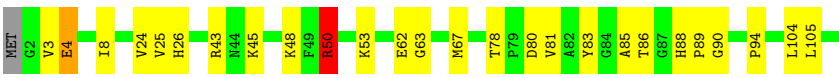


• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:

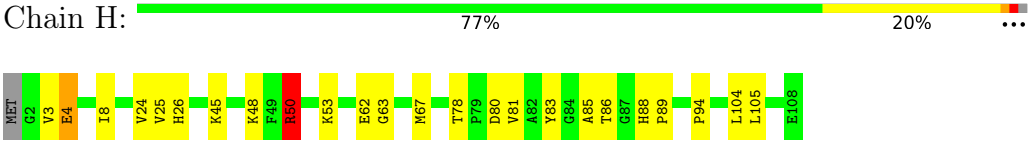
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:



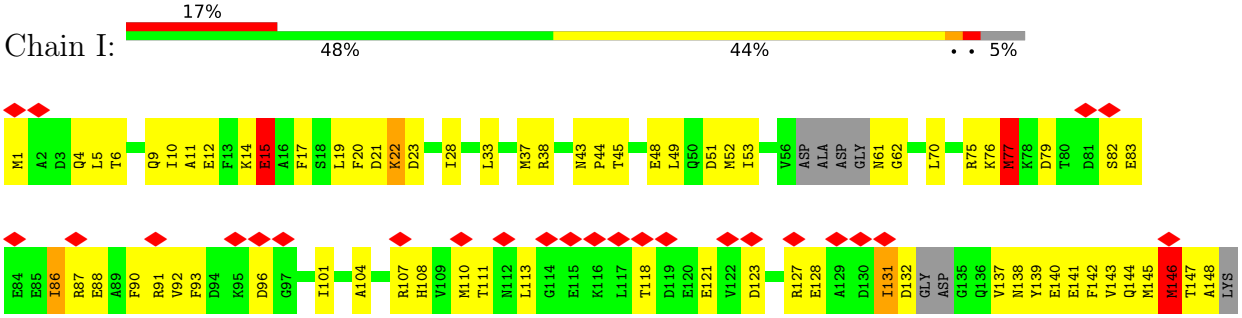
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



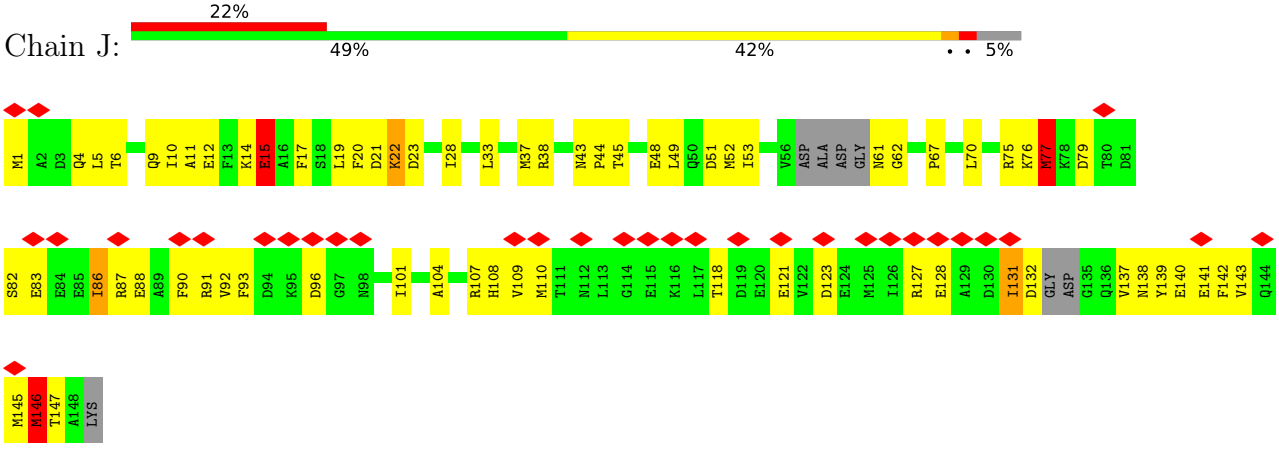
• Molecule 3: Calmodulin-1

Chain I:



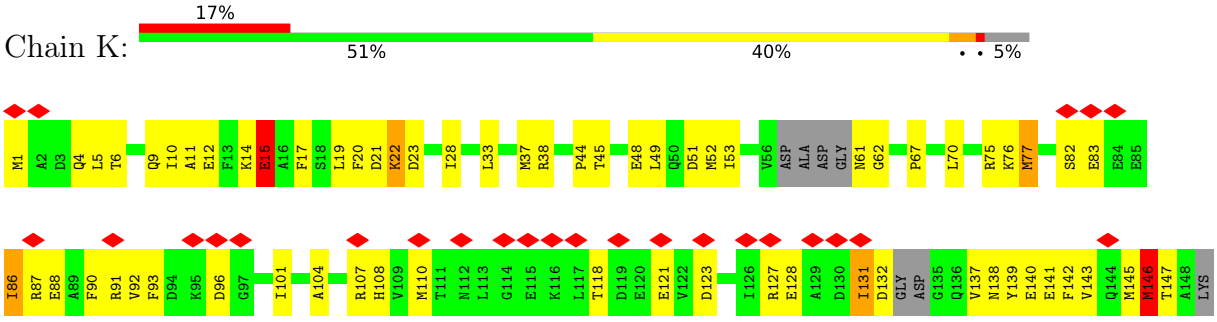
• Molecule 3: Calmodulin-1

Chain J:



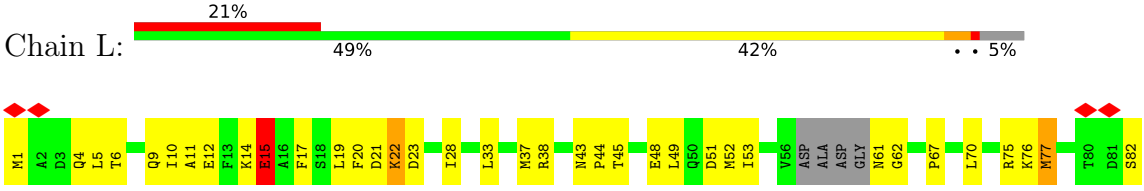
• Molecule 3: Calmodulin-1

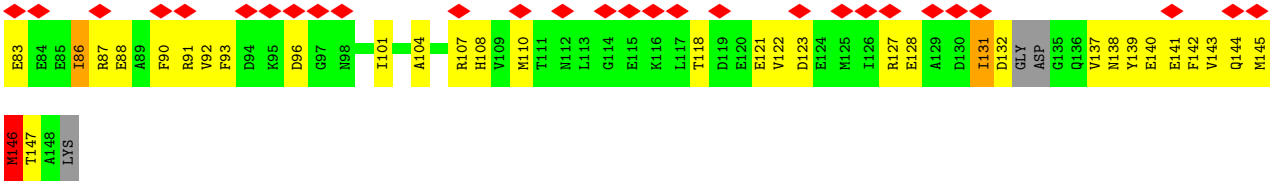
Chain K:



• Molecule 3: Calmodulin-1

Chain L:




E83
E84
E85
I86
R87
E88
A89
F90
R91
V92
F93
D94
K95
D96
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N98
I101
A104
R107
H108
V109
M110
T111
N112
L113
G114
E115
K116
L117
T118
D119
E120
E121
V122
D123
E124
M125
I126
R127
E128
A129
D130
I131
D132
GLY
ASP
G135
Q136
V137
N138
Y139
E140
E141
F142
V143
Q144
M145
M146
T147
A148
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102257	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	58	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.728	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.033	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.26	0/35720	0.50	7/48254 (0.0%)
1	B	0.26	0/35720	0.50	7/48254 (0.0%)
1	C	0.26	0/35720	0.50	7/48254 (0.0%)
1	D	0.26	0/35720	0.50	7/48254 (0.0%)
2	E	0.30	0/834	0.61	2/1123 (0.2%)
2	F	0.31	0/834	0.61	2/1123 (0.2%)
2	G	0.31	0/834	0.61	2/1123 (0.2%)
2	H	0.31	0/834	0.61	2/1123 (0.2%)
3	I	0.38	0/1122	0.80	6/1504 (0.4%)
3	J	0.38	0/1122	0.79	6/1504 (0.4%)
3	K	0.38	1/1122 (0.1%)	0.80	6/1504 (0.4%)
3	L	0.38	0/1122	0.80	6/1504 (0.4%)
All	All	0.27	1/150704 (0.0%)	0.51	60/203524 (0.0%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	15	GLU	CG-CD	-5.00	1.44	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	77	MET	CB-CG-SD	8.44	137.71	112.40
3	K	77	MET	CB-CG-SD	8.44	137.72	112.40
3	L	77	MET	CB-CG-SD	8.43	137.69	112.40
3	I	77	MET	CB-CG-SD	8.43	137.68	112.40
1	C	1729	MET	CB-CG-SD	-8.12	88.05	112.40
1	A	1729	MET	CB-CG-SD	-8.11	88.08	112.40
1	B	1729	MET	CB-CG-SD	-8.11	88.08	112.40
1	D	1729	MET	CB-CG-SD	-8.10	88.11	112.40
3	L	15	GLU	CA-CB-CG	7.23	129.30	113.40
3	I	15	GLU	CA-CB-CG	7.21	129.27	113.40
3	J	15	GLU	CA-CB-CG	7.21	129.25	113.40
3	K	15	GLU	CA-CB-CG	7.20	129.24	113.40
1	D	3231	MET	CA-CB-CG	6.69	124.68	113.30
1	B	3231	MET	CA-CB-CG	6.68	124.66	113.30
1	A	3231	MET	CA-CB-CG	6.68	124.65	113.30
1	C	3231	MET	CA-CB-CG	6.66	124.62	113.30
1	B	3461	MET	CB-CG-SD	6.64	132.32	112.40
1	A	3461	MET	CA-CB-CG	6.63	124.58	113.30
1	C	3461	MET	CA-CB-CG	6.63	124.57	113.30
1	A	3461	MET	CB-CG-SD	6.62	132.27	112.40
1	C	3461	MET	CB-CG-SD	6.62	132.28	112.40
1	D	3461	MET	CA-CB-CG	6.62	124.56	113.30
1	D	3461	MET	CB-CG-SD	6.62	132.27	112.40
1	B	3461	MET	CA-CB-CG	6.61	124.54	113.30
3	L	146	MET	CB-CG-SD	6.57	132.12	112.40
3	J	146	MET	CB-CG-SD	6.56	132.08	112.40
3	K	146	MET	CB-CG-SD	6.56	132.07	112.40
3	I	146	MET	CB-CG-SD	6.55	132.06	112.40
2	H	50	ARG	CG-CD-NE	6.22	124.85	111.80
2	F	50	ARG	CG-CD-NE	6.21	124.84	111.80
2	E	50	ARG	CG-CD-NE	6.20	124.82	111.80
2	G	50	ARG	CG-CD-NE	6.19	124.80	111.80
3	I	146	MET	CA-CB-CG	6.12	123.70	113.30
3	K	146	MET	CA-CB-CG	6.12	123.70	113.30
3	L	146	MET	CA-CB-CG	6.11	123.69	113.30
3	J	146	MET	CA-CB-CG	6.10	123.67	113.30
3	I	77	MET	CA-CB-CG	6.07	123.61	113.30
3	J	77	MET	CA-CB-CG	6.06	123.60	113.30
3	L	77	MET	CA-CB-CG	6.06	123.60	113.30
3	K	77	MET	CA-CB-CG	6.03	123.56	113.30
2	E	4	GLU	CA-CB-CG	5.95	126.50	113.40
2	H	4	GLU	CA-CB-CG	5.95	126.50	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	4	GLU	CA-CB-CG	5.95	126.49	113.40
2	G	4	GLU	CA-CB-CG	5.93	126.45	113.40
1	D	3320	LEU	CA-CB-CG	5.59	128.17	115.30
1	A	3320	LEU	CA-CB-CG	5.58	128.13	115.30
1	B	3320	LEU	CA-CB-CG	5.57	128.12	115.30
1	C	3320	LEU	CA-CB-CG	5.57	128.11	115.30
1	D	3231	MET	CB-CG-SD	5.55	129.05	112.40
1	A	3231	MET	CB-CG-SD	5.55	129.04	112.40
1	C	3231	MET	CB-CG-SD	5.54	129.03	112.40
1	B	3231	MET	CB-CG-SD	5.54	129.01	112.40
1	D	3491	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	3491	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	3491	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	3491	LEU	CA-CB-CG	5.16	127.16	115.30
3	L	23	ASP	CB-CG-OD1	5.07	122.86	118.30
3	I	23	ASP	CB-CG-OD1	5.05	122.84	118.30
3	K	23	ASP	CB-CG-OD1	5.04	122.84	118.30
3	J	23	ASP	CB-CG-OD1	5.04	122.83	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3190	ARG	Sidechain
1	A	3381	ARG	Sidechain
1	B	3190	ARG	Sidechain
1	B	3381	ARG	Sidechain
1	C	3190	ARG	Sidechain
1	C	3381	ARG	Sidechain
1	D	3190	ARG	Sidechain
1	D	3381	ARG	Sidechain

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	34959	0	34588	639	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	34959	0	34588	638	0
1	C	34959	0	34588	651	0
1	D	34959	0	34588	634	0
2	E	818	0	821	16	0
2	F	818	0	821	15	0
2	G	818	0	821	18	0
2	H	818	0	821	15	0
3	I	1112	0	1053	84	0
3	J	1112	0	1053	69	0
3	K	1112	0	1053	70	0
3	L	1112	0	1053	72	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	62	0	24	11	0
5	B	62	0	24	10	0
5	C	62	0	24	10	0
5	D	62	0	24	11	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	11	0	4	0	0
7	B	11	0	4	0	0
7	C	11	0	4	0	0
7	D	11	0	4	0	0
All	All	147856	0	145960	2850	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 10.

All (2850) 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)
3:L:128:GLU:CB	3:L:131:ILE:CD1	1.83	1.57
3:L:128:GLU:HB3	3:L:131:ILE:CD1	1.11	1.56
3:J:128:GLU:HB3	3:J:131:ILE:CD1	1.11	1.55
3:I:128:GLU:HB3	3:I:131:ILE:CD1	1.11	1.54
3:K:128:GLU:HB3	3:K:131:ILE:CD1	1.11	1.54
3:K:128:GLU:CB	3:K:131:ILE:CD1	1.83	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:GLU:CB	3:I:131:ILE:CD1	1.83	1.51
3:J:128:GLU:CB	3:J:131:ILE:CD1	1.83	1.50
1:C:3427:ASN:CB	1:C:3463:THR:HB	1.49	1.43
1:D:3427:ASN:CB	1:D:3463:THR:HB	1.48	1.43
1:A:3427:ASN:CB	1:A:3463:THR:HB	1.49	1.41
1:B:3427:ASN:CB	1:B:3463:THR:HB	1.48	1.41
1:B:3375:ARG:NH2	1:B:3437:SER:OG	1.56	1.37
1:D:3375:ARG:NH2	1:D:3437:SER:OG	1.56	1.33
1:A:3375:ARG:NH2	1:A:3437:SER:OG	1.56	1.33
1:C:3375:ARG:NH2	1:C:3437:SER:OG	1.56	1.33
1:B:3427:ASN:CG	1:B:3463:THR:O	1.68	1.32
1:D:3427:ASN:CG	1:D:3463:THR:O	1.68	1.30
1:A:3427:ASN:CG	1:A:3463:THR:O	1.68	1.29
1:C:3427:ASN:CG	1:C:3463:THR:O	1.68	1.29
1:A:897:LYS:HE3	5:A:5005:ATP:N6	1.53	1.24
1:D:897:LYS:HE3	5:D:5005:ATP:N6	1.52	1.24
1:B:897:LYS:HE3	5:B:5005:ATP:N6	1.53	1.23
1:C:897:LYS:HE3	5:C:5005:ATP:N6	1.52	1.22
1:D:897:LYS:CE	5:D:5005:ATP:N6	2.06	1.19
1:B:897:LYS:CE	5:B:5005:ATP:N6	2.06	1.18
1:C:897:LYS:CE	5:C:5005:ATP:N6	2.06	1.18
1:A:897:LYS:CE	5:A:5005:ATP:N6	2.06	1.18
1:D:3427:ASN:CB	1:D:3463:THR:CB	2.22	1.18
1:C:3427:ASN:CB	1:C:3463:THR:CB	2.22	1.17
1:B:3427:ASN:ND2	1:B:3463:THR:O	1.77	1.16
1:C:3427:ASN:ND2	1:C:3463:THR:O	1.77	1.16
1:D:3427:ASN:ND2	1:D:3463:THR:O	1.77	1.16
1:A:3427:ASN:CB	1:A:3463:THR:CB	2.22	1.16
1:A:3427:ASN:ND2	1:A:3463:THR:O	1.77	1.15
1:B:3427:ASN:CB	1:B:3463:THR:CB	2.22	1.15
1:D:3427:ASN:HB2	1:D:3463:THR:CB	1.76	1.14
1:A:3427:ASN:HB2	1:A:3463:THR:CB	1.76	1.14
1:B:3427:ASN:HB2	1:B:3463:THR:CB	1.76	1.14
1:C:3427:ASN:HB2	1:C:3463:THR:CB	1.76	1.13
3:K:128:GLU:CB	3:K:131:ILE:HD12	1.63	1.09
1:D:897:LYS:CE	5:D:5005:ATP:HN62	1.65	1.08
1:A:897:LYS:CE	5:A:5005:ATP:HN62	1.65	1.07
1:B:3423:ASN:O	1:B:3425:ILE:HD12	1.55	1.07
1:C:3423:ASN:O	1:C:3425:ILE:HD12	1.55	1.07
3:L:128:GLU:CB	3:L:131:ILE:HD12	1.63	1.06
1:B:897:LYS:CE	5:B:5005:ATP:HN62	1.65	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:LYS:CE	5:C:5005:ATP:HN62	1.65	1.06
1:A:3423:ASN:O	1:A:3425:ILE:HD12	1.55	1.06
3:L:128:GLU:HB3	3:L:131:ILE:HD13	1.07	1.06
3:K:128:GLU:HB3	3:K:131:ILE:HD13	1.07	1.06
3:J:132:ASP:O	3:J:137:VAL:HG21	1.56	1.05
3:I:128:GLU:CB	3:I:131:ILE:HD12	1.63	1.05
1:D:3423:ASN:O	1:D:3425:ILE:HD12	1.55	1.05
3:J:128:GLU:HB3	3:J:131:ILE:HD13	1.07	1.04
3:I:128:GLU:HB3	3:I:131:ILE:HD13	1.07	1.04
3:I:132:ASP:O	3:I:137:VAL:HG21	1.56	1.04
3:J:128:GLU:CB	3:J:131:ILE:HD12	1.63	1.04
3:K:132:ASP:O	3:K:137:VAL:HG21	1.56	1.04
1:C:3375:ARG:CZ	1:C:3437:SER:OG	2.06	1.03
1:B:3375:ARG:CZ	1:B:3437:SER:OG	2.06	1.03
3:L:132:ASP:O	3:L:137:VAL:HG21	1.56	1.02
3:I:128:GLU:CG	3:I:131:ILE:CD1	2.37	1.02
3:J:128:GLU:CG	3:J:131:ILE:CD1	2.37	1.02
1:D:3375:ARG:CZ	1:D:3437:SER:OG	2.06	1.02
1:A:3375:ARG:CZ	1:A:3437:SER:OG	2.06	1.02
3:K:128:GLU:CB	3:K:131:ILE:HD11	1.90	1.01
1:D:3427:ASN:HB2	1:D:3463:THR:OG1	1.59	1.01
1:A:3596:LYS:HB2	3:I:146:MET:CE	1.91	1.01
3:L:128:GLU:CB	3:L:131:ILE:HD11	1.90	1.01
3:L:128:GLU:CG	3:L:131:ILE:CD1	2.37	1.01
1:C:3427:ASN:HB2	1:C:3463:THR:OG1	1.59	1.01
3:J:128:GLU:CB	3:J:131:ILE:HD11	1.90	1.01
3:K:128:GLU:CG	3:K:131:ILE:CD1	2.37	1.01
1:B:3427:ASN:HB2	1:B:3463:THR:OG1	1.59	1.00
1:B:3427:ASN:HB3	1:B:3463:THR:HB	1.01	1.00
1:A:3427:ASN:HB2	1:A:3463:THR:OG1	1.59	1.00
1:A:3427:ASN:HB3	1:A:3463:THR:HB	1.01	1.00
1:A:897:LYS:HE3	5:A:5005:ATP:HN62	1.13	0.99
1:D:3427:ASN:HB3	1:D:3463:THR:HB	1.01	0.98
3:I:128:GLU:CB	3:I:131:ILE:HD11	1.90	0.98
3:L:132:ASP:O	3:L:137:VAL:CG2	2.13	0.96
3:K:132:ASP:O	3:K:137:VAL:CG2	2.13	0.96
1:C:3427:ASN:HB3	1:C:3463:THR:HB	1.01	0.96
3:J:132:ASP:O	3:J:137:VAL:CG2	2.13	0.95
3:I:132:ASP:O	3:I:137:VAL:CG2	2.13	0.95
1:B:897:LYS:HE3	5:B:5005:ATP:HN62	1.13	0.95
1:C:897:LYS:HE3	5:C:5005:ATP:HN62	1.13	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3427:ASN:HB3	1:C:3463:THR:CB	1.93	0.94
1:A:1959:ALA:HB2	3:I:108:HIS:HB3	1.48	0.93
3:J:128:GLU:HB3	3:J:131:ILE:HD12	0.93	0.93
3:K:128:GLU:HB3	3:K:131:ILE:HD12	0.93	0.93
1:B:3427:ASN:ND2	1:B:3463:THR:C	2.23	0.92
1:C:3427:ASN:ND2	1:C:3463:THR:C	2.23	0.92
1:A:3427:ASN:ND2	1:A:3463:THR:C	2.23	0.92
3:I:128:GLU:HB3	3:I:131:ILE:HD12	0.93	0.92
1:D:3427:ASN:ND2	1:D:3463:THR:C	2.23	0.92
3:J:128:GLU:CA	3:J:131:ILE:HD12	2.00	0.91
3:I:128:GLU:CA	3:I:131:ILE:HD12	2.00	0.91
3:L:128:GLU:HB3	3:L:131:ILE:HD12	0.93	0.91
1:D:897:LYS:HE3	5:D:5005:ATP:HN62	1.13	0.91
1:C:3650:GLU:HG2	1:C:3651:PRO:HD3	1.53	0.90
1:B:897:LYS:HE2	5:B:5005:ATP:N6	1.87	0.90
1:C:897:LYS:HE2	5:C:5005:ATP:N6	1.87	0.90
1:A:3650:GLU:HG2	1:A:3651:PRO:HD3	1.53	0.90
1:C:3509:ILE:HD12	1:C:3552:LEU:HD21	1.54	0.90
3:K:128:GLU:CA	3:K:131:ILE:HD12	2.01	0.90
1:A:3509:ILE:HD12	1:A:3552:LEU:HD21	1.54	0.90
3:L:128:GLU:CG	3:L:131:ILE:HD11	2.02	0.90
1:B:3650:GLU:HG2	1:B:3651:PRO:HD3	1.53	0.90
1:D:3650:GLU:HG2	1:D:3651:PRO:HD3	1.53	0.90
3:J:128:GLU:CG	3:J:131:ILE:HD11	2.01	0.90
1:D:3509:ILE:HD12	1:D:3552:LEU:HD21	1.54	0.90
1:D:3427:ASN:HB3	1:D:3463:THR:CB	1.93	0.89
3:L:128:GLU:CA	3:L:131:ILE:HD12	2.00	0.89
1:B:3509:ILE:HD12	1:B:3552:LEU:HD21	1.54	0.89
3:K:128:GLU:CG	3:K:131:ILE:HD11	2.02	0.88
1:A:3596:LYS:HB2	3:I:146:MET:HE1	1.53	0.88
3:K:128:GLU:CA	3:K:131:ILE:CD1	2.52	0.88
3:I:132:ASP:C	3:I:137:VAL:CG2	2.43	0.87
3:I:128:GLU:CA	3:I:131:ILE:CD1	2.52	0.87
3:J:132:ASP:C	3:J:137:VAL:CG2	2.43	0.87
3:J:128:GLU:CA	3:J:131:ILE:CD1	2.52	0.87
3:K:132:ASP:C	3:K:137:VAL:CG2	2.43	0.87
3:L:128:GLU:CA	3:L:131:ILE:CD1	2.52	0.87
1:A:3427:ASN:HB3	1:A:3463:THR:CB	1.93	0.87
1:D:897:LYS:HE2	5:D:5005:ATP:N6	1.87	0.87
3:L:132:ASP:C	3:L:137:VAL:CG2	2.43	0.87
1:A:897:LYS:HE2	5:A:5005:ATP:N6	1.87	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:GLU:CG	3:I:131:ILE:HD13	2.05	0.85
1:B:3427:ASN:HB3	1:B:3463:THR:CB	1.93	0.85
3:I:128:GLU:CG	3:I:131:ILE:HD11	2.01	0.84
3:L:128:GLU:CG	3:L:131:ILE:HD13	2.05	0.84
3:L:128:GLU:CB	3:L:131:ILE:HD13	1.75	0.84
1:A:897:LYS:HE3	5:A:5005:ATP:C6	2.13	0.84
1:D:3378:ASP:OD2	1:D:3434:ASP:OD2	1.96	0.83
1:D:3427:ASN:HB2	1:D:3463:THR:HB	1.38	0.83
1:B:3378:ASP:OD2	1:B:3434:ASP:OD2	1.96	0.83
1:A:3378:ASP:OD2	1:A:3434:ASP:OD2	1.96	0.83
1:D:897:LYS:HE3	5:D:5005:ATP:C6	2.13	0.83
3:J:128:GLU:CG	3:J:131:ILE:HD13	2.05	0.83
3:K:128:GLU:CG	3:K:131:ILE:HD13	2.05	0.83
1:B:2830:ASN:HD22	1:C:1435:GLY:HA2	1.44	0.83
1:C:3378:ASP:OD2	1:C:3434:ASP:OD2	1.96	0.83
1:B:897:LYS:HE3	5:B:5005:ATP:C6	2.13	0.82
1:B:943:LEU:HD21	1:B:999:LEU:HD22	1.62	0.82
1:C:897:LYS:HE3	5:C:5005:ATP:C6	2.13	0.82
1:A:943:LEU:HD21	1:A:999:LEU:HD22	1.62	0.82
1:A:1956:ALA:HA	3:I:108:HIS:HE1	1.45	0.82
1:C:4834:PRO:HB3	1:C:4843:ARG:HD3	1.62	0.82
1:A:4834:PRO:HB3	1:A:4843:ARG:HD3	1.62	0.81
1:C:3427:ASN:HB2	1:C:3463:THR:HB	1.38	0.81
1:C:3595:ARG:HA	1:C:3818:GLY:HA3	1.62	0.81
3:K:128:GLU:CB	3:K:131:ILE:HD13	1.75	0.81
1:B:4834:PRO:HB3	1:B:4843:ARG:HD3	1.62	0.81
1:C:943:LEU:HD21	1:C:999:LEU:HD22	1.62	0.81
3:I:128:GLU:CB	3:I:131:ILE:HD13	1.75	0.81
1:D:3595:ARG:HA	1:D:3818:GLY:HA3	1.62	0.81
1:D:4834:PRO:HB3	1:D:4843:ARG:HD3	1.62	0.81
1:D:943:LEU:HD21	1:D:999:LEU:HD22	1.62	0.80
1:B:3397:ARG:HH21	1:B:3550:ARG:HD2	1.47	0.80
1:D:3397:ARG:HH21	1:D:3550:ARG:HD2	1.47	0.80
1:B:3595:ARG:HA	1:B:3818:GLY:HA3	1.62	0.80
1:A:3397:ARG:HH21	1:A:3550:ARG:HD2	1.47	0.80
1:A:3595:ARG:HA	1:A:3818:GLY:HA3	1.62	0.80
1:A:996:VAL:HG13	1:A:1050:LEU:HD22	1.64	0.79
1:C:3397:ARG:HH21	1:C:3550:ARG:HD2	1.47	0.79
1:D:996:VAL:HG13	1:D:1050:LEU:HD22	1.64	0.79
1:C:996:VAL:HG13	1:C:1050:LEU:HD22	1.64	0.79
3:K:128:GLU:HG2	3:K:131:ILE:HD13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:128:GLU:O	3:K:131:ILE:HD12	1.84	0.77
3:J:128:GLU:CB	3:J:131:ILE:HD13	1.75	0.77
1:B:996:VAL:HG13	1:B:1050:LEU:HD22	1.64	0.77
3:I:128:GLU:HG2	3:I:131:ILE:HD13	1.66	0.77
3:L:128:GLU:O	3:L:131:ILE:HD12	1.84	0.77
1:C:3227:ARG:HH12	1:C:3290:ILE:HD12	1.50	0.77
1:B:3308:ASN:OD1	1:B:3437:SER:HB3	1.85	0.77
1:C:3308:ASN:OD1	1:C:3437:SER:HB3	1.84	0.77
1:D:3373:LEU:HD11	1:D:3395:LEU:HD21	1.67	0.77
1:B:1751:ILE:HG13	1:B:1839:LEU:HD23	1.66	0.76
1:A:1751:ILE:HG13	1:A:1839:LEU:HD23	1.66	0.76
3:I:128:GLU:O	3:I:131:ILE:HD12	1.84	0.76
1:A:3308:ASN:OD1	1:A:3437:SER:HB3	1.84	0.76
3:J:128:GLU:HG2	3:J:131:ILE:HD13	1.66	0.76
1:D:3227:ARG:HH12	1:D:3290:ILE:HD12	1.50	0.76
1:D:3509:ILE:CD1	1:D:3552:LEU:HD21	2.15	0.76
3:J:128:GLU:O	3:J:131:ILE:HD12	1.84	0.76
1:B:3227:ARG:HH12	1:B:3290:ILE:HD12	1.50	0.76
1:C:1751:ILE:HG13	1:C:1839:LEU:HD23	1.66	0.76
1:B:3509:ILE:CD1	1:B:3552:LEU:HD21	2.15	0.76
1:D:3308:ASN:OD1	1:D:3437:SER:HB3	1.85	0.76
1:A:3509:ILE:CD1	1:A:3552:LEU:HD21	2.15	0.76
1:D:1751:ILE:HG13	1:D:1839:LEU:HD23	1.67	0.76
1:C:3509:ILE:CD1	1:C:3552:LEU:HD21	2.15	0.76
3:L:128:GLU:HG2	3:L:131:ILE:HD13	1.66	0.75
1:C:2425:SER:O	1:D:142:LYS:NZ	2.19	0.75
1:B:3832:ASP:HB3	1:B:3835:PHE:HB3	1.69	0.75
1:C:3832:ASP:HB3	1:C:3835:PHE:HB3	1.69	0.75
1:A:3373:LEU:HD11	1:A:3395:LEU:HD21	1.67	0.75
1:D:3832:ASP:HB3	1:D:3835:PHE:HB3	1.69	0.75
1:B:3250:TRP:O	1:B:3256:ASN:ND2	2.20	0.75
1:B:3373:LEU:HD11	1:B:3395:LEU:HD21	1.67	0.75
1:C:3373:LEU:HD11	1:C:3395:LEU:HD21	1.67	0.75
1:A:3227:ARG:HH12	1:A:3290:ILE:HD12	1.50	0.74
1:A:1956:ALA:HA	3:I:108:HIS:CE1	2.22	0.74
1:A:3832:ASP:HB3	1:A:3835:PHE:HB3	1.69	0.74
1:D:3250:TRP:O	1:D:3256:ASN:ND2	2.20	0.74
1:A:2988:ARG:HH12	1:A:2995:HIS:HB2	1.52	0.74
1:D:2988:ARG:HH12	1:D:2995:HIS:HB2	1.52	0.74
1:A:3250:TRP:O	1:A:3256:ASN:ND2	2.20	0.74
1:C:3493:LYS:NZ	1:C:3558:LEU:HB3	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2988:ARG:HH12	1:B:2995:HIS:HB2	1.52	0.74
1:C:3250:TRP:O	1:C:3256:ASN:ND2	2.20	0.74
1:B:3493:LYS:NZ	1:B:3558:LEU:HB3	2.03	0.73
3:L:128:GLU:C	3:L:131:ILE:HD12	2.09	0.73
1:C:2988:ARG:HH12	1:C:2995:HIS:HB2	1.52	0.73
1:A:3148:VAL:HG12	1:A:3151:GLN:HE21	1.54	0.73
3:J:87:ARG:HE	3:J:90:PHE:HE1	1.37	0.73
1:D:3493:LYS:NZ	1:D:3558:LEU:HB3	2.03	0.73
3:I:143:VAL:HA	3:I:146:MET:HG3	1.71	0.72
3:J:143:VAL:HA	3:J:146:MET:HG3	1.71	0.72
1:B:3148:VAL:HG12	1:B:3151:GLN:HE21	1.54	0.72
1:D:3022:PHE:HB3	1:D:3025:ASP:HB2	1.71	0.72
3:K:128:GLU:C	3:K:131:ILE:HD12	2.09	0.72
1:A:3493:LYS:NZ	1:A:3558:LEU:HB3	2.03	0.72
3:K:87:ARG:HE	3:K:90:PHE:HE1	1.37	0.72
3:I:128:GLU:C	3:I:131:ILE:HD12	2.09	0.72
1:C:3022:PHE:HB3	1:C:3025:ASP:HB2	1.71	0.72
1:D:3378:ASP:OD2	1:D:3434:ASP:OD1	2.07	0.72
1:D:3148:VAL:HG12	1:D:3151:GLN:HE21	1.54	0.72
3:I:87:ARG:HE	3:I:90:PHE:HE1	1.37	0.72
1:C:3378:ASP:OD2	1:C:3434:ASP:OD1	2.07	0.72
3:K:143:VAL:HA	3:K:146:MET:HG3	1.71	0.72
1:B:3378:ASP:OD2	1:B:3434:ASP:OD1	2.07	0.72
1:B:3493:LYS:NZ	1:B:3558:LEU:CB	2.53	0.72
1:A:3022:PHE:HB3	1:A:3025:ASP:HB2	1.71	0.71
3:L:87:ARG:HE	3:L:90:PHE:HE1	1.37	0.71
3:L:143:VAL:HA	3:L:146:MET:HG3	1.71	0.71
1:C:3148:VAL:HG12	1:C:3151:GLN:HE21	1.54	0.71
1:B:3022:PHE:HB3	1:B:3025:ASP:HB2	1.71	0.71
1:C:2235:ARG:HG2	1:C:2297:ARG:HH12	1.56	0.71
1:C:4903:HIS:H	1:D:4183:LYS:HD2	1.54	0.71
3:J:128:GLU:C	3:J:131:ILE:HD12	2.09	0.71
1:B:2235:ARG:HG2	1:B:2297:ARG:HH12	1.55	0.71
1:D:2235:ARG:HG2	1:D:2297:ARG:HH12	1.55	0.71
1:A:2235:ARG:HG2	1:A:2297:ARG:HH12	1.55	0.71
1:A:3378:ASP:OD2	1:A:3434:ASP:CG	2.29	0.71
1:A:3378:ASP:OD2	1:A:3434:ASP:OD1	2.07	0.71
1:A:3493:LYS:NZ	1:A:3558:LEU:CB	2.53	0.71
1:C:3493:LYS:NZ	1:C:3558:LEU:CB	2.53	0.71
1:D:3493:LYS:NZ	1:D:3558:LEU:CB	2.53	0.71
1:C:3378:ASP:OD2	1:C:3434:ASP:CG	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2916:SER:OG	1:A:2920:ARG:NH2	2.24	0.71
1:B:2916:SER:OG	1:B:2920:ARG:NH2	2.24	0.70
1:D:2916:SER:OG	1:D:2920:ARG:NH2	2.24	0.70
1:D:3378:ASP:OD2	1:D:3434:ASP:CG	2.29	0.70
3:K:14:LYS:HG2	1:C:2153:LYS:HD3	1.72	0.70
1:B:2752:LYS:HA	1:B:2754:GLN:HE22	1.56	0.70
1:B:3378:ASP:OD2	1:B:3434:ASP:CG	2.29	0.70
1:C:2916:SER:OG	1:C:2920:ARG:NH2	2.24	0.70
1:D:894:VAL:O	1:D:898:ILE:HD12	1.92	0.70
1:D:3184:TYR:HA	1:D:3192:ARG:HH12	1.57	0.70
1:C:2752:LYS:HA	1:C:2754:GLN:HE22	1.56	0.70
1:C:3184:TYR:HA	1:C:3192:ARG:HH12	1.57	0.70
1:B:4609:LYS:HD2	1:B:4615:LEU:HD13	1.74	0.69
1:C:4609:LYS:HD2	1:C:4615:LEU:HD13	1.74	0.69
1:C:1685:LEU:HB3	1:C:1706:LEU:HD12	1.74	0.69
1:B:1685:LEU:HB3	1:B:1706:LEU:HD12	1.74	0.69
1:A:2752:LYS:HA	1:A:2754:GLN:HE22	1.56	0.69
1:D:2761:LYS:HE2	1:D:2761:LYS:HA	1.74	0.69
1:A:3184:TYR:HA	1:A:3192:ARG:HH12	1.57	0.69
1:A:894:VAL:O	1:A:898:ILE:HD12	1.92	0.69
1:C:894:VAL:O	1:C:898:ILE:HD12	1.92	0.69
1:D:1685:LEU:HB3	1:D:1706:LEU:HD12	1.74	0.69
1:D:4609:LYS:HD2	1:D:4615:LEU:HD13	1.74	0.69
1:A:2761:LYS:HE2	1:A:2761:LYS:HA	1.74	0.69
1:A:3597:ARG:HH22	3:I:148:ALA:HB3	1.56	0.69
1:B:3184:TYR:HA	1:B:3192:ARG:HH12	1.57	0.69
1:D:2752:LYS:HA	1:D:2754:GLN:HE22	1.56	0.69
1:A:1685:LEU:HB3	1:A:1706:LEU:HD12	1.74	0.69
1:B:2979:ARG:HG3	1:B:3039:THR:HG22	1.75	0.68
1:A:4609:LYS:HD2	1:A:4615:LEU:HD13	1.74	0.68
1:C:3525:ARG:HA	1:C:3528:MET:SD	2.34	0.68
1:A:3525:ARG:HA	1:A:3528:MET:SD	2.34	0.68
1:B:2761:LYS:HA	1:B:2761:LYS:HE2	1.74	0.68
1:B:3525:ARG:HA	1:B:3528:MET:SD	2.34	0.68
1:B:894:VAL:O	1:B:898:ILE:HD12	1.92	0.68
1:C:2761:LYS:HE2	1:C:2761:LYS:HA	1.74	0.68
1:D:3409:SER:HB3	1:D:3412:PHE:CE2	2.29	0.68
3:L:128:GLU:HG2	3:L:131:ILE:CD1	2.21	0.68
1:A:3409:SER:HB3	1:A:3412:PHE:CE2	2.29	0.67
3:K:132:ASP:C	3:K:137:VAL:HG22	2.14	0.67
1:A:2979:ARG:HG3	1:A:3039:THR:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:128:GLU:HG2	3:J:131:ILE:CD1	2.21	0.67
1:C:2764:SER:OG	1:C:2767:GLU:OE1	2.13	0.67
1:D:3525:ARG:HA	1:D:3528:MET:SD	2.34	0.67
1:B:3148:VAL:HA	1:B:3151:GLN:HG2	1.77	0.67
1:C:2979:ARG:HG3	1:C:3039:THR:HG22	1.75	0.67
1:D:2979:ARG:HG3	1:D:3039:THR:HG22	1.75	0.67
1:A:4602:ARG:HH12	1:A:4627:LYS:HB3	1.59	0.67
1:C:114:LEU:HB2	1:C:117:HIS:CD2	2.30	0.67
1:D:114:LEU:HB2	1:D:117:HIS:CD2	2.30	0.67
1:A:3148:VAL:HA	1:A:3151:GLN:HG2	1.77	0.67
3:I:132:ASP:C	3:I:137:VAL:HG22	2.14	0.67
1:B:4818:TYR:OH	1:C:4847:ASP:OD2	2.10	0.67
1:B:3409:SER:HB3	1:B:3412:PHE:CE2	2.29	0.67
1:C:3409:SER:HB3	1:C:3412:PHE:CE2	2.29	0.67
3:I:6:THR:OG1	3:I:9:GLN:OE1	2.13	0.67
1:B:114:LEU:HB2	1:B:117:HIS:CD2	2.30	0.67
1:D:1239:PHE:O	1:D:1807:ARG:NH2	2.28	0.67
1:C:4602:ARG:HH12	1:C:4627:LYS:HB3	1.59	0.66
1:B:2425:SER:O	1:C:142:LYS:NZ	2.29	0.66
1:D:4602:ARG:HH12	1:D:4627:LYS:HB3	1.59	0.66
1:A:142:LYS:NZ	1:D:2425:SER:O	2.27	0.66
3:J:132:ASP:C	3:J:137:VAL:HG22	2.14	0.66
1:C:3148:VAL:HA	1:C:3151:GLN:HG2	1.77	0.66
1:D:2764:SER:OG	1:D:2767:GLU:OE1	2.13	0.66
1:A:2764:SER:OG	1:A:2767:GLU:OE1	2.13	0.66
3:K:6:THR:OG1	3:K:9:GLN:OE1	2.13	0.66
1:B:4602:ARG:HH12	1:B:4627:LYS:HB3	1.59	0.66
1:A:114:LEU:HB2	1:A:117:HIS:CD2	2.30	0.66
1:B:2764:SER:OG	1:B:2767:GLU:OE1	2.13	0.66
1:D:3148:VAL:HA	1:D:3151:GLN:HG2	1.77	0.66
3:L:132:ASP:C	3:L:137:VAL:HG22	2.14	0.65
1:A:1239:PHE:O	1:A:1807:ARG:NH2	2.28	0.65
3:J:6:THR:OG1	3:J:9:GLN:OE1	2.13	0.65
1:B:1239:PHE:O	1:B:1807:ARG:NH2	2.28	0.65
1:C:3427:ASN:HB2	1:C:3463:THR:HG1	1.61	0.65
1:B:3412:PHE:O	1:B:3416:GLU:HB2	1.97	0.65
1:B:3427:ASN:HB2	1:B:3463:THR:HB	1.38	0.65
1:C:3412:PHE:O	1:C:3416:GLU:HB2	1.97	0.65
1:D:3412:PHE:O	1:D:3416:GLU:HB2	1.97	0.65
1:D:3427:ASN:CB	1:D:3463:THR:O	2.45	0.65
1:D:3499:LYS:HE3	1:D:3564:LYS:HZ2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3427:ASN:CB	1:A:3463:THR:O	2.45	0.64
1:C:1239:PHE:O	1:C:1807:ARG:NH2	2.28	0.64
1:A:1959:ALA:CB	3:I:108:HIS:HB3	2.26	0.64
1:B:3427:ASN:CB	1:B:3463:THR:O	2.45	0.64
1:D:1766:PRO:HG3	1:D:1780:PRO:HB3	1.80	0.64
1:A:1766:PRO:HG3	1:A:1780:PRO:HB3	1.80	0.64
3:I:128:GLU:HG2	3:I:131:ILE:CD1	2.21	0.64
1:B:3477:GLY:HA2	1:B:3480:ILE:HD12	1.79	0.64
1:C:1766:PRO:HG3	1:C:1780:PRO:HB3	1.80	0.64
1:B:1766:PRO:HG3	1:B:1780:PRO:HB3	1.80	0.64
1:C:3427:ASN:CB	1:C:3463:THR:O	2.45	0.64
1:C:3478:LEU:HD21	1:D:1233:GLN:HB3	1.78	0.64
1:C:3324:GLU:HG2	1:C:3327:LYS:HZ3	1.63	0.64
1:B:3695:MET:HB3	1:B:3731:LEU:HD11	1.80	0.64
1:A:3477:GLY:HA2	1:A:3480:ILE:HD12	1.79	0.63
1:D:3477:GLY:HA2	1:D:3480:ILE:HD12	1.79	0.63
1:A:3695:MET:HB3	1:A:3731:LEU:HD11	1.80	0.63
1:B:4664:ASP:OD1	1:B:4674:LYS:NZ	2.29	0.63
3:L:6:THR:OG1	3:L:9:GLN:OE1	2.13	0.63
1:D:4052:MET:HE2	1:D:4063:THR:HG23	1.79	0.63
1:D:4751:LYS:HA	1:D:4754:ARG:HE	1.64	0.63
1:A:3412:PHE:O	1:A:3416:GLU:HB2	1.97	0.63
1:C:4751:LYS:HA	1:C:4754:ARG:HE	1.63	0.63
3:L:138:ASN:O	3:L:142:PHE:HB2	1.98	0.63
3:K:138:ASN:O	3:K:142:PHE:HB2	1.98	0.63
1:B:222:GLU:HB2	1:B:349:MET:HG3	1.80	0.63
2:G:83:TYR:OH	1:C:1768:PHE:O	2.15	0.63
1:B:3499:LYS:HE3	1:B:3564:LYS:NZ	2.14	0.63
1:A:3037:GLY:HA2	1:A:3040:LEU:HD13	1.81	0.63
1:B:4144:ARG:HB3	1:B:4961:GLN:HE22	1.64	0.63
1:B:4751:LYS:HA	1:B:4754:ARG:HE	1.64	0.63
1:A:2556:SER:HB2	1:A:2569:ILE:HG21	1.81	0.62
1:A:3596:LYS:HB2	3:I:146:MET:HE3	1.76	0.62
1:C:3499:LYS:HE3	1:C:3564:LYS:NZ	2.14	0.62
1:C:4664:ASP:OD1	1:C:4674:LYS:NZ	2.29	0.62
1:A:4751:LYS:HA	1:A:4754:ARG:HE	1.64	0.62
1:C:2830:ASN:HD22	1:D:1435:GLY:HA2	1.63	0.62
1:C:4169:LYS:NZ	5:C:5002:ATP:O1B	2.32	0.62
1:D:3695:MET:HB3	1:D:3731:LEU:HD11	1.80	0.62
1:A:4664:ASP:OD1	1:A:4674:LYS:NZ	2.29	0.62
3:I:138:ASN:O	3:I:142:PHE:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:138:ASN:O	3:J:142:PHE:HB2	1.98	0.62
1:C:3499:LYS:HE3	1:C:3564:LYS:HZ2	1.64	0.62
1:D:4169:LYS:NZ	5:D:5002:ATP:O1B	2.32	0.62
1:A:4144:ARG:HB3	1:A:4961:GLN:HE22	1.64	0.62
1:A:4169:LYS:NZ	5:A:5002:ATP:O1B	2.32	0.62
1:A:4622:SER:OG	1:A:4624:ASP:OD1	2.18	0.62
1:B:2556:SER:HB2	1:B:2569:ILE:HG21	1.81	0.62
1:B:4052:MET:HE2	1:B:4063:THR:HG23	1.79	0.62
1:B:4169:LYS:NZ	5:B:5002:ATP:O1B	2.32	0.62
1:A:222:GLU:HB2	1:A:349:MET:HG3	1.80	0.62
1:C:3477:GLY:HA2	1:C:3480:ILE:HD12	1.79	0.62
1:D:4622:SER:OG	1:D:4624:ASP:OD1	2.18	0.62
3:J:15:GLU:OE1	3:J:15:GLU:N	2.32	0.62
1:B:3653:GLU:HG2	1:B:3655:ASP:H	1.65	0.62
1:C:897:LYS:HB2	1:C:902:TRP:HB2	1.82	0.62
1:C:3695:MET:HB3	1:C:3731:LEU:HD11	1.80	0.62
1:A:4052:MET:HE2	1:A:4063:THR:HG23	1.80	0.62
3:I:83:GLU:OE2	3:I:87:ARG:NH1	2.31	0.62
1:C:4144:ARG:HB3	1:C:4961:GLN:HE22	1.64	0.62
1:C:4590:TYR:HA	1:C:4593:LEU:HB3	1.82	0.62
1:D:222:GLU:HB2	1:D:349:MET:HG3	1.80	0.62
1:D:3037:GLY:HA2	1:D:3040:LEU:HD13	1.81	0.62
1:D:3499:LYS:HE3	1:D:3564:LYS:NZ	2.14	0.62
1:A:4775:ALA:HA	1:A:4817:MET:HE1	1.80	0.62
3:K:128:GLU:HG2	3:K:131:ILE:CD1	2.21	0.62
1:C:4052:MET:HE2	1:C:4063:THR:HG23	1.81	0.62
1:D:897:LYS:HB2	1:D:902:TRP:HB2	1.82	0.62
1:D:4144:ARG:HB3	1:D:4961:GLN:HE22	1.64	0.62
1:A:3499:LYS:HE3	1:A:3564:LYS:NZ	2.14	0.62
1:B:3037:GLY:HA2	1:B:3040:LEU:HD13	1.81	0.62
1:C:3653:GLU:HG2	1:C:3655:ASP:H	1.65	0.62
1:C:4775:ALA:HA	1:C:4817:MET:HE1	1.81	0.62
1:D:3324:GLU:HG2	1:D:3327:LYS:HZ3	1.65	0.62
1:A:3653:GLU:HG2	1:A:3655:ASP:H	1.65	0.61
1:C:222:GLU:HB2	1:C:349:MET:HG3	1.80	0.61
1:D:3653:GLU:HG2	1:D:3655:ASP:H	1.65	0.61
1:C:3037:GLY:HA2	1:C:3040:LEU:HD13	1.81	0.61
3:L:83:GLU:OE2	3:L:87:ARG:NH1	2.31	0.61
1:B:163:HIS:HB2	1:B:182:ILE:HG13	1.83	0.61
1:A:3274:ASN:HB2	1:A:3314:LEU:HD11	1.82	0.61
1:B:4590:TYR:HA	1:B:4593:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ARG:HH11	1:B:15:ARG:HG3	1.66	0.61
1:B:3274:ASN:HB2	1:B:3314:LEU:HD11	1.82	0.61
1:B:3464:SER:HB3	1:B:3467:VAL:HG22	1.83	0.61
1:C:3482:ALA:H	1:C:3485:ASP:HB3	1.65	0.61
1:A:4590:TYR:HA	1:A:4593:LEU:HB3	1.82	0.61
1:C:15:ARG:HH11	1:C:15:ARG:HG3	1.66	0.61
1:C:3493:LYS:HZ2	1:C:3558:LEU:HB2	1.65	0.61
1:A:163:HIS:HB2	1:A:182:ILE:HG13	1.83	0.61
1:A:3559:PHE:HD1	1:A:3563:GLN:HE21	1.48	0.61
1:D:3493:LYS:HZ2	1:D:3558:LEU:HB2	1.65	0.61
1:D:4590:TYR:HA	1:D:4593:LEU:HB3	1.82	0.61
1:A:2920:ARG:NH1	1:A:2981:TYR:OH	2.34	0.61
1:B:3493:LYS:HZ2	1:B:3558:LEU:HB2	1.64	0.61
1:C:3464:SER:HB3	1:C:3467:VAL:HG22	1.83	0.61
1:D:314:LEU:HD11	1:D:372:LEU:HD11	1.83	0.61
1:A:3522:PRO:HA	1:A:3525:ARG:HG2	1.83	0.60
3:I:15:GLU:OE1	3:I:15:GLU:N	2.32	0.60
1:C:2556:SER:HB2	1:C:2569:ILE:HG21	1.81	0.60
1:D:2556:SER:HB2	1:D:2569:ILE:HG21	1.81	0.60
1:D:2920:ARG:NH1	1:D:2981:TYR:OH	2.34	0.60
1:D:3522:PRO:HA	1:D:3525:ARG:HG2	1.83	0.60
1:A:314:LEU:HD11	1:A:372:LEU:HD11	1.83	0.60
1:B:3482:ALA:H	1:B:3485:ASP:HB3	1.65	0.60
1:C:163:HIS:HB2	1:C:182:ILE:HG13	1.83	0.60
1:C:2920:ARG:NH1	1:C:2981:TYR:OH	2.34	0.60
1:C:3522:PRO:HA	1:C:3525:ARG:HG2	1.83	0.60
1:D:3274:ASN:HB2	1:D:3314:LEU:HD11	1.82	0.60
1:A:137:ARG:NE	1:A:139:SER:OG	2.35	0.60
1:B:3522:PRO:HA	1:B:3525:ARG:HG2	1.83	0.60
1:C:4622:SER:OG	1:C:4624:ASP:OD1	2.18	0.60
1:D:323:ASP:O	1:D:325:LYS:N	2.33	0.60
1:D:799:LYS:HG2	1:D:1620:GLN:HG3	1.83	0.60
1:A:897:LYS:HB2	1:A:902:TRP:HB2	1.82	0.60
1:B:2920:ARG:NH1	1:B:2981:TYR:OH	2.34	0.60
1:B:3559:PHE:HD1	1:B:3563:GLN:HE21	1.48	0.60
1:A:3596:LYS:HD3	3:I:146:MET:O	2.02	0.60
1:D:1839:LEU:HD12	1:D:1842:ILE:HD11	1.84	0.60
1:D:3559:PHE:HD1	1:D:3563:GLN:HE21	1.48	0.60
1:A:3482:ALA:H	1:A:3485:ASP:HB3	1.65	0.60
1:B:4622:SER:OG	1:B:4624:ASP:OD1	2.18	0.60
1:C:137:ARG:NE	1:C:139:SER:OG	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:HIS:HB2	1:D:182:ILE:HG13	1.83	0.60
3:J:83:GLU:OE2	3:J:87:ARG:NH1	2.31	0.60
3:K:15:GLU:OE1	3:K:15:GLU:N	2.32	0.60
1:C:799:LYS:HG2	1:C:1620:GLN:HG3	1.83	0.60
1:C:2830:ASN:ND2	1:D:1435:GLY:HA2	2.16	0.60
1:B:897:LYS:HB2	1:B:902:TRP:HB2	1.82	0.60
1:C:3559:PHE:HD1	1:C:3563:GLN:HE21	1.48	0.60
1:A:3464:SER:HB3	1:A:3467:VAL:HG22	1.83	0.60
1:A:4637:THR:HG21	1:A:4705:TYR:HB2	1.84	0.60
1:B:541:ILE:HD11	1:B:574:VAL:HG13	1.84	0.60
3:J:138:ASN:O	3:J:142:PHE:CB	2.50	0.60
1:D:15:ARG:HH11	1:D:15:ARG:HG3	1.66	0.60
1:A:1839:LEU:HD12	1:A:1842:ILE:HD11	1.84	0.59
3:I:138:ASN:O	3:I:142:PHE:CB	2.50	0.59
3:K:83:GLU:OE2	3:K:87:ARG:NH1	2.31	0.59
1:B:555:LEU:HD11	1:B:578:VAL:HG11	1.84	0.59
1:C:3274:ASN:HB2	1:C:3314:LEU:HD11	1.82	0.59
1:D:3482:ALA:H	1:D:3485:ASP:HB3	1.65	0.59
1:A:799:LYS:HG2	1:A:1620:GLN:HG3	1.84	0.59
1:B:137:ARG:NE	1:B:139:SER:OG	2.35	0.59
1:D:137:ARG:NE	1:D:139:SER:OG	2.35	0.59
1:D:2139:GLU:HG3	1:D:2192:MET:HB2	1.84	0.59
1:D:3464:SER:HB3	1:D:3467:VAL:HG22	1.83	0.59
1:B:1839:LEU:HD12	1:B:1842:ILE:HD11	1.84	0.59
1:C:3022:PHE:HD2	1:C:3029:ILE:HD13	1.67	0.59
1:D:925:PRO:HB2	1:D:928:GLU:HB2	1.84	0.59
1:C:314:LEU:HD11	1:C:372:LEU:HD11	1.83	0.59
1:C:541:ILE:HD11	1:C:574:VAL:HG13	1.84	0.59
1:D:4637:THR:HG21	1:D:4705:TYR:HB2	1.84	0.59
1:A:541:ILE:HD11	1:A:574:VAL:HG13	1.84	0.59
1:C:925:PRO:HB2	1:C:928:GLU:HB2	1.85	0.59
1:A:3597:ARG:NH2	3:I:148:ALA:HB3	2.18	0.59
3:K:138:ASN:O	3:K:142:PHE:CB	2.50	0.59
1:B:799:LYS:HG2	1:B:1620:GLN:HG3	1.83	0.59
1:B:4187:GLU:OE1	1:B:4949:TRP:NE1	2.31	0.59
1:C:323:ASP:O	1:C:325:LYS:N	2.33	0.59
1:A:925:PRO:HB2	1:A:928:GLU:HB2	1.85	0.59
1:A:1129:GLY:HA3	1:A:1145:TRP:HB3	1.84	0.59
1:A:2139:GLU:HG3	1:A:2192:MET:HB2	1.84	0.59
1:B:1936:LEU:HD11	1:B:1976:LEU:HD22	1.84	0.59
1:D:1129:GLY:HA3	1:D:1145:TRP:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1936:LEU:HD11	1:D:1976:LEU:HD22	1.84	0.59
1:D:4187:GLU:OE1	1:D:4949:TRP:NE1	2.31	0.59
3:L:138:ASN:O	3:L:142:PHE:CB	2.50	0.59
1:B:3022:PHE:HD2	1:B:3029:ILE:HD13	1.68	0.59
1:B:4775:ALA:HA	1:B:4817:MET:HE1	1.84	0.59
1:C:555:LEU:HD11	1:C:578:VAL:HG11	1.85	0.59
1:C:1839:LEU:HD12	1:C:1842:ILE:HD11	1.84	0.59
1:A:15:ARG:HG3	1:A:15:ARG:HH11	1.66	0.59
1:A:555:LEU:HD11	1:A:578:VAL:HG11	1.85	0.59
1:A:3022:PHE:HD2	1:A:3029:ILE:HD13	1.68	0.59
1:A:4187:GLU:OE1	1:A:4949:TRP:NE1	2.31	0.59
1:B:314:LEU:HD11	1:B:372:LEU:HD11	1.83	0.59
1:B:4818:TYR:HE1	1:C:4847:ASP:HB2	1.66	0.59
1:D:3022:PHE:HD2	1:D:3029:ILE:HD13	1.68	0.59
1:A:1936:LEU:HD11	1:A:1976:LEU:HD22	1.84	0.58
1:D:841:LYS:O	1:D:848:ARG:NH2	2.34	0.58
1:D:4775:ALA:HA	1:D:4817:MET:HE1	1.83	0.58
1:C:1129:GLY:HA3	1:C:1145:TRP:HB3	1.84	0.58
1:C:1936:LEU:HD11	1:C:1976:LEU:HD22	1.84	0.58
1:C:3348:MET:SD	1:C:3353:LEU:HB2	2.44	0.58
1:B:3348:MET:SD	1:B:3353:LEU:HB2	2.44	0.58
1:C:4637:THR:HG21	1:C:4705:TYR:HB2	1.84	0.58
1:D:541:ILE:HD11	1:D:574:VAL:HG13	1.84	0.58
2:H:50:ARG:HB3	2:H:50:ARG:HH11	1.69	0.58
3:L:15:GLU:OE1	3:L:15:GLU:N	2.32	0.58
1:C:1962:THR:HA	1:C:1965:PHE:HD2	1.69	0.58
1:A:3804:ASP:H	1:A:3829:VAL:HG13	1.68	0.58
1:C:2823:PRO:O	1:C:2824:ARG:NH1	2.37	0.58
1:D:3651:PRO:HB2	1:D:3652:PRO:HD3	1.85	0.58
3:J:109:VAL:HB	1:B:3603:PHE:HZ	1.69	0.58
3:L:128:GLU:CA	3:L:131:ILE:HD11	2.29	0.58
1:B:323:ASP:O	1:B:325:LYS:N	2.33	0.58
1:B:1129:GLY:HA3	1:B:1145:TRP:HB3	1.84	0.58
1:C:3246:MET:HG2	1:C:3268:LEU:HD11	1.85	0.58
1:C:3804:ASP:H	1:C:3829:VAL:HG13	1.68	0.58
1:D:555:LEU:HD11	1:D:578:VAL:HG11	1.85	0.58
1:D:3348:MET:SD	1:D:3353:LEU:HB2	2.44	0.58
1:A:841:LYS:O	1:A:848:ARG:NH2	2.34	0.58
1:A:3269:ASN:HB3	1:A:3271:GLU:HG3	1.86	0.58
3:J:6:THR:H	3:J:9:GLN:NE2	2.02	0.58
1:B:3269:ASN:HB3	1:B:3271:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1960:ARG:NH2	3:I:111:THR:OG1	2.32	0.58
1:A:2823:PRO:O	1:A:2824:ARG:NH1	2.37	0.58
1:A:3348:MET:SD	1:A:3353:LEU:HB2	2.44	0.58
1:B:925:PRO:HB2	1:B:928:GLU:HB2	1.85	0.58
1:B:2139:GLU:HG3	1:B:2192:MET:HB2	1.84	0.58
1:D:2823:PRO:O	1:D:2824:ARG:NH1	2.37	0.58
1:D:2895:PHE:HA	1:D:2898:ILE:HG12	1.86	0.58
1:A:1962:THR:HA	1:A:1965:PHE:HD2	1.69	0.58
1:B:2744:GLY:HA2	1:B:2753:VAL:HG13	1.86	0.58
1:C:2322:ARG:O	1:C:2326:ARG:HG2	2.04	0.58
1:D:1097:LYS:NZ	1:D:1198:GLY:O	2.37	0.58
2:F:50:ARG:HB3	2:F:50:ARG:HH11	1.69	0.57
3:I:6:THR:H	3:I:9:GLN:NE2	2.02	0.57
1:B:1962:THR:HA	1:B:1965:PHE:HD2	1.69	0.57
1:B:4637:THR:HG21	1:B:4705:TYR:HB2	1.84	0.57
1:C:2139:GLU:HG3	1:C:2192:MET:HB2	1.84	0.57
1:C:2744:GLY:HA2	1:C:2753:VAL:HG13	1.86	0.57
1:C:3651:PRO:HB2	1:C:3652:PRO:HD3	1.85	0.57
1:C:3892:TYR:O	1:C:3957:LYS:NZ	2.37	0.57
1:D:1962:THR:HA	1:D:1965:PHE:HD2	1.69	0.57
1:D:2792:THR:HG23	1:D:2794:GLU:H	1.69	0.57
1:A:2792:THR:HG23	1:A:2794:GLU:H	1.69	0.57
1:A:2895:PHE:HA	1:A:2898:ILE:HG12	1.86	0.57
1:A:3320:LEU:HD23	1:A:3321:PRO:HD3	1.86	0.57
1:B:2545:ILE:HD12	1:B:2580:LEU:HD21	1.86	0.57
1:B:3246:MET:HG2	1:B:3268:LEU:HD11	1.85	0.57
1:B:3534:LEU:HD13	1:B:3537:ARG:HG3	1.86	0.57
1:D:3892:TYR:O	1:D:3957:LYS:NZ	2.37	0.57
2:E:50:ARG:HB3	2:E:50:ARG:HH11	1.69	0.57
1:C:2826:ILE:HD12	1:D:1501:ASN:HD21	1.69	0.57
1:D:4913:HIS:O	5:D:5002:ATP:N6	2.37	0.57
1:A:2322:ARG:O	1:A:2326:ARG:HG2	2.04	0.57
3:K:6:THR:H	3:K:9:GLN:NE2	2.02	0.57
3:L:6:THR:H	3:L:9:GLN:NE2	2.02	0.57
1:B:1097:LYS:NZ	1:B:1198:GLY:O	2.37	0.57
1:B:2322:ARG:O	1:B:2326:ARG:HG2	2.04	0.57
1:C:2758:LYS:HE3	1:C:2763:LEU:HA	1.87	0.57
1:A:4913:HIS:O	5:A:5002:ATP:N6	2.37	0.57
1:B:2895:PHE:HA	1:B:2898:ILE:HG12	1.86	0.57
1:B:4913:HIS:O	5:B:5002:ATP:N6	2.37	0.57
1:C:1097:LYS:NZ	1:C:1198:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3246:MET:HG2	1:D:3268:LEU:HD11	1.85	0.57
3:I:82:SER:O	3:I:86:ILE:HG22	2.04	0.57
1:C:2895:PHE:HA	1:C:2898:ILE:HG12	1.86	0.57
1:C:4913:HIS:O	5:C:5002:ATP:N6	2.37	0.57
1:D:3269:ASN:HB3	1:D:3271:GLU:HG3	1.86	0.57
1:D:3320:LEU:HD23	1:D:3321:PRO:HD3	1.86	0.57
1:D:3804:ASP:H	1:D:3829:VAL:HG13	1.68	0.57
1:A:394:HIS:CE1	1:A:396:GLU:HG3	2.40	0.57
1:A:1097:LYS:NZ	1:A:1198:GLY:O	2.37	0.57
1:A:1951:LEU:HD12	1:A:1958:THR:HG21	1.86	0.57
1:A:1963:LYS:HG3	3:I:113:LEU:HD22	1.87	0.57
1:A:2545:ILE:HD12	1:A:2580:LEU:HD21	1.86	0.57
1:B:1951:LEU:HD12	1:B:1958:THR:HG21	1.86	0.57
1:B:3324:GLU:HG2	1:B:3327:LYS:HZ3	1.69	0.57
1:B:3651:PRO:HB2	1:B:3652:PRO:HD3	1.85	0.57
1:C:3269:ASN:HB3	1:C:3271:GLU:HG3	1.86	0.57
1:D:1951:LEU:HD12	1:D:1958:THR:HG21	1.86	0.57
1:D:3274:ASN:OD1	1:D:3275:THR:N	2.38	0.57
1:D:3406:TRP:HA	1:D:3412:PHE:CE2	2.40	0.57
1:D:3534:LEU:HD13	1:D:3537:ARG:HG3	1.86	0.57
1:A:3184:TYR:HA	1:A:3192:ARG:NH1	2.20	0.57
2:G:50:ARG:HB3	2:G:50:ARG:HH11	1.69	0.57
3:J:82:SER:O	3:J:86:ILE:HG22	2.04	0.57
1:B:981:MET:HE1	1:B:1056:THR:HG23	1.87	0.57
1:C:3715:GLU:O	1:C:3719:MET:HG2	2.05	0.57
1:D:2545:ILE:HD12	1:D:2580:LEU:HD21	1.86	0.57
1:D:2744:GLY:HA2	1:D:2753:VAL:HG13	1.86	0.57
1:A:3406:TRP:HA	1:A:3412:PHE:CE2	2.40	0.57
1:A:3651:PRO:HB2	1:A:3652:PRO:HD3	1.85	0.57
1:A:3715:GLU:O	1:A:3719:MET:HG2	2.05	0.57
1:B:2823:PRO:O	1:B:2824:ARG:NH1	2.37	0.57
1:B:3804:ASP:H	1:B:3829:VAL:HG13	1.68	0.57
1:C:394:HIS:CE1	1:C:396:GLU:HG3	2.40	0.57
1:D:249:SER:HA	1:D:257:ARG:NH2	2.20	0.57
1:A:981:MET:HE1	1:A:1056:THR:HG23	1.87	0.57
1:A:1682:GLU:HG2	1:A:1683:PRO:HD3	1.86	0.57
1:A:1911:GLN:OE1	1:A:2090:ARG:NH1	2.33	0.57
1:A:3246:MET:HG2	1:A:3268:LEU:HD11	1.85	0.57
1:A:3427:ASN:OD1	1:A:3463:THR:O	2.22	0.57
1:C:875:PRO:HD2	1:C:878:LEU:HD12	1.86	0.57
1:C:1682:GLU:HG2	1:C:1683:PRO:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:394:HIS:CE1	1:D:396:GLU:HG3	2.40	0.57
1:A:1243:THR:HG22	1:A:1808:ASP:HB2	1.87	0.56
1:B:1911:GLN:OE1	1:B:2090:ARG:NH1	2.32	0.56
1:C:4640:PHE:HB3	1:C:4641:PRO:HD3	1.87	0.56
1:D:1682:GLU:HG2	1:D:1683:PRO:HD3	1.86	0.56
1:A:3324:GLU:HG2	1:A:3327:LYS:HZ3	1.69	0.56
3:K:82:SER:O	3:K:86:ILE:HG22	2.04	0.56
3:K:128:GLU:CA	3:K:131:ILE:HD11	2.29	0.56
1:C:2792:THR:HG23	1:C:2794:GLU:H	1.69	0.56
1:D:601:LEU:HG	1:D:610:VAL:HG11	1.87	0.56
1:A:249:SER:HA	1:A:257:ARG:NH2	2.20	0.56
1:A:558:LEU:HG	1:A:571:ILE:HG23	1.86	0.56
1:A:601:LEU:HG	1:A:610:VAL:HG11	1.87	0.56
1:A:875:PRO:HD2	1:A:878:LEU:HD12	1.86	0.56
1:A:1272:ARG:NH2	1:A:1582:CYS:SG	2.79	0.56
1:A:3534:LEU:HD13	1:A:3537:ARG:HG3	1.86	0.56
1:B:249:SER:HA	1:B:257:ARG:NH2	2.20	0.56
1:B:394:HIS:CE1	1:B:396:GLU:HG3	2.40	0.56
1:B:2758:LYS:HE3	1:B:2763:LEU:HA	1.87	0.56
1:B:2792:THR:HG23	1:B:2794:GLU:H	1.69	0.56
1:B:3406:TRP:HA	1:B:3412:PHE:CE2	2.40	0.56
1:B:3715:GLU:O	1:B:3719:MET:HG2	2.05	0.56
1:B:3892:TYR:O	1:B:3957:LYS:NZ	2.37	0.56
1:C:3320:LEU:HD23	1:C:3321:PRO:HD3	1.86	0.56
1:C:3406:TRP:HA	1:C:3412:PHE:CE2	2.40	0.56
1:D:558:LEU:HG	1:D:571:ILE:HG23	1.86	0.56
1:D:2758:LYS:HE3	1:D:2763:LEU:HA	1.87	0.56
1:D:3184:TYR:HA	1:D:3192:ARG:NH1	2.20	0.56
1:D:3715:GLU:O	1:D:3719:MET:HG2	2.05	0.56
1:D:4640:PHE:HB3	1:D:4641:PRO:HD3	1.88	0.56
2:H:24:VAL:HG22	2:H:48:LYS:HG2	1.88	0.56
3:L:82:SER:O	3:L:86:ILE:HG22	2.04	0.56
1:B:476:GLN:NE2	1:B:3678:GLU:OE1	2.39	0.56
1:B:3184:TYR:HA	1:B:3192:ARG:NH1	2.20	0.56
1:B:3493:LYS:HZ2	1:B:3558:LEU:CB	2.18	0.56
1:C:2426:LEU:HD21	1:D:143:LEU:HD22	1.86	0.56
1:C:3534:LEU:HD13	1:C:3537:ARG:HG3	1.86	0.56
1:D:1272:ARG:NH2	1:D:1582:CYS:SG	2.79	0.56
1:B:3320:LEU:HD23	1:B:3321:PRO:HD3	1.86	0.56
1:B:4640:PHE:HB3	1:B:4641:PRO:HD3	1.88	0.56
1:D:1243:THR:HG22	1:D:1808:ASP:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2322:ARG:O	1:D:2326:ARG:HG2	2.04	0.56
1:D:4028:SER:O	1:D:4033:LYS:NZ	2.36	0.56
1:A:1495:SER:OG	1:A:1496:PRO:HD2	2.06	0.56
1:B:1682:GLU:HG2	1:B:1683:PRO:HD3	1.86	0.56
1:C:2743:TYR:HA	1:C:2757:MET:HE1	1.86	0.56
1:A:1176:THR:HG22	1:A:1181:ILE:HA	1.88	0.56
1:A:2171:VAL:HG21	1:A:2199:PHE:CD2	2.41	0.56
1:C:249:SER:HA	1:C:257:ARG:NH2	2.20	0.56
1:C:1272:ARG:NH2	1:C:1582:CYS:SG	2.79	0.56
1:D:476:GLN:NE2	1:D:3678:GLU:OE1	2.39	0.56
1:A:2744:GLY:HA2	1:A:2753:VAL:HG13	1.86	0.56
1:B:1176:THR:HG22	1:B:1181:ILE:HA	1.88	0.56
1:B:1272:ARG:NH2	1:B:1582:CYS:SG	2.79	0.56
1:B:2171:VAL:HG21	1:B:2199:PHE:CD2	2.41	0.56
1:B:2830:ASN:ND2	1:C:1435:GLY:HA2	2.20	0.56
1:C:1951:LEU:HD12	1:C:1958:THR:HG21	1.86	0.56
1:C:2545:ILE:HD12	1:C:2580:LEU:HD21	1.86	0.56
1:C:3594:GLN:HA	1:C:3597:ARG:HD3	1.88	0.56
1:D:3594:GLN:HA	1:D:3597:ARG:HD3	1.88	0.56
1:A:323:ASP:O	1:A:325:LYS:N	2.33	0.56
1:A:3274:ASN:OD1	1:A:3275:THR:N	2.38	0.56
1:A:4640:PHE:HB3	1:A:4641:PRO:HD3	1.88	0.56
2:G:24:VAL:HG22	2:G:48:LYS:HG2	1.88	0.56
1:C:246:THR:HG21	1:C:267:VAL:HG11	1.88	0.56
1:C:476:GLN:NE2	1:C:3678:GLU:OE1	2.39	0.56
1:C:601:LEU:HG	1:C:610:VAL:HG11	1.87	0.56
1:C:981:MET:HE1	1:C:1056:THR:HG23	1.88	0.56
1:C:3184:TYR:HA	1:C:3192:ARG:NH1	2.20	0.56
1:C:4053:GLU:OE2	1:C:4060:GLN:NE2	2.39	0.56
1:A:2758:LYS:HE3	1:A:2763:LEU:HA	1.87	0.56
3:J:92:VAL:HG12	3:J:93:PHE:HD1	1.71	0.56
1:B:2488:LEU:HD21	1:B:2548:LEU:HD22	1.88	0.56
1:B:2743:TYR:HA	1:B:2757:MET:HE1	1.88	0.56
1:B:3594:GLN:HA	1:B:3597:ARG:HD3	1.88	0.56
1:B:3778:LEU:HB2	1:B:3854:PHE:CZ	2.41	0.56
1:D:875:PRO:HD2	1:D:878:LEU:HD12	1.86	0.56
1:D:1176:THR:HG22	1:D:1181:ILE:HA	1.88	0.56
1:D:2171:VAL:HG21	1:D:2199:PHE:CD2	2.41	0.56
1:D:4664:ASP:OD1	1:D:4674:LYS:NZ	2.29	0.56
1:A:419:ILE:HG21	1:A:492:GLU:HG3	1.88	0.55
1:A:476:GLN:NE2	1:A:3678:GLU:OE1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2743:TYR:HA	1:A:2757:MET:HE1	1.88	0.55
2:F:50:ARG:HB3	2:F:50:ARG:NH1	2.22	0.55
1:B:558:LEU:HG	1:B:571:ILE:HG23	1.86	0.55
1:C:558:LEU:HG	1:C:571:ILE:HG23	1.86	0.55
1:C:1243:THR:HG22	1:C:1808:ASP:HB2	1.87	0.55
1:A:3594:GLN:HA	1:A:3597:ARG:HD3	1.88	0.55
2:E:24:VAL:HG22	2:E:48:LYS:HG2	1.88	0.55
3:K:92:VAL:HG12	3:K:93:PHE:HD1	1.71	0.55
1:B:1243:THR:HG22	1:B:1808:ASP:HB2	1.87	0.55
1:B:2610:LEU:HD13	1:B:2644:LEU:HD21	1.89	0.55
1:C:1495:SER:OG	1:C:1496:PRO:HD2	2.06	0.55
1:C:2171:VAL:HG21	1:C:2199:PHE:CD2	2.41	0.55
1:C:2325:ILE:HD12	1:D:207:PHE:CZ	2.42	0.55
1:C:2610:LEU:HD13	1:C:2644:LEU:HD21	1.89	0.55
1:C:3274:ASN:OD1	1:C:3275:THR:N	2.38	0.55
1:D:2743:TYR:HA	1:D:2757:MET:HE1	1.88	0.55
1:A:246:THR:HG21	1:A:267:VAL:HG11	1.88	0.55
1:A:4053:GLU:OE2	1:A:4060:GLN:NE2	2.39	0.55
1:B:246:THR:HG21	1:B:267:VAL:HG11	1.88	0.55
1:B:875:PRO:HD2	1:B:878:LEU:HD12	1.86	0.55
1:B:4019:MET:HG2	1:B:4066:LEU:HD11	1.89	0.55
1:B:4053:GLU:OE2	1:B:4060:GLN:NE2	2.39	0.55
1:D:1495:SER:OG	1:D:1496:PRO:HD2	2.06	0.55
1:A:2488:LEU:HD21	1:A:2548:LEU:HD22	1.89	0.55
1:A:3892:TYR:O	1:A:3957:LYS:NZ	2.37	0.55
1:B:3274:ASN:OD1	1:B:3275:THR:N	2.38	0.55
1:C:4155:SER:O	1:C:4159:GLN:HG2	2.07	0.55
1:D:4019:MET:HG2	1:D:4066:LEU:HD11	1.89	0.55
1:A:2947:SER:HA	1:A:2952:GLU:HA	1.88	0.55
1:A:4019:MET:HG2	1:A:4066:LEU:HD11	1.89	0.55
1:A:3778:LEU:HB2	1:A:3854:PHE:CZ	2.41	0.55
2:F:24:VAL:HG22	2:F:48:LYS:HG2	1.88	0.55
2:H:50:ARG:HB3	2:H:50:ARG:NH1	2.22	0.55
1:B:601:LEU:HG	1:B:610:VAL:HG11	1.87	0.55
1:C:3250:TRP:NE1	1:C:3309:LYS:HG2	2.22	0.55
1:C:4187:GLU:OE1	1:C:4949:TRP:NE1	2.31	0.55
1:D:419:ILE:HG21	1:D:492:GLU:HG3	1.88	0.55
2:G:50:ARG:HB3	2:G:50:ARG:NH1	2.22	0.55
3:L:14:LYS:HG2	1:D:2153:LYS:HD3	1.89	0.55
1:B:2789:ILE:HD11	1:B:2901:TYR:HB3	1.88	0.55
1:C:2947:SER:HA	1:C:2952:GLU:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:THR:HG21	1:D:267:VAL:HG11	1.88	0.55
1:A:3234:VAL:O	1:A:3238:ILE:HB	2.07	0.55
1:A:3493:LYS:HZ2	1:A:3558:LEU:HB2	1.72	0.55
1:B:841:LYS:O	1:B:848:ARG:NH2	2.34	0.55
1:B:3499:LYS:HE3	1:B:3564:LYS:HZ2	1.71	0.55
1:C:4019:MET:HG2	1:C:4066:LEU:HD11	1.89	0.55
1:D:11:ILE:HD12	1:D:176:ARG:HG2	1.89	0.55
1:D:3778:LEU:HB2	1:D:3854:PHE:CZ	2.41	0.55
1:D:4053:GLU:OE2	1:D:4060:GLN:NE2	2.39	0.55
1:A:2405:GLU:OE1	1:A:2407:HIS:ND1	2.39	0.55
2:E:50:ARG:HB3	2:E:50:ARG:NH1	2.22	0.55
1:B:11:ILE:HD12	1:B:176:ARG:HG2	1.89	0.55
1:B:2947:SER:HA	1:B:2952:GLU:HA	1.88	0.55
1:B:4028:SER:O	1:B:4033:LYS:NZ	2.36	0.55
1:C:1176:THR:HG22	1:C:1181:ILE:HA	1.88	0.55
1:D:2947:SER:HA	1:D:2952:GLU:HA	1.88	0.55
1:D:3250:TRP:NE1	1:D:3309:LYS:HG2	2.22	0.55
1:B:164:PRO:HB3	1:B:169:ARG:HB2	1.89	0.55
1:B:419:ILE:HG21	1:B:492:GLU:HG3	1.88	0.55
1:B:1495:SER:OG	1:B:1496:PRO:HD2	2.06	0.55
1:B:3188:SER:OG	1:B:3190:ARG:NH1	2.40	0.55
1:C:1937:GLN:NE2	1:C:3608:LEU:O	2.40	0.55
1:C:4028:SER:O	1:C:4033:LYS:NZ	2.36	0.55
1:D:2610:LEU:HD13	1:D:2644:LEU:HD21	1.89	0.55
1:A:4155:SER:O	1:A:4159:GLN:HG2	2.07	0.54
1:B:1937:GLN:NE2	1:B:3608:LEU:O	2.40	0.54
1:C:3778:LEU:HB2	1:C:3854:PHE:CZ	2.41	0.54
1:D:2488:LEU:HD21	1:D:2548:LEU:HD22	1.89	0.54
3:K:4:GLN:HG2	3:K:5:LEU:HD12	1.90	0.54
1:C:2789:ILE:HD11	1:C:2901:TYR:HB3	1.88	0.54
1:A:1937:GLN:NE2	1:A:3608:LEU:O	2.40	0.54
1:A:2610:LEU:HD13	1:A:2644:LEU:HD21	1.89	0.54
3:I:92:VAL:HG12	3:I:93:PHE:HD1	1.71	0.54
3:J:4:GLN:HG2	3:J:5:LEU:HD12	1.90	0.54
1:C:3188:SER:OG	1:C:3190:ARG:NH1	2.40	0.54
1:C:3493:LYS:HZ2	1:C:3558:LEU:CB	2.18	0.54
1:D:629:GLN:OE1	1:D:1669:ASN:ND2	2.38	0.54
1:D:3072:MET:SD	1:D:3139:ALA:HB3	2.48	0.54
1:D:3234:VAL:O	1:D:3238:ILE:HB	2.07	0.54
1:D:3493:LYS:HZ2	1:D:3558:LEU:CB	2.18	0.54
3:I:107:ARG:HG2	3:I:121:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:128:GLU:CA	3:I:131:ILE:HD11	2.29	0.54
3:L:92:VAL:HG12	3:L:93:PHE:HD1	1.71	0.54
1:B:4155:SER:O	1:B:4159:GLN:HG2	2.07	0.54
1:C:2146:LEU:O	1:C:2150:MET:HG2	2.08	0.54
1:C:2787:TRP:HE1	1:C:2905:ARG:HH21	1.56	0.54
1:C:2837:LEU:HA	1:C:2840:MET:HE3	1.90	0.54
1:D:1273:ILE:HB	1:D:1282:CYS:HB2	1.90	0.54
1:D:1937:GLN:NE2	1:D:3608:LEU:O	2.40	0.54
1:D:2690:GLU:HB2	1:D:2692:GLN:HE22	1.72	0.54
1:A:1273:ILE:HB	1:A:1282:CYS:HB2	1.90	0.54
1:A:3072:MET:SD	1:A:3139:ALA:HB3	2.48	0.54
3:I:4:GLN:HG2	3:I:5:LEU:HD12	1.90	0.54
3:L:33:LEU:O	3:L:37:MET:HG2	2.08	0.54
1:D:896:ASN:O	1:D:900:LEU:HG	2.08	0.54
1:D:2146:LEU:O	1:D:2150:MET:HG2	2.08	0.54
1:A:1117:TRP:HB3	1:A:1201:PHE:HB3	1.90	0.54
1:A:1564:MET:SD	1:A:1565:PRO:HD2	2.48	0.54
1:A:2690:GLU:HB2	1:A:2692:GLN:HE22	1.72	0.54
1:B:2405:GLU:OE1	1:B:2407:HIS:ND1	2.39	0.54
1:B:3427:ASN:OD1	1:B:3463:THR:O	2.22	0.54
1:D:1117:TRP:HB3	1:D:1201:PHE:HB3	1.90	0.54
1:A:896:ASN:O	1:A:900:LEU:HG	2.08	0.54
1:A:3188:SER:OG	1:A:3190:ARG:NH1	2.40	0.54
3:K:33:LEU:O	3:K:37:MET:HG2	2.08	0.54
1:B:1048:ASP:OD1	1:B:1049:SER:N	2.41	0.54
1:B:1564:MET:SD	1:B:1565:PRO:HD2	2.48	0.54
1:B:3250:TRP:NE1	1:B:3309:LYS:HG2	2.22	0.54
1:C:164:PRO:HB3	1:C:169:ARG:HB2	1.89	0.54
1:D:2789:ILE:HD11	1:D:2901:TYR:HB3	1.89	0.54
1:A:4028:SER:O	1:A:4033:LYS:NZ	2.36	0.54
3:I:128:GLU:HG3	3:I:131:ILE:HD11	1.89	0.54
3:J:107:ARG:HG2	3:J:121:GLU:HG3	1.89	0.54
3:K:140:GLU:O	3:K:143:VAL:HG22	2.08	0.54
1:B:2690:GLU:HB2	1:B:2692:GLN:HE22	1.72	0.54
1:C:141:ASP:HB3	1:C:144:ALA:HB3	1.90	0.54
1:C:3507:ASP:OD1	1:C:3510:ARG:NH2	2.41	0.54
1:D:4155:SER:O	1:D:4159:GLN:HG2	2.07	0.54
1:B:1722:ASN:O	1:B:1919:ARG:NH2	2.41	0.54
1:B:2146:LEU:O	1:B:2150:MET:HG2	2.08	0.54
1:B:3234:VAL:O	1:B:3238:ILE:HB	2.07	0.54
1:A:2146:LEU:O	1:A:2150:MET:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2683:SER:OG	1:A:2685:TYR:O	2.25	0.54
1:A:3493:LYS:HZ2	1:A:3558:LEU:CB	2.19	0.54
1:C:659:ILE:HD11	1:C:826:VAL:HG22	1.90	0.54
1:C:1273:ILE:HB	1:C:1282:CYS:HB2	1.90	0.54
1:D:1048:ASP:OD1	1:D:1049:SER:N	2.41	0.54
1:A:11:ILE:HD12	1:A:176:ARG:HG2	1.89	0.53
3:I:33:LEU:O	3:I:37:MET:HG2	2.08	0.53
3:J:140:GLU:O	3:J:143:VAL:HG22	2.08	0.53
1:B:659:ILE:HD11	1:B:826:VAL:HG22	1.90	0.53
1:B:2787:TRP:HE1	1:B:2905:ARG:HH21	1.56	0.53
1:C:2488:LEU:HD21	1:C:2548:LEU:HD22	1.89	0.53
1:C:2561:LEU:O	1:C:2566:ARG:NH1	2.42	0.53
1:C:3072:MET:SD	1:C:3139:ALA:HB3	2.48	0.53
1:C:3234:VAL:O	1:C:3238:ILE:HB	2.07	0.53
1:D:141:ASP:HB3	1:D:144:ALA:HB3	1.90	0.53
3:J:138:ASN:HD21	3:J:141:GLU:HB2	1.74	0.53
3:K:11:ALA:O	3:K:15:GLU:OE1	2.26	0.53
3:L:107:ARG:HG2	3:L:121:GLU:HG3	1.89	0.53
1:B:896:ASN:O	1:B:900:LEU:HG	2.08	0.53
1:C:141:ASP:O	1:C:143:LEU:N	2.41	0.53
1:C:896:ASN:O	1:C:900:LEU:HG	2.08	0.53
1:D:1564:MET:SD	1:D:1565:PRO:HD2	2.48	0.53
1:A:164:PRO:HB3	1:A:169:ARG:HB2	1.90	0.53
1:A:3145:SER:HB3	1:A:3148:VAL:HG22	1.91	0.53
1:A:3499:LYS:HE3	1:A:3564:LYS:HZ2	1.71	0.53
3:I:138:ASN:HD21	3:I:141:GLU:HB2	1.74	0.53
3:L:11:ALA:O	3:L:15:GLU:OE1	2.26	0.53
1:B:3072:MET:SD	1:B:3139:ALA:HB3	2.48	0.53
1:C:1564:MET:SD	1:C:1565:PRO:HD2	2.48	0.53
1:C:2405:GLU:OE1	1:C:2407:HIS:ND1	2.39	0.53
1:A:2789:ILE:HD11	1:A:2901:TYR:HB3	1.89	0.53
2:G:78:THR:OG1	2:G:80:ASP:OD1	2.23	0.53
1:B:3507:ASP:OD1	1:B:3510:ARG:NH2	2.41	0.53
1:C:2202:TYR:O	1:C:2206:ILE:HG12	2.09	0.53
1:C:2690:GLU:HB2	1:C:2692:GLN:HE22	1.72	0.53
1:D:981:MET:HE1	1:D:1056:THR:HG23	1.89	0.53
1:D:2202:TYR:O	1:D:2206:ILE:HG12	2.09	0.53
1:D:3507:ASP:OD1	1:D:3510:ARG:NH2	2.41	0.53
1:A:1722:ASN:O	1:A:1919:ARG:NH2	2.41	0.53
1:B:1273:ILE:HB	1:B:1282:CYS:HB2	1.90	0.53
1:B:3145:SER:HB3	1:B:3148:VAL:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ILE:HD12	1:C:176:ARG:HG2	1.89	0.53
1:C:419:ILE:HG21	1:C:492:GLU:HG3	1.88	0.53
1:C:629:GLN:OE1	1:C:1669:ASN:ND2	2.37	0.53
1:C:2683:SER:OG	1:C:2685:TYR:O	2.25	0.53
1:D:2787:TRP:HE1	1:D:2905:ARG:HH21	1.56	0.53
1:D:3188:SER:OG	1:D:3190:ARG:NH1	2.40	0.53
1:A:1973:ILE:HG21	1:A:3620:PHE:HA	1.91	0.53
1:A:2202:TYR:O	1:A:2206:ILE:HG12	2.08	0.53
3:J:33:LEU:O	3:J:37:MET:HG2	2.08	0.53
3:K:138:ASN:HD21	3:K:141:GLU:HB2	1.74	0.53
3:L:4:GLN:HG2	3:L:5:LEU:HD12	1.90	0.53
3:L:140:GLU:O	3:L:143:VAL:HG22	2.08	0.53
1:C:3145:SER:HB3	1:C:3148:VAL:HG22	1.91	0.53
1:D:141:ASP:O	1:D:143:LEU:N	2.41	0.53
1:D:164:PRO:HB3	1:D:169:ARG:HB2	1.89	0.53
1:D:1722:ASN:O	1:D:1919:ARG:NH2	2.41	0.53
1:D:4637:THR:HG22	1:D:4639:SER:H	1.74	0.53
1:A:141:ASP:O	1:A:143:LEU:N	2.41	0.53
1:A:1048:ASP:OD1	1:A:1049:SER:N	2.41	0.53
1:A:2561:LEU:O	1:A:2566:ARG:NH1	2.42	0.53
1:A:3250:TRP:NE1	1:A:3309:LYS:HG2	2.22	0.53
2:F:50:ARG:NH1	2:F:53:LYS:HG3	2.24	0.53
1:B:4637:THR:HG22	1:B:4639:SER:H	1.74	0.53
1:C:841:LYS:O	1:C:848:ARG:NH2	2.34	0.53
1:C:1722:ASN:O	1:C:1919:ARG:NH2	2.41	0.53
1:D:1973:ILE:HG21	1:D:3620:PHE:HA	1.91	0.53
1:A:3507:ASP:OD1	1:A:3510:ARG:NH2	2.41	0.53
3:K:107:ARG:HG2	3:K:121:GLU:HG3	1.89	0.53
1:B:1117:TRP:HB3	1:B:1201:PHE:HB3	1.90	0.53
1:B:1973:ILE:HG21	1:B:3620:PHE:HA	1.91	0.53
1:B:2202:TYR:O	1:B:2206:ILE:HG12	2.08	0.53
1:B:2837:LEU:HA	1:B:2840:MET:HE3	1.91	0.53
1:C:983:LEU:O	1:C:1055:ARG:NH2	2.41	0.53
1:C:1048:ASP:OD1	1:C:1049:SER:N	2.41	0.53
1:C:1117:TRP:HB3	1:C:1201:PHE:HB3	1.90	0.53
1:C:2730:ASP:OD1	1:C:2821:TYR:OH	2.27	0.53
1:D:1911:GLN:OE1	1:D:2090:ARG:NH1	2.33	0.53
1:A:2285:TYR:OH	1:A:2380:ASP:O	2.27	0.53
1:A:4753:LEU:HG	1:B:4773:LEU:HD22	1.90	0.53
1:B:4775:ALA:HA	1:B:4817:MET:CE	2.39	0.53
1:C:4637:THR:HG22	1:C:4639:SER:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4775:ALA:HA	1:C:4817:MET:CE	2.39	0.53
1:A:2787:TRP:HE1	1:A:2905:ARG:HH21	1.56	0.53
1:A:4637:THR:HG22	1:A:4639:SER:H	1.74	0.53
2:H:8:ILE:HA	1:D:730:LEU:HD11	1.90	0.53
3:I:140:GLU:O	3:I:143:VAL:HG22	2.08	0.53
3:L:49:LEU:O	3:L:53:ILE:HG12	2.09	0.53
1:B:2730:ASP:OD1	1:B:2821:TYR:OH	2.27	0.53
1:C:1973:ILE:HG21	1:C:3620:PHE:HA	1.91	0.53
1:D:897:LYS:CD	5:D:5005:ATP:HN62	2.22	0.53
1:A:141:ASP:HB3	1:A:144:ALA:HB3	1.90	0.52
1:A:1960:ARG:HH22	3:I:111:THR:CB	2.22	0.52
1:A:3280:ILE:O	1:A:3284:ILE:HG12	2.09	0.52
1:C:2826:ILE:HA	1:D:1501:ASN:HD21	1.73	0.52
1:C:3427:ASN:OD1	1:C:3463:THR:O	2.22	0.52
1:D:2730:ASP:OD1	1:D:2821:TYR:OH	2.27	0.52
1:A:1089:ARG:HB3	1:A:1204:VAL:HG23	1.91	0.52
1:A:2730:ASP:OD1	1:A:2821:TYR:OH	2.27	0.52
2:G:50:ARG:NH1	2:G:53:LYS:HG3	2.24	0.52
3:J:128:GLU:CA	3:J:131:ILE:HD11	2.29	0.52
3:K:49:LEU:O	3:K:53:ILE:HG12	2.09	0.52
3:L:87:ARG:HA	3:L:90:PHE:CE1	2.45	0.52
3:L:138:ASN:HD21	3:L:141:GLU:HB2	1.74	0.52
2:H:50:ARG:NH1	2:H:53:LYS:HG3	2.24	0.52
3:J:11:ALA:O	3:J:15:GLU:OE1	2.27	0.52
3:L:143:VAL:O	3:L:147:THR:HG22	2.10	0.52
1:B:515:ALA:HB2	1:B:523:GLY:HA3	1.91	0.52
1:B:983:LEU:O	1:B:1055:ARG:NH2	2.41	0.52
1:C:3280:ILE:O	1:C:3284:ILE:HG12	2.09	0.52
1:D:515:ALA:HB2	1:D:523:GLY:HA3	1.91	0.52
1:A:2722:ASN:O	1:A:2726:GLU:HG3	2.10	0.52
3:I:11:ALA:O	3:I:15:GLU:OE1	2.26	0.52
3:I:87:ARG:HA	3:I:90:PHE:CE1	2.45	0.52
3:J:87:ARG:HA	3:J:90:PHE:CE1	2.45	0.52
1:B:132:CYS:SG	1:B:187:SER:OG	2.68	0.52
1:C:132:CYS:SG	1:C:187:SER:OG	2.68	0.52
1:D:2285:TYR:OH	1:D:2380:ASP:O	2.27	0.52
1:D:2561:LEU:O	1:D:2566:ARG:NH1	2.42	0.52
1:A:2837:LEU:HA	1:A:2840:MET:HE3	1.92	0.52
2:E:50:ARG:NH1	2:E:53:LYS:HG3	2.24	0.52
3:K:87:ARG:HA	3:K:90:PHE:CE1	2.45	0.52
1:C:2285:TYR:OH	1:C:2380:ASP:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:659:ILE:HD11	1:D:826:VAL:HG22	1.90	0.52
1:D:2072:GLU:O	1:D:3660:ARG:NH1	2.43	0.52
1:D:3145:SER:HB3	1:D:3148:VAL:HG22	1.91	0.52
1:D:3280:ILE:O	1:D:3284:ILE:HG12	2.09	0.52
1:A:544:ASN:HB3	1:A:547:ASN:HB2	1.91	0.52
1:A:849:ASP:OD1	1:A:1214:ARG:NE	2.43	0.52
1:A:2929:LEU:HD13	1:A:2971:ILE:HG12	1.91	0.52
1:A:3596:LYS:HD3	3:I:147:THR:HA	1.91	0.52
1:B:544:ASN:HB3	1:B:547:ASN:HB2	1.91	0.52
1:B:3414:ARG:NH1	1:B:3417:GLN:OE1	2.43	0.52
1:D:983:LEU:O	1:D:1055:ARG:NH2	2.41	0.52
1:D:2837:LEU:HA	1:D:2840:MET:HE3	1.91	0.52
1:A:659:ILE:HD11	1:A:826:VAL:HG22	1.90	0.52
1:A:983:LEU:O	1:A:1055:ARG:NH2	2.41	0.52
1:A:4775:ALA:HA	1:A:4817:MET:CE	2.39	0.52
1:B:270:HIS:CD2	1:B:491:GLU:HG3	2.45	0.52
1:B:2561:LEU:O	1:B:2566:ARG:NH1	2.42	0.52
1:C:1089:ARG:HB3	1:C:1204:VAL:HG23	1.91	0.52
1:C:1911:GLN:OE1	1:C:2090:ARG:NH1	2.33	0.52
1:C:2436:ILE:HG22	1:C:2491:GLY:HA3	1.92	0.52
1:D:849:ASP:OD1	1:D:1214:ARG:NE	2.43	0.52
1:D:2722:ASN:O	1:D:2726:GLU:HG3	2.10	0.52
1:A:629:GLN:OE1	1:A:1669:ASN:ND2	2.38	0.52
1:B:2285:TYR:OH	1:B:2380:ASP:O	2.27	0.52
1:C:3250:TRP:HB2	1:C:3273:MET:CE	2.40	0.52
1:A:515:ALA:HB2	1:A:523:GLY:HA3	1.91	0.52
2:E:80:ASP:OD1	2:E:81:VAL:N	2.43	0.52
3:I:49:LEU:O	3:I:53:ILE:HG12	2.09	0.52
3:K:143:VAL:O	3:K:147:THR:HG22	2.10	0.52
1:B:3250:TRP:HB2	1:B:3273:MET:CE	2.40	0.52
1:B:4170:ARG:NH1	5:B:5002:ATP:O2G	2.40	0.52
1:C:544:ASN:HB3	1:C:547:ASN:HB2	1.91	0.52
1:C:814:LEU:HD12	1:C:815:PRO:HD2	1.92	0.52
1:C:3729:ALA:HA	1:C:3732:HIS:CD2	2.45	0.52
1:D:1009:ARG:O	1:D:1013:ARG:NE	2.42	0.52
1:D:2683:SER:OG	1:D:2685:TYR:O	2.25	0.52
1:D:3414:ARG:NH1	1:D:3417:GLN:OE1	2.43	0.52
1:A:2541:HIS:O	1:A:2545:ILE:HG12	2.10	0.52
1:A:3729:ALA:HA	1:A:3732:HIS:CD2	2.45	0.52
1:B:629:GLN:OE1	1:B:1669:ASN:ND2	2.37	0.52
1:B:849:ASP:OD1	1:B:1214:ARG:NE	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:HIS:CD2	1:C:491:GLU:HG3	2.45	0.52
1:C:849:ASP:OD1	1:C:1214:ARG:NE	2.43	0.52
1:C:2722:ASN:O	1:C:2726:GLU:HG3	2.10	0.52
1:C:2929:LEU:HD13	1:C:2971:ILE:HG12	1.91	0.52
1:D:544:ASN:HB3	1:D:547:ASN:HB2	1.91	0.52
1:D:562:LEU:HD22	1:D:600:LEU:HD22	1.92	0.52
1:D:1089:ARG:HB3	1:D:1204:VAL:HG23	1.91	0.52
3:I:143:VAL:O	3:I:147:THR:HG22	2.10	0.51
1:D:2405:GLU:OE1	1:D:2407:HIS:ND1	2.39	0.51
1:D:3250:TRP:HB2	1:D:3273:MET:CE	2.40	0.51
1:D:4775:ALA:HA	1:D:4817:MET:CE	2.39	0.51
1:A:562:LEU:HD22	1:A:600:LEU:HD22	1.92	0.51
1:A:814:LEU:HD12	1:A:815:PRO:HD2	1.92	0.51
1:A:3414:ARG:NH1	1:A:3417:GLN:OE1	2.43	0.51
3:J:49:LEU:O	3:J:53:ILE:HG12	2.09	0.51
1:B:141:ASP:HB3	1:B:144:ALA:HB3	1.90	0.51
1:B:562:LEU:HD22	1:B:600:LEU:HD22	1.92	0.51
1:B:2541:HIS:O	1:B:2545:ILE:HG12	2.10	0.51
1:C:562:LEU:HD22	1:C:600:LEU:HD22	1.92	0.51
1:C:2072:GLU:O	1:C:3660:ARG:NH1	2.43	0.51
1:D:1549:SER:OG	1:D:1551:ASN:O	2.28	0.51
1:A:730:LEU:HD11	2:E:8:ILE:HA	1.93	0.51
1:A:1549:SER:OG	1:A:1551:ASN:O	2.28	0.51
1:A:2478:ILE:HD13	1:A:2527:LEU:HD11	1.92	0.51
1:B:2072:GLU:O	1:B:3660:ARG:NH1	2.43	0.51
1:C:1009:ARG:O	1:C:1013:ARG:NE	2.42	0.51
1:C:3414:ARG:NH1	1:C:3417:GLN:OE1	2.43	0.51
1:C:4170:ARG:NH1	5:C:5002:ATP:O2G	2.40	0.51
1:D:132:CYS:SG	1:D:187:SER:OG	2.68	0.51
1:A:132:CYS:SG	1:A:187:SER:OG	2.68	0.51
1:A:1966:ARG:HB2	3:I:113:LEU:HD13	1.92	0.51
2:F:26:HIS:CD2	2:F:105:LEU:HD11	2.46	0.51
2:F:80:ASP:OD1	2:F:81:VAL:N	2.43	0.51
3:L:128:GLU:HA	3:L:131:ILE:HD11	1.93	0.51
1:B:1089:ARG:HB3	1:B:1204:VAL:HG23	1.91	0.51
1:B:1549:SER:OG	1:B:1551:ASN:O	2.28	0.51
1:B:3280:ILE:O	1:B:3284:ILE:HG12	2.09	0.51
1:C:1118:SER:HB3	1:C:1204:VAL:HG11	1.93	0.51
1:C:1549:SER:OG	1:C:1551:ASN:O	2.28	0.51
1:C:2541:HIS:O	1:C:2545:ILE:HG12	2.10	0.51
1:D:814:LEU:HD12	1:D:815:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2929:LEU:HD13	1:D:2971:ILE:HG12	1.91	0.51
1:D:3427:ASN:OD1	1:D:3463:THR:O	2.22	0.51
1:A:270:HIS:CD2	1:A:491:GLU:HG3	2.45	0.51
1:A:1009:ARG:O	1:A:1013:ARG:NE	2.42	0.51
1:A:1772:SER:OG	1:A:1774:GLU:OE1	2.28	0.51
2:G:80:ASP:OD1	2:G:81:VAL:N	2.43	0.51
1:B:2478:ILE:HD13	1:B:2527:LEU:HD11	1.91	0.51
1:C:4747:ALA:HA	1:C:4753:LEU:HB3	1.92	0.51
1:D:3729:ALA:HA	1:D:3732:HIS:CD2	2.45	0.51
1:D:4747:ALA:HA	1:D:4753:LEU:HB3	1.92	0.51
1:A:3427:ASN:HD21	1:A:3464:SER:HA	1.76	0.51
2:E:26:HIS:CD2	2:E:105:LEU:HD11	2.46	0.51
2:G:26:HIS:CD2	2:G:105:LEU:HD11	2.46	0.51
1:B:141:ASP:O	1:B:143:LEU:N	2.41	0.51
1:B:2436:ILE:HG22	1:B:2491:GLY:HA3	1.92	0.51
1:B:4045:LYS:HD3	1:B:4078:LEU:HD23	1.93	0.51
1:C:2478:ILE:HD13	1:C:2527:LEU:HD11	1.92	0.51
1:C:3324:GLU:HG2	1:C:3327:LYS:NZ	2.26	0.51
1:D:1118:SER:HB3	1:D:1204:VAL:HG11	1.93	0.51
1:D:2478:ILE:HD13	1:D:2527:LEU:HD11	1.92	0.51
1:D:2779:LEU:HA	1:D:2782:MET:HG2	1.92	0.51
1:D:4045:LYS:HD3	1:D:4078:LEU:HD23	1.93	0.51
1:A:466:PRO:HG2	1:A:479:LEU:HG	1.93	0.51
1:A:2072:GLU:O	1:A:3660:ARG:NH1	2.43	0.51
2:H:26:HIS:CD2	2:H:105:LEU:HD11	2.46	0.51
1:B:1118:SER:HB3	1:B:1204:VAL:HG11	1.93	0.51
1:B:2929:LEU:HD13	1:B:2971:ILE:HG12	1.91	0.51
1:B:3015:VAL:HG23	1:B:3029:ILE:HD12	1.93	0.51
1:B:3427:ASN:HD21	1:B:3464:SER:HA	1.76	0.51
1:C:1932:PHE:CE1	1:C:1996:LEU:HB2	2.46	0.51
1:C:3047:LYS:HD2	1:C:3048:THR:HG23	1.93	0.51
1:D:1932:PHE:CE1	1:D:1996:LEU:HB2	2.46	0.51
1:D:3015:VAL:HG23	1:D:3029:ILE:HD12	1.93	0.51
1:A:1118:SER:HB3	1:A:1204:VAL:HG11	1.93	0.51
1:A:3493:LYS:NZ	1:A:3558:LEU:HB2	2.24	0.51
1:A:4045:LYS:HD3	1:A:4078:LEU:HD23	1.93	0.51
1:C:732:LEU:HB3	1:C:779:PHE:CZ	2.46	0.51
1:C:897:LYS:CD	5:C:5005:ATP:HN62	2.22	0.51
1:C:4045:LYS:HD3	1:C:4078:LEU:HD23	1.93	0.51
1:D:270:HIS:CD2	1:D:491:GLU:HG3	2.45	0.51
1:D:2541:HIS:O	1:D:2545:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3015:VAL:HG23	1:A:3029:ILE:HD12	1.93	0.51
1:A:3250:TRP:HB2	1:A:3273:MET:CE	2.40	0.51
3:J:143:VAL:O	3:J:147:THR:HG22	2.10	0.51
1:B:713:TRP:HZ2	1:B:1251:LEU:HD21	1.76	0.51
1:C:3015:VAL:HG23	1:C:3029:ILE:HD12	1.93	0.51
1:C:3803:LEU:HB2	1:C:3884:SER:HB2	1.93	0.51
1:D:3324:GLU:HG2	1:D:3327:LYS:NZ	2.26	0.51
1:A:3455:LYS:O	1:A:3459:TYR:HB3	2.11	0.51
2:H:80:ASP:OD1	2:H:81:VAL:N	2.43	0.51
3:K:128:GLU:HG3	3:K:131:ILE:HD11	1.89	0.51
1:B:466:PRO:HG2	1:B:479:LEU:HG	1.93	0.51
1:B:1729:MET:CE	1:B:1930:ASP:HB2	2.41	0.51
1:B:3493:LYS:NZ	1:B:3558:LEU:HB2	2.23	0.51
1:B:4620:GLN:OE1	1:B:4632:ARG:NH2	2.44	0.51
1:D:466:PRO:HG2	1:D:479:LEU:HG	1.93	0.51
1:D:2436:ILE:HG22	1:D:2491:GLY:HA3	1.92	0.51
1:A:4620:GLN:OE1	1:A:4632:ARG:NH2	2.44	0.50
3:I:12:GLU:HA	3:I:15:GLU:OE1	2.12	0.50
1:B:814:LEU:HD12	1:B:815:PRO:HD2	1.92	0.50
1:B:1220:ASP:O	1:B:1223:THR:OG1	2.28	0.50
1:B:2722:ASN:O	1:B:2726:GLU:HG3	2.10	0.50
1:B:3455:LYS:O	1:B:3459:TYR:HB3	2.11	0.50
1:B:3729:ALA:HA	1:B:3732:HIS:CD2	2.45	0.50
1:D:3427:ASN:HD21	1:D:3464:SER:HA	1.76	0.50
1:A:4625:ASP:OD1	1:A:4625:ASP:N	2.43	0.50
3:I:88:GLU:OE1	3:I:91:ARG:NH2	2.45	0.50
1:B:4827:ILE:O	1:B:4831:ILE:HG12	2.11	0.50
1:C:515:ALA:HB2	1:C:523:GLY:HA3	1.91	0.50
1:C:1729:MET:CE	1:C:1930:ASP:HB2	2.41	0.50
1:C:4620:GLN:OE1	1:C:4632:ARG:NH2	2.44	0.50
1:D:732:LEU:HB3	1:D:779:PHE:CZ	2.46	0.50
1:A:307:SER:HB3	1:A:327:THR:HG22	1.94	0.50
1:A:1932:PHE:CE1	1:A:1996:LEU:HB2	2.46	0.50
1:A:2779:LEU:HA	1:A:2782:MET:HG2	1.92	0.50
1:A:3803:LEU:HB2	1:A:3884:SER:HB2	1.93	0.50
1:A:4827:ILE:O	1:A:4831:ILE:HG12	2.12	0.50
1:B:732:LEU:HB3	1:B:779:PHE:CZ	2.46	0.50
1:B:2779:LEU:HA	1:B:2782:MET:HG2	1.92	0.50
1:C:466:PRO:HG2	1:C:479:LEU:HG	1.93	0.50
1:C:1428:TYR:OH	1:C:1444:GLY:O	2.30	0.50
1:D:258:ARG:NE	1:D:316:LEU:O	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3047:LYS:HD2	1:D:3048:THR:HG23	1.93	0.50
1:D:4827:ILE:O	1:D:4831:ILE:HG12	2.11	0.50
1:A:2436:ILE:HG22	1:A:2491:GLY:HA3	1.92	0.50
1:A:4747:ALA:HA	1:A:4753:LEU:HB3	1.92	0.50
3:J:12:GLU:HA	3:J:15:GLU:OE1	2.12	0.50
3:K:128:GLU:HA	3:K:131:ILE:HD11	1.93	0.50
1:B:1932:PHE:CE1	1:B:1996:LEU:HB2	2.46	0.50
1:B:3324:GLU:HG2	1:B:3327:LYS:NZ	2.26	0.50
1:C:3250:TRP:HB2	1:C:3273:MET:HE1	1.94	0.50
1:D:737:ILE:HD12	1:D:1482:ARG:HD3	1.94	0.50
1:A:317:MET:HB2	1:A:321:LYS:HD2	1.94	0.50
1:A:1729:MET:CE	1:A:1930:ASP:HB2	2.41	0.50
1:A:3047:LYS:HD2	1:A:3048:THR:HG23	1.93	0.50
3:L:12:GLU:HA	3:L:15:GLU:OE1	2.12	0.50
3:L:88:GLU:OE1	3:L:91:ARG:NH2	2.45	0.50
1:B:2834:SER:O	1:B:2838[A]:HIS:HB2	2.11	0.50
1:C:4014:LEU:HD13	1:C:4122:ALA:HB2	1.94	0.50
1:C:4637:THR:O	1:C:4650:LYS:NZ	2.41	0.50
1:C:4896:ASP:HA	1:C:4899:ASP:HB2	1.94	0.50
1:D:2322:ARG:HH22	1:D:2415:GLU:HG3	1.77	0.50
1:D:4014:LEU:HD13	1:D:4122:ALA:HB2	1.94	0.50
1:D:4620:GLN:OE1	1:D:4632:ARG:NH2	2.44	0.50
1:A:115:TYR:HE2	1:A:169:ARG:HB3	1.77	0.50
1:A:1428:TYR:OH	1:A:1444:GLY:O	2.30	0.50
3:L:61:ASN:CG	3:L:62:GLY:H	2.15	0.50
1:B:3076:LYS:O	1:B:3077:GLN:HG3	2.12	0.50
1:C:2779:LEU:HA	1:C:2782:MET:HG2	1.92	0.50
1:D:317:MET:HB2	1:D:321:LYS:HD2	1.94	0.50
1:D:3467:VAL:HB	1:D:3471:LYS:NZ	2.27	0.50
1:A:737:ILE:HD12	1:A:1482:ARG:HD3	1.94	0.50
1:A:2834:SER:O	1:A:2838[A]:HIS:HB2	2.11	0.50
1:A:3427:ASN:OD1	1:A:3465:LEU:CD2	2.60	0.50
3:K:61:ASN:CG	3:K:62:GLY:H	2.15	0.50
3:K:88:GLU:OE1	3:K:91:ARG:NH2	2.45	0.50
1:B:737:ILE:HD12	1:B:1482:ARG:HD3	1.94	0.50
1:B:1428:TYR:OH	1:B:1444:GLY:O	2.30	0.50
1:B:3336:GLU:HG3	1:B:3355:ILE:HG22	1.94	0.50
1:B:4014:LEU:HD13	1:B:4122:ALA:HB2	1.94	0.50
1:B:4747:ALA:HA	1:B:4753:LEU:HB3	1.92	0.50
1:C:559:ILE:HG23	1:C:562:LEU:HD12	1.93	0.50
1:C:713:TRP:HZ2	1:C:1251:LEU:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1772:SER:OG	1:C:1774:GLU:OE1	2.28	0.50
1:C:3427:ASN:HD21	1:C:3464:SER:HA	1.75	0.50
1:C:3455:LYS:O	1:C:3459:TYR:HB3	2.11	0.50
1:D:3455:LYS:O	1:D:3459:TYR:HB3	2.11	0.50
1:A:242:ASP:OD1	1:A:242:ASP:N	2.45	0.50
1:A:3280:ILE:CG2	1:A:3299:LEU:HD21	2.42	0.50
3:J:128:GLU:HG3	3:J:131:ILE:HD11	1.89	0.50
1:B:897:LYS:CD	5:B:5005:ATP:HN62	2.22	0.50
1:B:1001:GLU:OE2	1:B:1005:ASN:ND2	2.45	0.50
1:B:1772:SER:OG	1:B:1774:GLU:OE1	2.28	0.50
1:C:3427:ASN:CB	1:C:3463:THR:OG1	2.42	0.50
1:D:1428:TYR:OH	1:D:1444:GLY:O	2.30	0.50
1:D:1844:GLN:NE2	1:D:1853:GLU:OE1	2.45	0.50
1:A:3324:GLU:HG2	1:A:3327:LYS:NZ	2.26	0.50
3:J:128:GLU:HA	3:J:131:ILE:HD11	1.93	0.50
1:B:2920:ARG:HG3	1:B:2923:TYR:HB2	1.93	0.50
1:B:3427:ASN:OD1	1:B:3465:LEU:CD2	2.60	0.50
1:C:1729:MET:HE2	1:C:1930:ASP:HB2	1.94	0.50
1:C:2920:ARG:HG3	1:C:2923:TYR:HB2	1.93	0.50
1:C:3280:ILE:CG2	1:C:3299:LEU:HD21	2.42	0.50
1:C:4827:ILE:O	1:C:4831:ILE:HG12	2.12	0.50
1:D:115:TYR:HE2	1:D:169:ARG:HB3	1.77	0.50
1:D:2749:ASP:HA	1:D:2754:GLN:OE1	2.12	0.50
1:D:2857:LYS:HA	1:D:2860:LEU:HG	1.93	0.50
1:A:732:LEU:HB3	1:A:779:PHE:CZ	2.46	0.49
3:I:128:GLU:HA	3:I:131:ILE:HD11	1.93	0.49
3:J:67:PRO:HB2	1:B:2202:TYR:CZ	2.46	0.49
3:J:88:GLU:OE1	3:J:91:ARG:NH2	2.45	0.49
1:B:1009:ARG:O	1:B:1013:ARG:NE	2.42	0.49
1:B:4896:ASP:HA	1:B:4899:ASP:HB2	1.94	0.49
1:C:737:ILE:HD12	1:C:1482:ARG:HD3	1.94	0.49
1:C:3691:TYR:O	1:C:3695:MET:HG3	2.12	0.49
1:D:1729:MET:CE	1:D:1930:ASP:HB2	2.41	0.49
1:D:3280:ILE:CG2	1:D:3299:LEU:HD21	2.42	0.49
1:D:4116:GLN:HA	1:D:4119:LEU:HD12	1.94	0.49
1:D:4896:ASP:HA	1:D:4899:ASP:HB2	1.94	0.49
1:A:1729:MET:HE2	1:A:1930:ASP:HB2	1.94	0.49
1:A:1844:GLN:NE2	1:A:1853:GLU:OE1	2.45	0.49
1:A:2322:ARG:HH22	1:A:2415:GLU:HG3	1.77	0.49
1:A:3076:LYS:O	1:A:3077:GLN:HG3	2.12	0.49
2:G:8:ILE:HA	1:C:730:LEU:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2753:VAL:O	1:B:2753:VAL:HG12	2.12	0.49
1:B:3150:ARG:NH1	1:B:3151:GLN:HB3	2.28	0.49
1:B:3198:PRO:HG2	1:B:3204:VAL:HA	1.95	0.49
1:B:4116:GLN:HA	1:B:4119:LEU:HD12	1.94	0.49
1:C:1834:PHE:O	1:C:1835:HIS:ND1	2.45	0.49
1:C:1844:GLN:NE2	1:C:1853:GLU:OE1	2.45	0.49
1:C:2749:ASP:HA	1:C:2754:GLN:OE1	2.12	0.49
1:C:2834:SER:O	1:C:2838[A]:HIS:HB2	2.11	0.49
1:A:4014:LEU:HD13	1:A:4122:ALA:HB2	1.94	0.49
1:B:2171:VAL:HG21	1:B:2199:PHE:HD2	1.77	0.49
1:B:2749:ASP:HA	1:B:2754:GLN:OE1	2.12	0.49
1:B:2937:HIS:O	1:B:2940:ILE:HG22	2.12	0.49
1:B:3467:VAL:HB	1:B:3471:LYS:NZ	2.27	0.49
1:B:3691:TYR:O	1:B:3695:MET:HG3	2.12	0.49
1:C:2753:VAL:O	1:C:2753:VAL:HG12	2.13	0.49
1:C:4079:ASP:O	1:C:4082:GLU:HG3	2.12	0.49
1:D:59:PRO:HG3	1:D:296:ARG:CZ	2.43	0.49
1:D:242:ASP:OD1	1:D:242:ASP:N	2.45	0.49
1:D:1772:SER:OG	1:D:1774:GLU:OE1	2.28	0.49
1:A:1440:ASN:HB3	1:A:1546:GLN:HB3	1.95	0.49
1:A:2857:LYS:HA	1:A:2860:LEU:HG	1.93	0.49
1:A:2920:ARG:HG3	1:A:2923:TYR:HB2	1.93	0.49
1:A:3600:VAL:CG1	3:I:146:MET:SD	3.00	0.49
3:I:61:ASN:CG	3:I:62:GLY:H	2.15	0.49
3:J:61:ASN:CG	3:J:62:GLY:H	2.15	0.49
1:B:115:TYR:HE2	1:B:169:ARG:HB3	1.77	0.49
1:B:2834:SER:O	1:B:2838[B]:HIS:HB2	2.12	0.49
1:B:4079:ASP:O	1:B:4082:GLU:HG3	2.12	0.49
1:B:4796:SER:HB3	1:B:4803:ASP:H	1.77	0.49
1:C:3150:ARG:NH1	1:C:3151:GLN:HB3	2.28	0.49
1:C:3467:VAL:HB	1:C:3471:LYS:NZ	2.27	0.49
1:D:307:SER:HB3	1:D:327:THR:HG22	1.94	0.49
1:D:713:TRP:HZ2	1:D:1251:LEU:HD21	1.76	0.49
1:D:1001:GLU:OE2	1:D:1005:ASN:ND2	2.45	0.49
1:D:4637:THR:O	1:D:4650:LYS:NZ	2.41	0.49
1:A:114:LEU:HB2	1:A:117:HIS:HD2	1.77	0.49
1:A:2937:HIS:O	1:A:2940:ILE:HG22	2.12	0.49
1:A:3198:PRO:HG2	1:A:3204:VAL:HA	1.94	0.49
1:A:3467:VAL:HB	1:A:3471:LYS:NZ	2.27	0.49
3:J:51:ASP:OD1	3:J:52:MET:N	2.45	0.49
1:B:559:ILE:HG23	1:B:562:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1844:GLN:NE2	1:B:1853:GLU:OE1	2.45	0.49
1:B:3280:ILE:CG2	1:B:3299:LEU:HD21	2.42	0.49
1:C:2937:HIS:O	1:C:2940:ILE:HG22	2.12	0.49
1:D:2834:SER:O	1:D:2838[A]:HIS:HB2	2.11	0.49
1:D:3803:LEU:HB2	1:D:3884:SER:HB2	1.94	0.49
1:A:59:PRO:HG3	1:A:296:ARG:CZ	2.43	0.49
1:A:713:TRP:HZ2	1:A:1251:LEU:HD21	1.76	0.49
1:A:4896:ASP:HA	1:A:4899:ASP:HB2	1.94	0.49
1:B:2252:GLU:OE2	1:B:3819:MET:HG3	2.13	0.49
1:B:2322:ARG:HH22	1:B:2415:GLU:HG3	1.77	0.49
1:B:4172:PHE:O	1:B:4176:VAL:HG22	2.13	0.49
1:C:2154:VAL:HG13	1:C:2158:HIS:HD2	1.78	0.49
1:C:2322:ARG:HH22	1:C:2415:GLU:HG3	1.77	0.49
1:C:3076:LYS:O	1:C:3077:GLN:HG3	2.12	0.49
1:C:3198:PRO:HG2	1:C:3204:VAL:HA	1.94	0.49
1:C:4886:THR:O	1:C:4895:ASN:N	2.46	0.49
1:D:643:LEU:O	1:D:645:GLN:NE2	2.46	0.49
1:D:3134:LEU:HB2	1:D:3162:PHE:CE1	2.48	0.49
1:D:4796:SER:HB3	1:D:4803:ASP:H	1.77	0.49
1:A:2252:GLU:OE2	1:A:3819:MET:HG3	2.13	0.49
1:B:1440:ASN:HB3	1:B:1546:GLN:HB3	1.95	0.49
1:B:2338:GLU:HA	1:C:140:THR:HB	1.95	0.49
1:B:2683:SER:OG	1:B:2685:TYR:O	2.25	0.49
1:B:2857:LYS:HA	1:B:2860:LEU:HG	1.93	0.49
1:B:3803:LEU:HB2	1:B:3884:SER:HB2	1.93	0.49
1:C:307:SER:HB3	1:C:327:THR:HG22	1.94	0.49
1:C:3427:ASN:OD1	1:C:3465:LEU:CD2	2.60	0.49
1:C:4796:SER:HB3	1:C:4803:ASP:H	1.77	0.49
1:D:2154:VAL:HG13	1:D:2158:HIS:HD2	1.78	0.49
1:D:3076:LYS:O	1:D:3077:GLN:HG3	2.12	0.49
1:A:559:ILE:HG23	1:A:562:LEU:HD12	1.93	0.49
1:A:1001:GLU:OE2	1:A:1005:ASN:ND2	2.45	0.49
1:A:4079:ASP:O	1:A:4082:GLU:HG3	2.12	0.49
1:A:4796:SER:HB3	1:A:4803:ASP:H	1.77	0.49
3:L:128:GLU:HG3	3:L:131:ILE:HD11	1.89	0.49
1:B:3047:LYS:HD2	1:B:3048:THR:HG23	1.93	0.49
1:C:3493:LYS:NZ	1:C:3558:LEU:HB2	2.24	0.49
1:C:4172:PHE:O	1:C:4176:VAL:HG22	2.13	0.49
1:D:2920:ARG:HG3	1:D:2923:TYR:HB2	1.93	0.49
1:D:3638:ASP:OD1	1:D:3730:ARG:NH2	2.37	0.49
1:D:3691:TYR:O	1:D:3695:MET:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1834:PHE:O	1:A:1835:HIS:ND1	2.45	0.49
1:A:4116:GLN:HA	1:A:4119:LEU:HD12	1.94	0.49
1:B:59:PRO:HG3	1:B:296:ARG:CZ	2.43	0.49
1:C:1001:GLU:OE2	1:C:1005:ASN:ND2	2.45	0.49
1:C:2857:LYS:HA	1:C:2860:LEU:HG	1.93	0.49
1:C:3134:LEU:HB2	1:C:3162:PHE:CE1	2.48	0.49
1:D:1644:LEU:HD23	1:D:1651:LEU:HA	1.95	0.49
1:D:2171:VAL:HG21	1:D:2199:PHE:HD2	1.77	0.49
1:D:2753:VAL:O	1:D:2753:VAL:HG12	2.13	0.49
1:D:3198:PRO:HG2	1:D:3204:VAL:HA	1.95	0.49
1:D:3427:ASN:OD1	1:D:3465:LEU:CD2	2.60	0.49
1:A:897:LYS:CD	5:A:5005:ATP:HN62	2.22	0.49
1:A:2834:SER:O	1:A:2838[B]:HIS:HB2	2.12	0.49
1:A:3150:ARG:NH1	1:A:3151:GLN:HB3	2.28	0.49
1:A:3336:GLU:HG3	1:A:3355:ILE:HG22	1.94	0.49
1:A:3691:TYR:O	1:A:3695:MET:HG3	2.12	0.49
1:A:4172:PHE:O	1:A:4176:VAL:HG22	2.13	0.49
1:A:4196:THR:HB	1:A:4919:LEU:HD11	1.95	0.49
3:K:12:GLU:HA	3:K:15:GLU:OE1	2.12	0.49
1:B:643:LEU:O	1:B:645:GLN:NE2	2.46	0.49
1:B:2154:VAL:HG13	1:B:2158:HIS:HD2	1.78	0.49
1:B:4196:THR:HB	1:B:4919:LEU:HD11	1.95	0.49
1:C:59:PRO:HG3	1:C:296:ARG:CZ	2.43	0.49
1:C:866:PRO:HG2	1:C:1009:ARG:HH11	1.78	0.49
1:D:4079:ASP:O	1:D:4082:GLU:HG3	2.12	0.49
1:A:3638:ASP:OD1	1:A:3730:ARG:NH2	2.37	0.48
3:K:51:ASP:OD1	3:K:52:MET:N	2.45	0.48
1:B:866:PRO:HG2	1:B:1009:ARG:HH11	1.78	0.48
1:C:115:TYR:HE2	1:C:169:ARG:HB3	1.77	0.48
1:C:4196:THR:HB	1:C:4919:LEU:HD11	1.95	0.48
1:D:331:PHE:HE1	1:D:363:ILE:HG12	1.78	0.48
1:D:866:PRO:HG2	1:D:1009:ARG:HH11	1.78	0.48
1:D:2229:LEU:HB3	1:D:2297:ARG:HD3	1.95	0.48
1:D:4196:THR:HB	1:D:4919:LEU:HD11	1.95	0.48
1:A:866:PRO:HG3	1:A:1005:ASN:HB3	1.95	0.48
2:G:88:HIS:HD2	2:G:89:PRO:HD2	1.78	0.48
3:J:15:GLU:O	3:J:19:LEU:HG	2.13	0.48
1:B:307:SER:HB3	1:B:327:THR:HG22	1.94	0.48
1:B:2968:LEU:HB2	1:B:2969:PRO:HD3	1.96	0.48
1:B:3509:ILE:O	1:B:3513:ILE:HG12	2.14	0.48
1:C:2171:VAL:HG21	1:C:2199:PHE:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4116:GLN:HA	1:C:4119:LEU:HD12	1.94	0.48
1:D:1834:PHE:O	1:D:1835:HIS:ND1	2.45	0.48
1:A:2753:VAL:HG12	1:A:2753:VAL:O	2.13	0.48
1:A:2968:LEU:HB2	1:A:2969:PRO:HD3	1.95	0.48
1:B:1834:PHE:O	1:B:1835:HIS:ND1	2.45	0.48
1:C:2229:LEU:HB3	1:C:2297:ARG:HD3	1.95	0.48
1:C:2252:GLU:OE2	1:C:3819:MET:HG3	2.13	0.48
1:C:2834:SER:O	1:C:2838[B]:HIS:HB2	2.12	0.48
1:D:559:ILE:HG23	1:D:562:LEU:HD12	1.93	0.48
1:D:2252:GLU:OE2	1:D:3819:MET:HG3	2.13	0.48
1:D:2834:SER:O	1:D:2838[B]:HIS:HB2	2.12	0.48
1:D:3250:TRP:HB2	1:D:3273:MET:HE1	1.95	0.48
1:D:3467:VAL:HA	1:D:3470:LEU:HG	1.96	0.48
1:D:3509:ILE:O	1:D:3513:ILE:HG12	2.14	0.48
1:A:331:PHE:HE1	1:A:363:ILE:HG12	1.78	0.48
1:A:2154:VAL:HG13	1:A:2158:HIS:HD2	1.78	0.48
1:A:2171:VAL:HG21	1:A:2199:PHE:HD2	1.77	0.48
1:B:2736:LYS:HG3	1:B:2737:LEU:HD23	1.94	0.48
1:B:3134:LEU:HB2	1:B:3162:PHE:CE1	2.48	0.48
1:B:3496:PHE:CE2	1:B:3556:ASN:N	2.82	0.48
1:C:3404:ILE:O	1:C:3408:LYS:HG2	2.13	0.48
1:D:2582:PRO:HB3	1:D:2617:CYS:SG	2.54	0.48
1:D:2736:LYS:HG3	1:D:2737:LEU:HD23	1.94	0.48
1:D:2937:HIS:O	1:D:2940:ILE:HG22	2.12	0.48
1:A:866:PRO:HG2	1:A:1009:ARG:HH11	1.78	0.48
1:A:999:LEU:HD23	1:A:1050:LEU:HD21	1.96	0.48
1:A:1249:MET:HB3	1:A:1599:MET:HB3	1.96	0.48
1:A:2749:ASP:HA	1:A:2754:GLN:OE1	2.12	0.48
1:A:3397:ARG:NH2	1:A:3550:ARG:HD2	2.24	0.48
1:A:3467:VAL:HA	1:A:3470:LEU:HG	1.96	0.48
1:A:3740:VAL:HG13	1:A:3758:THR:HG22	1.95	0.48
1:A:4617:ILE:HG23	1:A:4665:ARG:HH22	1.78	0.48
2:F:88:HIS:HD2	2:F:89:PRO:HD2	1.78	0.48
3:I:51:ASP:OD1	3:I:52:MET:N	2.45	0.48
1:B:3122:ILE:HG22	1:B:3127:GLN:HG2	1.96	0.48
1:C:317:MET:HB2	1:C:321:LYS:HD2	1.94	0.48
1:D:2968:LEU:HB2	1:D:2969:PRO:HD3	1.95	0.48
1:D:3336:GLU:HG3	1:D:3355:ILE:HG22	1.94	0.48
1:D:3774:GLN:HB3	1:D:3854:PHE:HE2	1.79	0.48
2:E:88:HIS:HD2	2:E:89:PRO:HD2	1.78	0.48
3:L:15:GLU:O	3:L:19:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ASP:OD1	1:B:242:ASP:N	2.45	0.48
1:B:317:MET:HB2	1:B:321:LYS:HD2	1.94	0.48
1:C:1440:ASN:HB3	1:C:1546:GLN:HB3	1.95	0.48
1:C:2968:LEU:HB2	1:C:2969:PRO:HD3	1.96	0.48
1:D:999:LEU:HD23	1:D:1050:LEU:HD21	1.96	0.48
1:D:4170:ARG:NH1	5:D:5002:ATP:O2G	2.41	0.48
1:A:115:TYR:CE1	1:A:175:VAL:HG22	2.49	0.48
1:A:3134:LEU:HB2	1:A:3162:PHE:CE1	2.48	0.48
1:A:3427:ASN:OD1	1:A:3465:LEU:HD22	2.14	0.48
1:A:3509:ILE:O	1:A:3513:ILE:HG12	2.14	0.48
1:A:4933:HIS:HD2	1:A:4937:GLU:HB3	1.79	0.48
2:F:78:THR:OG1	2:F:80:ASP:OD1	2.23	0.48
3:I:15:GLU:O	3:I:19:LEU:HG	2.13	0.48
3:K:15:GLU:O	3:K:19:LEU:HG	2.14	0.48
1:B:891:GLU:HA	1:B:894:VAL:HG22	1.96	0.48
1:B:891:GLU:O	1:B:895:MET:HG3	2.13	0.48
1:B:895:MET:HA	1:B:898:ILE:HD13	1.96	0.48
1:B:2283:LYS:HE3	1:B:2285:TYR:HE1	1.79	0.48
1:B:3476:ILE:O	1:B:3480:ILE:HG13	2.14	0.48
1:C:891:GLU:O	1:C:895:MET:HG3	2.13	0.48
1:C:2283:LYS:HE3	1:C:2285:TYR:HE1	1.79	0.48
1:C:3476:ILE:O	1:C:3480:ILE:HG13	2.14	0.48
1:C:4617:ILE:HG23	1:C:4665:ARG:HH22	1.78	0.48
1:D:3122:ILE:HG22	1:D:3127:GLN:HG2	1.96	0.48
1:D:3476:ILE:O	1:D:3480:ILE:HG13	2.14	0.48
1:A:891:GLU:HA	1:A:894:VAL:HG22	1.96	0.48
1:A:4170:ARG:NH1	5:A:5002:ATP:O2G	2.40	0.48
2:H:88:HIS:HD2	2:H:89:PRO:HD2	1.78	0.48
3:K:108:HIS:HE1	1:C:1956:ALA:HA	1.79	0.48
1:B:4617:ILE:HG23	1:B:4665:ARG:HH22	1.78	0.48
1:C:2736:LYS:HG3	1:C:2737:LEU:HD23	1.94	0.48
1:C:4933:HIS:HD2	1:C:4937:GLU:HB3	1.79	0.48
1:D:891:GLU:O	1:D:895:MET:HG3	2.13	0.48
1:D:891:GLU:HA	1:D:894:VAL:HG22	1.96	0.48
1:D:3150:ARG:NH1	1:D:3151:GLN:HB3	2.27	0.48
1:D:3404:ILE:O	1:D:3408:LYS:HG2	2.13	0.48
1:D:4172:PHE:O	1:D:4176:VAL:HG22	2.13	0.48
1:D:4933:HIS:HD2	1:D:4937:GLU:HB3	1.79	0.48
1:A:882:ARG:CZ	1:A:937:LEU:HD12	2.44	0.48
1:A:2283:LYS:HE3	1:A:2285:TYR:HE1	1.79	0.48
1:A:2582:PRO:HB3	1:A:2617:CYS:SG	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3345:ARG:NH1	1:A:3347:ASP:OD1	2.44	0.48
1:A:3496:PHE:CE2	1:A:3556:ASN:N	2.82	0.48
1:B:2229:LEU:HB3	1:B:2297:ARG:HD3	1.95	0.48
1:B:2565:GLN:O	1:B:2569:ILE:HG13	2.14	0.48
1:C:986:ILE:O	1:C:1055:ARG:NH2	2.47	0.48
1:C:2582:PRO:HB3	1:C:2617:CYS:SG	2.54	0.48
1:C:3033:LEU:HD13	1:C:3104:MET:SD	2.54	0.48
1:D:986:ILE:O	1:D:1055:ARG:NH2	2.47	0.48
1:D:4617:ILE:HG23	1:D:4665:ARG:HH22	1.78	0.48
1:A:643:LEU:O	1:A:645:GLN:NE2	2.46	0.48
1:A:2229:LEU:HB3	1:A:2297:ARG:HD3	1.95	0.48
1:A:3122:ILE:HG22	1:A:3127:GLN:HG2	1.96	0.48
1:A:3404:ILE:O	1:A:3408:LYS:HG2	2.13	0.48
1:A:4615:LEU:HA	1:A:4619:GLU:HB2	1.96	0.48
1:A:4886:THR:O	1:A:4895:ASN:N	2.46	0.48
1:B:331:PHE:HE1	1:B:363:ILE:HG12	1.78	0.48
1:B:2582:PRO:HB3	1:B:2617:CYS:SG	2.54	0.48
1:B:4933:HIS:HD2	1:B:4937:GLU:HB3	1.79	0.48
1:C:514:PHE:CE2	1:C:522:ALA:HB1	2.49	0.48
1:C:1249:MET:HB3	1:C:1599:MET:HB3	1.96	0.48
1:C:1644:LEU:HD23	1:C:1651:LEU:HA	1.95	0.48
1:C:3122:ILE:HG22	1:C:3127:GLN:HG2	1.96	0.48
1:C:3427:ASN:OD1	1:C:3465:LEU:HD22	2.14	0.48
1:C:3496:PHE:CE2	1:C:3556:ASN:N	2.82	0.48
1:C:3740:VAL:HG13	1:C:3758:THR:HG22	1.95	0.48
1:C:3774:GLN:HB3	1:C:3854:PHE:HE2	1.79	0.48
1:D:882:ARG:CZ	1:D:937:LEU:HD12	2.44	0.48
1:A:1644:LEU:HD23	1:A:1651:LEU:HA	1.95	0.47
1:A:3476:ILE:O	1:A:3480:ILE:HG13	2.14	0.47
1:B:115:TYR:CE1	1:B:175:VAL:HG22	2.49	0.47
1:B:3033:LEU:HD13	1:B:3104:MET:SD	2.54	0.47
1:C:189:GLU:HG2	1:C:207:PHE:HE1	1.79	0.47
1:C:271:ALA:HB2	1:C:488:LEU:HD22	1.96	0.47
1:C:331:PHE:HE1	1:C:363:ILE:HG12	1.78	0.47
1:C:891:GLU:HA	1:C:894:VAL:HG22	1.96	0.47
1:C:3172:GLU:OE1	1:C:3266:THR:OG1	2.29	0.47
1:D:115:TYR:CE1	1:D:175:VAL:HG22	2.49	0.47
1:D:555:LEU:HD23	1:D:589:ILE:HD11	1.96	0.47
1:D:3496:PHE:CE2	1:D:3556:ASN:N	2.82	0.47
1:D:3697:LYS:HA	1:D:3700:HIS:CD2	2.49	0.47
1:A:891:GLU:O	1:A:895:MET:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3499:LYS:CE	1:A:3564:LYS:HZ1	2.27	0.47
1:B:986:ILE:O	1:B:1055:ARG:NH2	2.47	0.47
1:B:3297:LYS:HE3	1:B:3297:LYS:HB3	1.34	0.47
1:B:3404:ILE:O	1:B:3408:LYS:HG2	2.14	0.47
1:B:3697:LYS:HA	1:B:3700:HIS:CD2	2.49	0.47
1:C:643:LEU:O	1:C:645:GLN:NE2	2.46	0.47
1:C:2565:GLN:O	1:C:2569:ILE:HG13	2.14	0.47
1:C:2788:ARG:HB2	1:C:2904:SER:OG	2.14	0.47
1:C:3336:GLU:HG3	1:C:3355:ILE:HG22	1.94	0.47
1:C:3467:VAL:HA	1:C:3470:LEU:HG	1.96	0.47
1:D:189:GLU:HG2	1:D:207:PHE:HE1	1.79	0.47
1:D:514:PHE:CE2	1:D:522:ALA:HB1	2.49	0.47
1:D:928:GLU:HA	1:D:931:TYR:CE2	2.49	0.47
1:D:2283:LYS:HE3	1:D:2285:TYR:HE1	1.79	0.47
1:D:2758:LYS:HB2	1:D:2762:LEU:HD23	1.96	0.47
1:D:3454:ARG:N	1:D:3457:ASP:OD2	2.47	0.47
1:B:882:ARG:CZ	1:B:937:LEU:HD12	2.44	0.47
1:B:1644:LEU:HD23	1:B:1651:LEU:HA	1.95	0.47
1:B:2758:LYS:HB2	1:B:2762:LEU:HD23	1.96	0.47
1:C:2849:HIS:CE1	1:C:2877:LEU:HD11	2.50	0.47
1:C:3183:ILE:HG13	1:C:3187:LYS:HB2	1.96	0.47
1:C:3523:ALA:HA	1:C:3526:TRP:CD1	2.50	0.47
1:C:3638:ASP:OD1	1:C:3730:ARG:NH2	2.37	0.47
1:D:2788:ARG:HB2	1:D:2904:SER:OG	2.14	0.47
1:D:3145:SER:O	1:D:3149:GLU:HG2	2.14	0.47
1:A:514:PHE:CE2	1:A:522:ALA:HB1	2.49	0.47
1:A:895:MET:HA	1:A:898:ILE:HD13	1.96	0.47
1:A:1114:ARG:NH1	1:A:1128:LEU:O	2.45	0.47
1:A:1220:ASP:O	1:A:1223:THR:OG1	2.28	0.47
1:A:2736:LYS:HG3	1:A:2737:LEU:HD23	1.94	0.47
1:A:2767:GLU:O	1:A:2770:ILE:HG12	2.14	0.47
1:A:2849:HIS:CE1	1:A:2877:LEU:HD11	2.50	0.47
1:A:3454:ARG:N	1:A:3457:ASP:OD2	2.47	0.47
1:B:111:ARG:HD3	1:B:111:ARG:HA	1.69	0.47
1:B:514:PHE:CE2	1:B:522:ALA:HB1	2.49	0.47
1:B:2767:GLU:O	1:B:2770:ILE:HG12	2.14	0.47
1:C:555:LEU:HD23	1:C:589:ILE:HD11	1.97	0.47
1:C:882:ARG:CZ	1:C:937:LEU:HD12	2.44	0.47
1:C:895:MET:HA	1:C:898:ILE:HD13	1.96	0.47
1:D:2290:TRP:CZ2	1:D:2388:ILE:HG12	2.50	0.47
1:D:2849:HIS:CE1	1:D:2877:LEU:HD11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3740:VAL:HG13	1:D:3758:THR:HG22	1.95	0.47
1:A:928:GLU:HA	1:A:931:TYR:CE2	2.49	0.47
1:A:2508:SER:OG	1:A:2560:SER:OG	2.28	0.47
1:A:3697:LYS:HA	1:A:3700:HIS:CD2	2.49	0.47
1:B:1249:MET:HB3	1:B:1599:MET:HB3	1.96	0.47
1:C:866:PRO:HG3	1:C:1005:ASN:HB3	1.95	0.47
1:C:3509:ILE:O	1:C:3513:ILE:HG12	2.13	0.47
1:D:271:ALA:HB2	1:D:488:LEU:HD22	1.96	0.47
1:D:866:PRO:HG3	1:D:1005:ASN:HB3	1.95	0.47
1:D:2767:GLU:O	1:D:2770:ILE:HG12	2.14	0.47
1:D:4886:THR:O	1:D:4895:ASN:N	2.46	0.47
1:A:674:TYR:CE1	1:A:756:SER:HB3	2.49	0.47
1:A:877:HIS:HA	1:A:880:ARG:CD	2.45	0.47
1:A:986:ILE:O	1:A:1055:ARG:NH2	2.47	0.47
1:A:2565:GLN:O	1:A:2569:ILE:HG13	2.14	0.47
1:A:3172:GLU:OE1	1:A:3266:THR:OG1	2.28	0.47
1:A:3774:GLN:HB3	1:A:3854:PHE:HE2	1.79	0.47
1:B:866:PRO:HG3	1:B:1005:ASN:HB3	1.95	0.47
1:B:2788:ARG:HB2	1:B:2904:SER:OG	2.14	0.47
1:B:3072:MET:HG3	1:B:3140:LEU:HG	1.96	0.47
1:B:3462:GLN:OE1	1:C:1187:GLY:HA3	2.15	0.47
1:C:756:SER:HB2	1:C:769:ARG:HB2	1.97	0.47
1:C:877:HIS:HA	1:C:880:ARG:CD	2.45	0.47
1:C:928:GLU:HA	1:C:931:TYR:CE2	2.49	0.47
1:C:3145:SER:O	1:C:3149:GLU:HG2	2.14	0.47
1:C:3454:ARG:N	1:C:3457:ASP:OD2	2.47	0.47
1:D:877:HIS:HA	1:D:880:ARG:CD	2.45	0.47
1:D:3033:LEU:HD13	1:D:3104:MET:SD	2.54	0.47
1:D:3219:VAL:HA	1:D:3279:ASN:OD1	2.15	0.47
1:A:189:GLU:HG2	1:A:207:PHE:HE1	1.79	0.47
1:A:434:ASP:O	1:A:438:LYS:NZ	2.48	0.47
1:A:555:LEU:HD23	1:A:589:ILE:HD11	1.97	0.47
1:A:2758:LYS:HB2	1:A:2762:LEU:HD23	1.96	0.47
1:A:3033:LEU:HD13	1:A:3104:MET:SD	2.54	0.47
3:I:33:LEU:HD22	3:I:49:LEU:HD12	1.97	0.47
3:J:33:LEU:HD22	3:J:49:LEU:HD12	1.97	0.47
1:B:363:ILE:HD12	1:B:372:LEU:HD22	1.97	0.47
1:B:555:LEU:HD23	1:B:589:ILE:HD11	1.96	0.47
1:B:877:HIS:HA	1:B:880:ARG:CD	2.45	0.47
1:B:928:GLU:HA	1:B:931:TYR:CE2	2.49	0.47
1:B:1729:MET:HE2	1:B:1930:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3345:ARG:NH1	1:B:3347:ASP:OD1	2.44	0.47
1:B:3774:GLN:HB3	1:B:3854:PHE:HE2	1.79	0.47
1:B:4615:LEU:HA	1:B:4619:GLU:HB2	1.96	0.47
1:C:114:LEU:HB2	1:C:117:HIS:HD2	1.78	0.47
1:C:749:LEU:HD22	1:C:755:ILE:HD11	1.97	0.47
1:C:1929:SER:HG	1:C:3620:PHE:HD2	1.63	0.47
1:C:3184:TYR:CE2	1:C:3201:VAL:HA	2.50	0.47
1:C:3219:VAL:HA	1:C:3279:ASN:OD1	2.15	0.47
1:D:114:LEU:HB2	1:D:117:HIS:HD2	1.77	0.47
1:D:227:TYR:HB3	1:D:352:SER:HB2	1.97	0.47
1:D:434:ASP:O	1:D:438:LYS:NZ	2.48	0.47
1:D:674:TYR:CE1	1:D:756:SER:HB3	2.50	0.47
1:D:2508:SER:HG	1:D:2560:SER:HG	1.58	0.47
1:D:2565:GLN:O	1:D:2569:ILE:HG13	2.14	0.47
1:D:3427:ASN:OD1	1:D:3465:LEU:HD22	2.14	0.47
1:D:4928:LYS:HE2	1:D:4932:GLU:HG3	1.97	0.47
1:A:3920:LEU:O	1:A:3924:ILE:HG12	2.15	0.47
1:B:3184:TYR:CE2	1:B:3201:VAL:HA	2.50	0.47
1:B:3523:ALA:HA	1:B:3526:TRP:CD1	2.50	0.47
1:B:3740:VAL:HG13	1:B:3758:THR:HG22	1.95	0.47
1:B:3939:ARG:NH2	1:C:172:GLY:O	2.47	0.47
1:C:115:TYR:CE1	1:C:175:VAL:HG22	2.48	0.47
1:C:549:ALA:O	1:C:552:SER:OG	2.18	0.47
1:A:2290:TRP:CZ2	1:A:2388:ILE:HG12	2.50	0.47
1:A:4637:THR:O	1:A:4650:LYS:NZ	2.41	0.47
1:B:189:GLU:HG2	1:B:207:PHE:HE1	1.79	0.47
1:B:3219:VAL:HA	1:B:3279:ASN:OD1	2.15	0.47
1:B:3427:ASN:OD1	1:B:3465:LEU:HD22	2.14	0.47
1:B:3454:ARG:N	1:B:3457:ASP:OD2	2.47	0.47
1:B:3467:VAL:HA	1:B:3470:LEU:HG	1.96	0.47
1:B:3920:LEU:O	1:B:3924:ILE:HG12	2.15	0.47
1:C:674:TYR:CE1	1:C:756:SER:HB3	2.50	0.47
1:C:3548:VAL:O	1:C:3552:LEU:HG	2.15	0.47
1:D:895:MET:HA	1:D:898:ILE:HD13	1.96	0.47
1:D:3493:LYS:NZ	1:D:3558:LEU:HB2	2.23	0.47
1:D:3523:ALA:HA	1:D:3526:TRP:CD1	2.50	0.47
1:A:3072:MET:HG3	1:A:3140:LEU:HG	1.96	0.47
1:B:2290:TRP:CZ2	1:B:2388:ILE:HG12	2.50	0.47
1:B:2787:TRP:CH2	1:B:2840:MET:HB3	2.50	0.47
1:B:3560:HIS:O	1:B:3564:LYS:C	2.53	0.47
1:B:3638:ASP:OD1	1:B:3730:ARG:NH2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4091:ALA:C	1:B:4093:ASP:H	2.18	0.47
1:B:4590:TYR:OH	1:B:4718:SER:HB2	2.15	0.47
1:C:227:TYR:HB3	1:C:352:SER:HB2	1.97	0.47
1:C:2290:TRP:CZ2	1:C:2388:ILE:HG12	2.50	0.47
1:C:3697:LYS:HA	1:C:3700:HIS:CD2	2.49	0.47
1:C:4590:TYR:OH	1:C:4718:SER:HB2	2.15	0.47
1:D:1440:ASN:HB3	1:D:1546:GLN:HB3	1.95	0.47
1:D:3427:ASN:CB	1:D:3463:THR:OG1	2.43	0.47
1:D:4615:LEU:HA	1:D:4619:GLU:HB2	1.96	0.47
1:A:3774:GLN:HB3	1:A:3854:PHE:CE2	2.51	0.46
2:F:63:GLY:O	2:F:67:MET:HG3	2.16	0.46
3:I:96:ASP:OD1	3:I:96:ASP:N	2.48	0.46
3:K:96:ASP:OD1	3:K:96:ASP:N	2.48	0.46
3:L:38:ARG:HD2	3:L:44:PRO:HD2	1.97	0.46
1:B:756:SER:HB2	1:B:769:ARG:HB2	1.97	0.46
1:B:1429:SER:OG	1:B:1556:GLU:HB2	2.15	0.46
1:B:3499:LYS:CE	1:B:3564:LYS:HZ1	2.27	0.46
1:C:1429:SER:OG	1:C:1556:GLU:HB2	2.15	0.46
1:C:3072:MET:HG3	1:C:3140:LEU:HG	1.97	0.46
1:D:1249:MET:HB3	1:D:1599:MET:HB3	1.96	0.46
1:D:2765:GLU:HA	1:D:2768:LYS:HD2	1.97	0.46
1:D:3184:TYR:CE2	1:D:3201:VAL:HA	2.50	0.46
1:D:3774:GLN:HB3	1:D:3854:PHE:CE2	2.50	0.46
1:D:4091:ALA:C	1:D:4093:ASP:H	2.18	0.46
1:A:1114:ARG:HG2	1:A:1138:ASP:HB2	1.97	0.46
1:A:2788:ARG:HB2	1:A:2904:SER:OG	2.14	0.46
1:A:3183:ILE:HG13	1:A:3187:LYS:HB2	1.96	0.46
1:A:3184:TYR:CE2	1:A:3201:VAL:HA	2.50	0.46
1:B:749:LEU:HD22	1:B:755:ILE:HD11	1.97	0.46
1:B:999:LEU:HD23	1:B:1050:LEU:HD21	1.96	0.46
1:B:4661:TYR:HB3	1:B:4665:ARG:HH21	1.80	0.46
1:C:3560:HIS:O	1:C:3564:LYS:C	2.54	0.46
1:C:3774:GLN:O	1:C:3854:PHE:HZ	1.99	0.46
1:C:3920:LEU:O	1:C:3924:ILE:HG12	2.15	0.46
1:D:756:SER:HB2	1:D:769:ARG:HB2	1.97	0.46
1:D:3166:PHE:CE2	1:D:3168:VAL:HB	2.51	0.46
1:D:3560:HIS:O	1:D:3564:LYS:C	2.54	0.46
1:A:271:ALA:HB2	1:A:488:LEU:HD22	1.96	0.46
1:A:363:ILE:HD12	1:A:372:LEU:HD22	1.97	0.46
1:A:1010:ASP:OD1	1:A:1013:ARG:NH2	2.48	0.46
1:A:2153:LYS:HD3	3:I:14:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3145:SER:O	1:A:3149:GLU:HG2	2.15	0.46
1:A:3308:ASN:OD1	1:A:3437:SER:CB	2.61	0.46
1:A:3560:HIS:O	1:A:3564:LYS:C	2.54	0.46
1:A:4928:LYS:HE2	1:A:4932:GLU:HG3	1.97	0.46
1:B:271:ALA:HB2	1:B:488:LEU:HD22	1.96	0.46
1:B:2765:GLU:HA	1:B:2768:LYS:HD2	1.97	0.46
1:C:1010:ASP:OD1	1:C:1013:ARG:NH2	2.48	0.46
1:C:2767:GLU:O	1:C:2770:ILE:HG12	2.14	0.46
1:C:3505:VAL:HG23	1:C:3552:LEU:HD13	1.97	0.46
1:C:3774:GLN:HB3	1:C:3854:PHE:CE2	2.50	0.46
1:D:1269:GLU:HB2	1:D:1288:LYS:HE2	1.97	0.46
1:D:3183:ILE:HG13	1:D:3187:LYS:HB2	1.96	0.46
1:A:33:GLN:OE1	1:A:53:SER:OG	2.34	0.46
1:A:227:TYR:HB3	1:A:352:SER:HB2	1.97	0.46
1:A:2787:TRP:CH2	1:A:2840:MET:HB3	2.50	0.46
1:A:3250:TRP:CE2	1:A:3309:LYS:HG2	2.51	0.46
1:A:3548:VAL:O	1:A:3552:LEU:HG	2.15	0.46
1:A:3774:GLN:O	1:A:3854:PHE:HZ	1.99	0.46
1:A:4091:ALA:C	1:A:4093:ASP:H	2.18	0.46
1:A:4661:TYR:HB3	1:A:4665:ARG:HH21	1.80	0.46
3:K:38:ARG:HD2	3:K:44:PRO:HD2	1.97	0.46
1:B:1010:ASP:OD1	1:B:1013:ARG:NH2	2.48	0.46
1:B:3774:GLN:HB3	1:B:3854:PHE:CE2	2.50	0.46
1:B:3774:GLN:O	1:B:3854:PHE:HZ	1.99	0.46
1:B:4891:CYS:HB3	1:B:4913:HIS:CE1	2.50	0.46
1:C:999:LEU:HD23	1:C:1050:LEU:HD21	1.96	0.46
1:C:4091:ALA:C	1:C:4093:ASP:H	2.18	0.46
1:D:981:MET:HE1	1:D:1056:THR:HA	1.98	0.46
1:D:3505:VAL:HG23	1:D:3552:LEU:HD13	1.97	0.46
1:D:3774:GLN:O	1:D:3854:PHE:HZ	1.99	0.46
1:A:111:ARG:HD3	1:A:111:ARG:HA	1.69	0.46
1:A:1429:SER:OG	1:A:1556:GLU:HB2	2.15	0.46
2:H:63:GLY:O	2:H:67:MET:HG3	2.16	0.46
3:J:38:ARG:HD2	3:J:44:PRO:HD2	1.97	0.46
1:B:674:TYR:CE1	1:B:756:SER:HB3	2.50	0.46
1:B:1269:GLU:HB2	1:B:1288:LYS:HE2	1.98	0.46
1:B:3559:PHE:HA	1:B:3563:GLN:NE2	2.31	0.46
1:C:1718:ARG:HD3	1:C:1831:MET:HA	1.98	0.46
1:C:3335:SER:O	1:C:3339:HIS:ND1	2.49	0.46
1:C:4928:LYS:HE2	1:C:4932:GLU:HG3	1.97	0.46
1:D:1010:ASP:OD1	1:D:1013:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1114:ARG:HG2	1:D:1138:ASP:HB2	1.97	0.46
1:D:3250:TRP:CE2	1:D:3309:LYS:HG2	2.51	0.46
1:D:3307:ILE:HD11	1:D:3372:LEU:HD13	1.98	0.46
1:D:4590:TYR:OH	1:D:4718:SER:HB2	2.15	0.46
1:D:4863:GLN:O	1:D:4867:ILE:HG12	2.16	0.46
1:A:156:GLU:HG3	1:A:187:SER:HB3	1.98	0.46
1:A:1269:GLU:HB2	1:A:1288:LYS:HE2	1.98	0.46
1:A:3166:PHE:CE2	1:A:3168:VAL:HB	2.51	0.46
1:A:3307:ILE:HD11	1:A:3372:LEU:HD13	1.98	0.46
1:A:3523:ALA:HA	1:A:3526:TRP:CD1	2.50	0.46
1:A:3559:PHE:HA	1:A:3563:GLN:NE2	2.31	0.46
1:A:4634:VAL:HG13	1:A:4640:PHE:HE1	1.81	0.46
2:G:85:ALA:O	2:G:94:PRO:HB3	2.16	0.46
1:B:1718:ARG:HD3	1:B:1831:MET:HA	1.98	0.46
1:B:2849:HIS:CE1	1:B:2877:LEU:HD11	2.50	0.46
1:C:363:ILE:HD12	1:C:372:LEU:HD22	1.97	0.46
1:C:1114:ARG:NH1	1:C:1128:LEU:O	2.45	0.46
1:C:2758:LYS:HB2	1:C:2762:LEU:HD23	1.96	0.46
1:C:2787:TRP:CH2	1:C:2840:MET:HB3	2.51	0.46
1:D:878:LEU:HA	1:D:881:ILE:HG22	1.98	0.46
1:D:3920:LEU:O	1:D:3924:ILE:HG12	2.15	0.46
1:A:2765:GLU:HA	1:A:2768:LYS:HD2	1.97	0.46
3:I:38:ARG:HD2	3:I:44:PRO:HD2	1.97	0.46
1:B:227:TYR:HB3	1:B:352:SER:HB2	1.97	0.46
1:B:1114:ARG:HG2	1:B:1138:ASP:HB2	1.97	0.46
1:B:3145:SER:O	1:B:3149:GLU:HG2	2.14	0.46
1:B:3335:SER:O	1:B:3339:HIS:ND1	2.49	0.46
1:B:3401:GLU:HA	1:B:3404:ILE:HG12	1.98	0.46
1:C:878:LEU:HA	1:C:881:ILE:HG22	1.98	0.46
1:C:1825:PHE:CE1	1:C:1842:ILE:HD12	2.51	0.46
1:C:3374:ILE:HA	1:C:3377:VAL:HG22	1.97	0.46
1:C:3892:TYR:OH	1:C:3899:ASP:OD1	2.19	0.46
1:C:4615:LEU:HA	1:C:4619:GLU:HB2	1.96	0.46
1:D:1114:ARG:NH1	1:D:1128:LEU:O	2.45	0.46
1:D:2697:SER:O	1:D:2699:GLY:N	2.48	0.46
1:D:4891:CYS:HB3	1:D:4913:HIS:CE1	2.50	0.46
1:A:878:LEU:HA	1:A:881:ILE:HG22	1.98	0.46
1:A:1979:PHE:CZ	1:A:1996:LEU:HD23	2.51	0.46
1:A:4590:TYR:OH	1:A:4718:SER:HB2	2.15	0.46
3:K:10:ILE:HD11	3:K:70:LEU:HD11	1.98	0.46
1:B:3183:ILE:HG13	1:B:3187:LYS:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HD21	1:C:214:VAL:HG23	1.98	0.46
1:C:1014:GLN:HG2	1:C:1027:ARG:NH2	2.31	0.46
1:C:2508:SER:OG	1:C:2560:SER:OG	2.28	0.46
1:C:3166:PHE:CE2	1:C:3168:VAL:HB	2.51	0.46
1:C:3401:GLU:HA	1:C:3404:ILE:HG12	1.98	0.46
1:C:4891:CYS:HB3	1:C:4913:HIS:CE1	2.50	0.46
1:D:1979:PHE:CZ	1:D:1996:LEU:HD23	2.51	0.46
1:D:2187:ILE:HD13	1:D:2227:VAL:HG13	1.98	0.46
1:D:3072:MET:HG3	1:D:3140:LEU:HG	1.96	0.46
1:A:756:SER:HB2	1:A:769:ARG:HB2	1.97	0.46
1:A:3219:VAL:HA	1:A:3279:ASN:OD1	2.15	0.46
1:A:3250:TRP:HB2	1:A:3273:MET:HE1	1.98	0.46
2:H:85:ALA:O	2:H:94:PRO:HB3	2.16	0.46
3:K:67:PRO:HB2	1:C:2202:TYR:CZ	2.51	0.46
1:B:114:LEU:HB2	1:B:117:HIS:HD2	1.77	0.46
1:C:1269:GLU:HB2	1:C:1288:LYS:HE2	1.98	0.46
1:C:4863:GLN:O	1:C:4867:ILE:HG12	2.16	0.46
1:D:181:LEU:HD21	1:D:214:VAL:HG23	1.98	0.46
1:D:749:LEU:HD22	1:D:755:ILE:HD11	1.97	0.46
1:D:1429:SER:OG	1:D:1556:GLU:HB2	2.15	0.46
1:D:2658:GLU:HB3	1:D:2661:LEU:HB3	1.98	0.46
1:D:2787:TRP:CH2	1:D:2840:MET:HB3	2.50	0.46
1:D:3335:SER:O	1:D:3339:HIS:ND1	2.49	0.46
1:A:2296:GLU:HG3	1:A:2390:THR:HG22	1.98	0.46
1:A:4863:GLN:O	1:A:4867:ILE:HG12	2.16	0.46
3:L:10:ILE:HD11	3:L:70:LEU:HD11	1.98	0.46
1:B:1825:PHE:CE1	1:B:1842:ILE:HD12	2.51	0.46
1:B:1979:PHE:CZ	1:B:1996:LEU:HD23	2.51	0.46
1:B:2142:MET:SD	1:B:2174:VAL:HG11	2.56	0.46
1:B:3505:VAL:HG23	1:B:3552:LEU:HD13	1.97	0.46
1:C:1708:ASP:HA	1:C:1712:SER:HB2	1.98	0.46
1:C:2658:GLU:HB3	1:C:2661:LEU:HB3	1.98	0.46
1:C:4661:TYR:HB3	1:C:4665:ARG:HH21	1.80	0.46
1:D:1718:ARG:HD3	1:D:1831:MET:HA	1.98	0.46
1:D:3427:ASN:HB2	1:D:3463:THR:HG1	1.76	0.46
1:A:4190:VAL:HG11	1:A:4949:TRP:CH2	2.52	0.45
3:L:33:LEU:HD22	3:L:49:LEU:HD12	1.97	0.45
3:L:51:ASP:OD1	3:L:52:MET:N	2.45	0.45
1:B:1014:GLN:HG2	1:B:1027:ARG:NH2	2.31	0.45
1:B:1986:CYS:O	1:B:1993:ARG:NH2	2.50	0.45
1:B:2607:LEU:HD23	1:B:2665:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3250:TRP:CE2	1:B:3309:LYS:HG2	2.51	0.45
1:B:3374:ILE:HA	1:B:3377:VAL:HG22	1.97	0.45
1:B:3548:VAL:O	1:B:3552:LEU:HG	2.15	0.45
1:B:4832:GLU:O	1:B:4843:ARG:NH2	2.49	0.45
1:B:4928:LYS:HE2	1:B:4932:GLU:HG3	1.97	0.45
1:C:3454:ARG:O	1:C:3458:ARG:HG2	2.16	0.45
1:C:4190:VAL:HG11	1:C:4949:TRP:CH2	2.52	0.45
1:D:801:ARG:HG2	1:D:1618:LEU:HA	1.98	0.45
1:D:2607:LEU:HD23	1:D:2665:ALA:HA	1.98	0.45
1:D:3454:ARG:O	1:D:3458:ARG:HG2	2.17	0.45
1:A:2697:SER:O	1:A:2699:GLY:N	2.48	0.45
2:E:45:LYS:HB2	2:E:45:LYS:HE2	1.68	0.45
2:F:45:LYS:HE2	2:F:45:LYS:HB2	1.68	0.45
3:K:33:LEU:HD22	3:K:49:LEU:HD12	1.97	0.45
1:B:948:CYS:HB3	1:B:1064:LEU:HD12	1.99	0.45
1:B:3250:TRP:HB2	1:B:3273:MET:HE1	1.98	0.45
1:C:1979:PHE:CZ	1:C:1996:LEU:HD23	2.51	0.45
1:C:2771:TYR:O	1:C:2774:PRO:HD2	2.16	0.45
1:C:3250:TRP:CE2	1:C:3309:LYS:HG2	2.51	0.45
1:C:3277:LEU:O	1:C:3281:LEU:HD23	2.16	0.45
1:C:4832:GLU:O	1:C:4843:ARG:NH2	2.50	0.45
1:D:363:ILE:HD12	1:D:372:LEU:HD22	1.97	0.45
1:D:1014:GLN:HG2	1:D:1027:ARG:NH2	2.31	0.45
1:D:1986:CYS:O	1:D:1993:ARG:NH2	2.49	0.45
1:A:749:LEU:HD22	1:A:755:ILE:HD11	1.97	0.45
1:A:1718:ARG:HD3	1:A:1831:MET:HA	1.98	0.45
1:A:2658:GLU:HB3	1:A:2661:LEU:HB3	1.98	0.45
1:A:3335:SER:O	1:A:3339:HIS:ND1	2.49	0.45
2:E:63:GLY:O	2:E:67:MET:HG3	2.16	0.45
3:J:10:ILE:HD11	3:J:70:LEU:HD11	1.98	0.45
3:L:61:ASN:OD1	3:L:62:GLY:N	2.49	0.45
1:B:181:LEU:HD21	1:B:214:VAL:HG23	1.98	0.45
1:B:587:ASN:OD1	1:B:2133:ARG:NH1	2.49	0.45
1:B:2296:GLU:HG3	1:B:2390:THR:HG22	1.98	0.45
1:B:2771:TYR:O	1:B:2774:PRO:HD2	2.16	0.45
1:B:3277:LEU:O	1:B:3281:LEU:HD23	2.16	0.45
1:B:3454:ARG:O	1:B:3458:ARG:HG2	2.16	0.45
1:B:4822:ARG:HG2	1:C:4851:PHE:CD2	2.51	0.45
1:C:513:HIS:O	1:C:517:VAL:HG23	2.17	0.45
1:C:1114:ARG:HG2	1:C:1138:ASP:HB2	1.97	0.45
1:C:2590:ARG:O	1:C:2593:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2765:GLU:HA	1:C:2768:LYS:HD2	1.97	0.45
1:A:1986:CYS:O	1:A:1993:ARG:NH2	2.50	0.45
1:A:2142:MET:SD	1:A:2174:VAL:HG11	2.56	0.45
1:A:2187:ILE:HD13	1:A:2227:VAL:HG13	1.98	0.45
1:A:2863:LYS:HE2	1:A:2865:GLY:O	2.17	0.45
1:A:4898:PHE:O	1:A:4904:GLY:HA3	2.17	0.45
3:L:11:ALA:O	3:L:14:LYS:HB3	2.17	0.45
1:C:948:CYS:HB3	1:C:1064:LEU:HD12	1.98	0.45
1:C:3154:ALA:O	1:C:3157:GLU:HG3	2.17	0.45
1:C:3345:ARG:NH1	1:C:3347:ASP:OD1	2.44	0.45
1:D:1825:PHE:CE1	1:D:1842:ILE:HD12	2.51	0.45
1:D:2296:GLU:HG3	1:D:2390:THR:HG22	1.99	0.45
1:D:3345:ARG:NH1	1:D:3347:ASP:OD1	2.44	0.45
1:D:3401:GLU:HA	1:D:3404:ILE:HG12	1.98	0.45
1:D:3559:PHE:HA	1:D:3563:GLN:NE2	2.31	0.45
1:D:3892:TYR:OH	1:D:3899:ASP:OD1	2.19	0.45
1:D:4832:GLU:O	1:D:4843:ARG:NH2	2.50	0.45
1:A:2771:TYR:O	1:A:2774:PRO:HD2	2.16	0.45
1:A:3233:HIS:O	1:A:3237:VAL:HG22	2.17	0.45
1:A:3426:ASN:HD22	1:A:3426:ASN:HA	1.63	0.45
1:A:3454:ARG:O	1:A:3458:ARG:HG2	2.16	0.45
1:A:4832:GLU:O	1:A:4843:ARG:NH2	2.50	0.45
1:A:4891:CYS:HB3	1:A:4913:HIS:CE1	2.50	0.45
1:B:434:ASP:O	1:B:438:LYS:NZ	2.48	0.45
1:B:866:PRO:HG2	1:B:1009:ARG:NH1	2.32	0.45
1:B:3233:HIS:O	1:B:3237:VAL:HG22	2.17	0.45
1:B:3861:GLN:H	1:B:3867:THR:HG23	1.82	0.45
1:B:4898:PHE:O	1:B:4904:GLY:HA3	2.17	0.45
1:C:801:ARG:HA	1:C:1617:TRP:O	2.17	0.45
1:C:1986:CYS:O	1:C:1993:ARG:NH2	2.50	0.45
1:C:2187:ILE:HD13	1:C:2227:VAL:HG13	1.98	0.45
1:C:2911:GLU:HG2	1:C:2912:LEU:HD23	1.99	0.45
1:D:624:ALA:HB2	1:D:1667:LEU:HD12	1.99	0.45
1:D:644:LEU:HD13	1:D:1630:LEU:HD21	1.99	0.45
1:D:2142:MET:SD	1:D:2174:VAL:HG11	2.56	0.45
1:D:4634:VAL:HG13	1:D:4640:PHE:HE1	1.81	0.45
1:A:1708:ASP:HA	1:A:1712:SER:HB2	1.98	0.45
1:A:1960:ARG:HA	1:A:1960:ARG:HE	1.82	0.45
1:A:3505:VAL:HG23	1:A:3552:LEU:HD13	1.97	0.45
2:E:85:ALA:O	2:E:94:PRO:HB3	2.16	0.45
2:G:63:GLY:O	2:G:67:MET:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:801:ARG:HG2	1:B:1618:LEU:HA	1.98	0.45
1:B:2187:ILE:HD13	1:B:2227:VAL:HG13	1.98	0.45
1:B:3166:PHE:CE2	1:B:3168:VAL:HB	2.51	0.45
1:B:4634:VAL:HG13	1:B:4640:PHE:HE1	1.81	0.45
1:B:4863:GLN:O	1:B:4867:ILE:HG12	2.16	0.45
1:B:4886:THR:O	1:B:4895:ASN:N	2.46	0.45
1:C:434:ASP:O	1:C:438:LYS:NZ	2.48	0.45
1:C:866:PRO:HG2	1:C:1009:ARG:NH1	2.32	0.45
1:D:33:GLN:OE1	1:D:53:SER:OG	2.34	0.45
1:D:587:ASN:OD1	1:D:2133:ARG:NH1	2.49	0.45
1:D:1708:ASP:HA	1:D:1712:SER:HB2	1.98	0.45
1:D:2590:ARG:O	1:D:2593:VAL:HG12	2.17	0.45
1:D:3374:ILE:HA	1:D:3377:VAL:HG22	1.97	0.45
1:D:3548:VAL:O	1:D:3552:LEU:HG	2.15	0.45
1:A:181:LEU:HD21	1:A:214:VAL:HG23	1.98	0.45
1:A:1825:PHE:CE1	1:A:1842:ILE:HD12	2.51	0.45
1:A:3374:ILE:HA	1:A:3377:VAL:HG22	1.97	0.45
1:A:3401:GLU:HA	1:A:3404:ILE:HG12	1.98	0.45
2:F:85:ALA:O	2:F:94:PRO:HB3	2.16	0.45
2:H:78:THR:OG1	2:H:80:ASP:OD1	2.23	0.45
3:I:11:ALA:O	3:I:14:LYS:HB3	2.17	0.45
3:I:61:ASN:OD1	3:I:62:GLY:N	2.49	0.45
3:J:96:ASP:N	3:J:96:ASP:OD1	2.48	0.45
1:B:801:ARG:HA	1:B:1617:TRP:O	2.17	0.45
1:B:878:LEU:HA	1:B:881:ILE:HG22	1.98	0.45
1:B:1114:ARG:NH1	1:B:1128:LEU:O	2.45	0.45
1:B:1960:ARG:HA	1:B:1960:ARG:HE	1.82	0.45
1:B:3167:PRO:HA	1:B:3248:ARG:NH2	2.32	0.45
1:B:3553:ASP:O	1:B:3557:VAL:HG23	2.17	0.45
1:C:188:SER:HB2	1:C:190:ARG:HH11	1.82	0.45
1:C:644:LEU:HD13	1:C:1630:LEU:HD21	1.99	0.45
1:C:3307:ILE:HD11	1:C:3372:LEU:HD13	1.98	0.45
1:C:4509:VAL:HG11	1:C:4579:HIS:HB2	1.99	0.45
1:C:4634:VAL:HG13	1:C:4640:PHE:HE1	1.81	0.45
1:D:801:ARG:HA	1:D:1617:TRP:O	2.17	0.45
1:D:2771:TYR:O	1:D:2774:PRO:HD2	2.16	0.45
1:D:2863:LYS:HE2	1:D:2865:GLY:O	2.17	0.45
1:D:3154:ALA:O	1:D:3157:GLU:HG3	2.17	0.45
1:D:4661:TYR:HB3	1:D:4665:ARG:HH21	1.80	0.45
1:A:587:ASN:OD1	1:A:2133:ARG:NH1	2.49	0.45
1:A:624:ALA:HB2	1:A:1667:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:MET:HE1	1:A:1056:THR:HA	1.99	0.45
1:A:1014:GLN:HG2	1:A:1027:ARG:NH2	2.31	0.45
1:A:2607:LEU:HD23	1:A:2665:ALA:HA	1.98	0.45
1:A:4589:GLY:O	1:A:4590:TYR:HB3	2.17	0.45
3:J:11:ALA:O	3:J:14:LYS:HB3	2.17	0.45
1:B:1113:MET:HB2	1:B:1156:TRP:HZ2	1.82	0.45
1:B:2255:LEU:O	1:B:3810:ARG:NH1	2.47	0.45
1:B:2863:LYS:HE2	1:B:2865:GLY:O	2.17	0.45
1:B:4509:VAL:HG11	1:B:4579:HIS:HB2	1.99	0.45
1:C:1960:ARG:HA	1:C:1960:ARG:HE	1.82	0.45
1:C:2787:TRP:HA	1:C:2906:GLY:HA3	1.99	0.45
1:C:3861:GLN:H	1:C:3867:THR:HG23	1.82	0.45
1:D:188:SER:HB2	1:D:190:ARG:HH11	1.82	0.45
1:D:3233:HIS:O	1:D:3237:VAL:HG22	2.17	0.45
1:D:3370:TYR:HB3	1:D:3465:LEU:HD12	1.99	0.45
1:A:513:HIS:O	1:A:517:VAL:HG23	2.17	0.45
1:A:801:ARG:HG2	1:A:1618:LEU:HA	1.98	0.45
2:G:45:LYS:HB2	2:G:45:LYS:HE2	1.68	0.45
3:I:10:ILE:HD11	3:I:70:LEU:HD11	1.98	0.45
3:K:11:ALA:O	3:K:14:LYS:HB3	2.17	0.45
1:B:2658:GLU:HB3	1:B:2661:LEU:HB3	1.98	0.45
1:B:2911:GLU:HG2	1:B:2912:LEU:HD23	1.99	0.45
1:C:976:TYR:O	1:C:978:PRO:HD3	2.17	0.45
1:C:981:MET:HE1	1:C:1056:THR:HA	1.99	0.45
1:C:2863:LYS:HE2	1:C:2865:GLY:O	2.17	0.45
1:C:3559:PHE:HA	1:C:3563:GLN:NE2	2.31	0.45
1:C:3651:PRO:CB	1:C:3652:PRO:HD3	2.47	0.45
1:C:3872:ILE:HA	1:C:3875:VAL:HG12	1.99	0.45
1:D:2075:ILE:HG22	1:D:2077:ASP:H	1.82	0.45
1:D:2605:MET:HB3	1:D:2606:PRO:HD3	1.99	0.45
1:D:3651:PRO:CB	1:D:3652:PRO:HD3	2.47	0.45
1:D:4190:VAL:HG11	1:D:4949:TRP:CH2	2.52	0.45
1:A:1113:MET:HB2	1:A:1156:TRP:HZ2	1.82	0.45
1:A:1910:LEU:HB2	1:A:2087:LEU:HD21	1.99	0.45
1:A:2075:ILE:HG22	1:A:2077:ASP:H	1.82	0.45
1:A:3312:PRO:HA	1:A:3376:PHE:HZ	1.82	0.45
1:A:3313:GLN:HA	1:A:3316:LYS:HD3	1.99	0.45
1:A:4480:PHE:O	1:A:4484:ILE:HG23	2.17	0.45
3:K:61:ASN:OD1	3:K:62:GLY:N	2.49	0.45
1:B:188:SER:HB2	1:B:190:ARG:HH11	1.82	0.45
1:B:2590:ARG:O	1:B:2593:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2596:VAL:HG21	1:B:2610:LEU:HD11	1.99	0.45
1:B:3307:ILE:HD11	1:B:3372:LEU:HD13	1.98	0.45
1:C:801:ARG:HG2	1:C:1618:LEU:HA	1.98	0.45
1:C:1113:MET:HB2	1:C:1156:TRP:HZ2	1.82	0.45
1:C:1910:LEU:HB2	1:C:2087:LEU:HD21	1.99	0.45
1:C:2607:LEU:HD23	1:C:2665:ALA:HA	1.98	0.45
1:C:3397:ARG:NH2	1:C:3550:ARG:HD2	2.24	0.45
1:D:976:TYR:O	1:D:978:PRO:HD3	2.17	0.45
1:D:1960:ARG:HA	1:D:1960:ARG:HE	1.82	0.45
1:D:3312:PRO:HA	1:D:3376:PHE:HZ	1.82	0.45
1:D:4898:PHE:O	1:D:4904:GLY:HA3	2.17	0.45
1:A:188:SER:HB2	1:A:190:ARG:HH11	1.82	0.44
2:H:25:VAL:HG12	2:H:104:LEU:HA	1.99	0.44
1:B:513:HIS:O	1:B:517:VAL:HG23	2.17	0.44
1:B:995:MET:HE3	1:B:995:MET:HB3	1.87	0.44
1:B:2605:MET:HB3	1:B:2606:PRO:HD3	1.99	0.44
1:C:156:GLU:HG3	1:C:187:SER:HB3	1.98	0.44
1:C:258:ARG:NE	1:C:316:LEU:O	2.33	0.44
1:C:881:ILE:O	1:C:885:LEU:HD23	2.18	0.44
1:C:2075:ILE:HG22	1:C:2077:ASP:H	1.82	0.44
1:C:3399:VAL:HG21	1:C:3473:LEU:HD22	2.00	0.44
1:C:3840:PHE:HE1	1:C:3874:THR:HG23	1.82	0.44
1:D:156:GLU:HG3	1:D:187:SER:HB3	1.98	0.44
1:D:866:PRO:HG2	1:D:1009:ARG:NH1	2.32	0.44
1:D:1910:LEU:HB2	1:D:2087:LEU:HD21	1.99	0.44
1:D:2482:ASP:OD1	1:D:2483:PHE:N	2.50	0.44
1:A:644:LEU:HD13	1:A:1630:LEU:HD21	1.99	0.44
1:A:2590:ARG:O	1:A:2593:VAL:HG12	2.17	0.44
1:A:3167:PRO:HA	1:A:3248:ARG:NH2	2.32	0.44
1:A:3496:PHE:HE2	1:A:3552:LEU:O	2.00	0.44
2:E:25:VAL:HG12	2:E:104:LEU:HA	1.99	0.44
1:B:33:GLN:OE1	1:B:53:SER:OG	2.34	0.44
1:B:4190:VAL:HG11	1:B:4949:TRP:CH2	2.52	0.44
1:B:4589:GLY:O	1:B:4590:TYR:HB3	2.17	0.44
1:C:587:ASN:OD1	1:C:2133:ARG:NH1	2.49	0.44
1:C:2142:MET:SD	1:C:2174:VAL:HG11	2.56	0.44
1:C:2296:GLU:HG3	1:C:2390:THR:HG22	1.99	0.44
1:C:2697:SER:O	1:C:2699:GLY:N	2.48	0.44
1:C:3553:ASP:O	1:C:3557:VAL:HG23	2.17	0.44
1:C:3840:PHE:CE1	1:C:3874:THR:HG23	2.53	0.44
1:C:4589:GLY:O	1:C:4590:TYR:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:HIS:O	1:D:517:VAL:HG23	2.17	0.44
1:D:3277:LEU:O	1:D:3281:LEU:HD23	2.16	0.44
1:A:976:TYR:O	1:A:978:PRO:HD3	2.17	0.44
1:A:2605:MET:HB3	1:A:2606:PRO:HD3	1.99	0.44
1:A:3277:LEU:O	1:A:3281:LEU:HD23	2.16	0.44
1:A:3426:ASN:C	1:A:3428:MET:H	2.21	0.44
1:A:3840:PHE:CE1	1:A:3874:THR:HG23	2.53	0.44
1:B:76:ARG:HH11	1:B:80:GLU:HG3	1.82	0.44
1:B:1708:ASP:HA	1:B:1712:SER:HB2	1.98	0.44
1:B:1910:LEU:HB2	1:B:2087:LEU:HD21	1.99	0.44
1:B:2075:ILE:HG22	1:B:2077:ASP:H	1.82	0.44
1:B:3313:GLN:HA	1:B:3316:LYS:HD3	1.99	0.44
1:B:3423:ASN:O	1:B:3425:ILE:CD1	2.46	0.44
1:C:2596:VAL:HG21	1:C:2610:LEU:HD11	1.99	0.44
1:C:3070:LYS:O	1:C:3073:GLU:HG3	2.17	0.44
1:C:4898:PHE:O	1:C:4904:GLY:HA3	2.17	0.44
1:D:1914:CYS:SG	1:D:2091:GLN:NE2	2.78	0.44
1:D:3174:HIS:ND1	1:D:3175:LEU:HG	2.33	0.44
1:D:3313:GLN:HA	1:D:3316:LYS:HD3	1.99	0.44
1:D:3553:ASP:O	1:D:3557:VAL:HG23	2.17	0.44
1:D:3861:GLN:H	1:D:3867:THR:HG23	1.82	0.44
1:A:948:CYS:HB3	1:A:1064:LEU:HD12	1.98	0.44
1:B:3427:ASN:CB	1:B:3463:THR:OG1	2.42	0.44
1:B:3840:PHE:CE1	1:B:3874:THR:HG23	2.53	0.44
1:B:4480:PHE:O	1:B:4484:ILE:HG23	2.17	0.44
1:C:1091:GLU:HB3	1:C:1094:TYR:CD2	2.53	0.44
1:C:3426:ASN:C	1:C:3428:MET:H	2.21	0.44
1:C:3545:GLU:HG2	1:C:3546:LYS:N	2.32	0.44
1:D:2580:LEU:HD23	1:D:2580:LEU:HA	1.81	0.44
1:D:4509:VAL:HG11	1:D:4579:HIS:HB2	1.99	0.44
1:A:1091:GLU:HB3	1:A:1094:TYR:CD2	2.53	0.44
1:A:3190:ARG:HG2	1:A:3191:GLU:OE1	2.17	0.44
1:A:3861:GLN:H	1:A:3867:THR:HG23	1.82	0.44
2:G:90:GLY:HA2	1:C:638:PRO:HD3	2.00	0.44
1:B:2482:ASP:OD1	1:B:2483:PHE:N	2.50	0.44
1:B:4610:LEU:HD11	1:B:4635:ILE:HG12	2.00	0.44
1:C:33:GLN:OE1	1:C:53:SER:OG	2.34	0.44
1:C:2605:MET:HB3	1:C:2606:PRO:HD3	1.99	0.44
1:C:3190:ARG:HG2	1:C:3191:GLU:OE1	2.17	0.44
1:C:3233:HIS:O	1:C:3237:VAL:HG22	2.17	0.44
1:C:3499:LYS:CE	1:C:3564:LYS:NZ	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4888:CYS:HB3	1:C:4891:CYS:SG	2.58	0.44
1:D:3399:VAL:HG21	1:D:3473:LEU:HD22	2.00	0.44
1:D:3840:PHE:HE1	1:D:3874:THR:HG23	1.82	0.44
1:A:2884:LYS:O	1:A:2887:GLU:HG3	2.18	0.44
1:A:3545:GLU:HG2	1:A:3546:LYS:N	2.32	0.44
1:A:3661:VAL:HG23	1:A:3666:GLN:HG2	2.00	0.44
1:A:4610:LEU:HD11	1:A:4635:ILE:HG12	2.00	0.44
3:L:21:ASP:OD1	3:L:22:LYS:N	2.51	0.44
3:L:96:ASP:OD1	3:L:96:ASP:N	2.48	0.44
1:B:258:ARG:NE	1:B:316:LEU:O	2.33	0.44
1:B:976:TYR:O	1:B:978:PRO:HD3	2.17	0.44
1:B:3190:ARG:HG2	1:B:3191:GLU:OE1	2.17	0.44
1:B:4752:THR:HG23	1:B:4753:LEU:HD12	2.00	0.44
1:C:76:ARG:HH11	1:C:80:GLU:HG3	1.82	0.44
1:C:624:ALA:HB2	1:C:1667:LEU:HD12	1.99	0.44
1:C:2062:ILE:O	1:C:2066:MET:HG2	2.18	0.44
1:C:3496:PHE:HE2	1:C:3552:LEU:O	2.00	0.44
1:C:4480:PHE:O	1:C:4484:ILE:HG23	2.17	0.44
1:C:4610:LEU:HD11	1:C:4635:ILE:HG12	2.00	0.44
1:C:4753:LEU:HG	1:D:4773:LEU:HD22	1.99	0.44
1:D:2193:VAL:HG11	1:D:2227:VAL:HG11	2.00	0.44
1:D:3123:LEU:HB3	1:D:3124:GLU:OE1	2.17	0.44
1:D:3872:ILE:HA	1:D:3875:VAL:HG12	1.99	0.44
1:D:4480:PHE:O	1:D:4484:ILE:HG23	2.18	0.44
1:D:4589:GLY:O	1:D:4590:TYR:HB3	2.16	0.44
1:D:4770:THR:HG23	1:D:4862:ILE:HG12	2.00	0.44
1:A:881:ILE:O	1:A:885:LEU:HD23	2.17	0.44
1:A:1896:MET:HG2	1:A:1896:MET:O	2.18	0.44
1:A:2773:TRP:NE1	1:A:2777:GLU:OE2	2.51	0.44
1:A:3123:LEU:HB3	1:A:3124:GLU:OE1	2.17	0.44
1:A:3427:ASN:HD22	1:A:3463:THR:C	2.18	0.44
1:A:3493:LYS:HZ3	1:A:3558:LEU:HB3	1.81	0.44
1:A:3553:ASP:O	1:A:3557:VAL:HG23	2.17	0.44
1:A:4770:THR:HG23	1:A:4862:ILE:HG12	2.00	0.44
1:B:2787:TRP:HA	1:B:2906:GLY:HA3	1.99	0.44
1:B:3070:LYS:O	1:B:3073:GLU:HG3	2.17	0.44
1:B:3154:ALA:O	1:B:3157:GLU:HG3	2.17	0.44
1:B:3399:VAL:HG21	1:B:3473:LEU:HD22	2.00	0.44
1:B:3426:ASN:C	1:B:3428:MET:H	2.21	0.44
1:B:4584:PHE:O	1:B:4587:ILE:HG22	2.18	0.44
1:C:3313:GLN:HA	1:C:3316:LYS:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3370:TYR:HB3	1:C:3465:LEU:HD12	1.99	0.44
1:C:3506:ARG:NH2	1:C:3549:GLU:OE1	2.42	0.44
1:D:3190:ARG:HG2	1:D:3191:GLU:OE1	2.17	0.44
1:A:514:PHE:HD2	1:A:526:TRP:HB2	1.83	0.44
1:A:758:CYS:HB3	1:A:819:TYR:CE2	2.53	0.44
1:A:1914:CYS:SG	1:A:2091:GLN:NE2	2.78	0.44
1:A:2176:VAL:HG22	1:A:2220:TYR:CZ	2.53	0.44
1:A:3070:LYS:O	1:A:3073:GLU:HG3	2.17	0.44
1:A:3154:ALA:O	1:A:3157:GLU:HG3	2.17	0.44
1:A:3215:MET:O	1:A:3219:VAL:HG23	2.18	0.44
1:A:4509:VAL:HG11	1:A:4579:HIS:HB2	1.99	0.44
1:B:156:GLU:HG3	1:B:187:SER:HB3	1.98	0.44
1:B:644:LEU:HD13	1:B:1630:LEU:HD21	1.99	0.44
1:B:981:MET:HE1	1:B:1056:THR:HA	1.99	0.44
1:B:3215:MET:O	1:B:3219:VAL:HG23	2.18	0.44
1:B:3840:PHE:HE1	1:B:3874:THR:HG23	1.82	0.44
1:C:2884:LYS:O	1:C:2887:GLU:HG3	2.18	0.44
1:C:3167:PRO:HA	1:C:3248:ARG:NH2	2.32	0.44
1:D:115:TYR:CD1	1:D:175:VAL:HG22	2.53	0.44
1:D:2062:ILE:O	1:D:2066:MET:HG2	2.18	0.44
1:D:2787:TRP:HA	1:D:2906:GLY:HA3	1.99	0.44
1:D:3297:LYS:HE3	1:D:3297:LYS:HB3	1.34	0.44
1:D:3426:ASN:C	1:D:3428:MET:H	2.21	0.44
1:A:115:TYR:CD1	1:A:175:VAL:HG22	2.53	0.44
1:A:866:PRO:HG2	1:A:1009:ARG:NH1	2.32	0.44
1:A:2193:VAL:HG11	1:A:2227:VAL:HG11	2.00	0.44
1:A:2482:ASP:OD1	1:A:2483:PHE:N	2.50	0.44
1:A:2787:TRP:HA	1:A:2906:GLY:HA3	1.99	0.44
1:A:3174:HIS:ND1	1:A:3175:LEU:HG	2.33	0.44
1:A:3399:VAL:HG21	1:A:3473:LEU:HD22	2.00	0.44
1:A:3653:GLU:OE1	1:A:3653:GLU:N	2.46	0.44
1:A:3872:ILE:HA	1:A:3875:VAL:HG12	1.99	0.44
1:A:4569:GLU:HB3	1:A:4570:PRO:HD3	2.00	0.44
2:F:83:TYR:OH	1:B:1768:PHE:O	2.29	0.44
1:B:758:CYS:HB3	1:B:819:TYR:CE2	2.53	0.44
1:B:2258:ARG:HB3	1:B:2260:PRO:HD2	2.00	0.44
1:B:3307:ILE:HD12	1:B:3375:ARG:HD3	2.00	0.44
1:B:3308:ASN:OD1	1:B:3437:SER:CB	2.61	0.44
1:B:3496:PHE:HE2	1:B:3552:LEU:O	2.00	0.44
1:B:3651:PRO:CB	1:B:3652:PRO:HD3	2.47	0.44
1:B:4637:THR:O	1:B:4650:LYS:NZ	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:758:CYS:HB3	1:C:819:TYR:CE2	2.53	0.44
1:C:2482:ASP:OD1	1:C:2483:PHE:N	2.50	0.44
1:C:2773:TRP:NE1	1:C:2777:GLU:OE2	2.51	0.44
1:C:4584:PHE:O	1:C:4587:ILE:HG22	2.18	0.44
1:D:948:CYS:HB3	1:D:1064:LEU:HD12	1.98	0.44
1:D:2773:TRP:NE1	1:D:2777:GLU:OE2	2.51	0.44
1:D:3215:MET:O	1:D:3219:VAL:HG23	2.18	0.44
1:D:3467:VAL:HB	1:D:3471:LYS:HZ1	1.83	0.44
1:D:4584:PHE:O	1:D:4587:ILE:HG22	2.18	0.44
1:A:801:ARG:HA	1:A:1617:TRP:O	2.17	0.43
1:A:2087:LEU:O	1:A:2091:GLN:HG2	2.18	0.43
1:A:3366:LEU:HG	1:A:3370:TYR:CD1	2.53	0.43
1:A:3370:TYR:HB3	1:A:3465:LEU:HD12	1.99	0.43
1:A:3651:PRO:CB	1:A:3652:PRO:HD3	2.47	0.43
1:A:3840:PHE:HE1	1:A:3874:THR:HG23	1.82	0.43
1:B:514:PHE:HD2	1:B:526:TRP:HB2	1.83	0.43
1:B:2759:PRO:O	1:B:2762:LEU:N	2.51	0.43
1:B:3872:ILE:HA	1:B:3875:VAL:HG12	1.99	0.43
1:B:4753:LEU:HD11	1:C:4769:LEU:HB3	2.00	0.43
1:C:115:TYR:CD1	1:C:175:VAL:HG22	2.53	0.43
1:C:3215:MET:O	1:C:3219:VAL:HG23	2.18	0.43
1:C:3366:LEU:HG	1:C:3370:TYR:CD1	2.53	0.43
1:C:3496:PHE:CE2	1:C:3555:ALA:HB3	2.53	0.43
1:C:3794:ALA:HB2	1:C:3868:VAL:HG11	2.00	0.43
1:C:4792:PHE:HB3	1:C:4843:ARG:NH2	2.33	0.43
1:D:514:PHE:HD2	1:D:526:TRP:HB2	1.83	0.43
1:D:881:ILE:O	1:D:885:LEU:HD23	2.18	0.43
1:D:3167:PRO:HA	1:D:3248:ARG:NH2	2.32	0.43
1:D:3366:LEU:HG	1:D:3370:TYR:CD1	2.53	0.43
1:A:1829:LEU:HG	1:A:1912:TYR:CE2	2.53	0.43
1:A:2596:VAL:HG21	1:A:2610:LEU:HD11	1.99	0.43
1:A:2911:GLU:HG2	1:A:2912:LEU:HD23	1.99	0.43
1:A:3324:GLU:HA	1:A:3327:LYS:HZ3	1.83	0.43
1:A:3627:SER:O	1:A:3631:THR:OG1	2.24	0.43
1:B:624:ALA:HB2	1:B:1667:LEU:HD12	1.99	0.43
1:B:881:ILE:O	1:B:885:LEU:HD23	2.18	0.43
1:B:1829:LEU:HG	1:B:1912:TYR:CE2	2.53	0.43
1:B:1896:MET:O	1:B:1896:MET:HG2	2.18	0.43
1:B:2087:LEU:O	1:B:2091:GLN:HG2	2.18	0.43
1:B:2176:VAL:HG22	1:B:2220:TYR:CZ	2.53	0.43
1:B:3123:LEU:HB3	1:B:3124:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3174:HIS:ND1	1:B:3175:LEU:HG	2.33	0.43
1:C:2082:ARG:HG3	1:C:3687:LEU:HD22	2.01	0.43
1:C:2176:VAL:HG22	1:C:2220:TYR:CZ	2.53	0.43
1:C:3307:ILE:HD12	1:C:3375:ARG:HD3	2.00	0.43
1:C:3496:PHE:HE2	1:C:3555:ALA:HB3	1.83	0.43
1:D:3070:LYS:O	1:D:3073:GLU:HG3	2.17	0.43
1:D:4606:VAL:HA	1:D:4609:LYS:HE2	2.01	0.43
1:D:4610:LEU:HD11	1:D:4635:ILE:HG12	2.00	0.43
1:A:3499:LYS:CE	1:A:3564:LYS:NZ	2.81	0.43
2:F:25:VAL:HG12	2:F:104:LEU:HA	1.99	0.43
3:J:21:ASP:OD1	3:J:22:LYS:N	2.51	0.43
3:K:21:ASP:OD1	3:K:22:LYS:N	2.51	0.43
3:K:108:HIS:CE1	1:C:1956:ALA:HA	2.53	0.43
1:B:2062:ILE:O	1:B:2066:MET:HG2	2.18	0.43
1:B:2082:ARG:HG3	1:B:3687:LEU:HD22	2.01	0.43
1:B:2884:LYS:O	1:B:2887:GLU:HG3	2.18	0.43
1:B:3483:PRO:O	1:B:3486:GLN:HB2	2.18	0.43
1:B:3763:ILE:HD11	1:B:3838:ASP:O	2.18	0.43
1:B:4162:LYS:HD2	1:B:4203:ALA:HB1	2.00	0.43
1:C:739:ARG:HD2	1:C:739:ARG:HA	1.81	0.43
1:C:2193:VAL:HG11	1:C:2227:VAL:HG11	2.00	0.43
1:C:3035:ILE:O	1:C:3039:THR:HG23	2.19	0.43
1:C:3123:LEU:HB3	1:C:3124:GLU:OE1	2.17	0.43
1:C:3312:PRO:HA	1:C:3376:PHE:HZ	1.82	0.43
1:C:3653:GLU:OE1	1:C:3653:GLU:N	2.47	0.43
1:C:4752:THR:HG23	1:C:4753:LEU:HD12	2.00	0.43
1:D:931:TYR:HA	1:D:934:GLN:HB2	2.01	0.43
1:D:1113:MET:HB2	1:D:1156:TRP:HZ2	1.82	0.43
1:D:4203:ALA:HA	1:D:4206:ILE:HG12	2.00	0.43
1:A:2062:ILE:O	1:A:2066:MET:HG2	2.18	0.43
1:A:3109:PHE:O	1:A:3165:ALA:HB2	2.19	0.43
3:I:17:PHE:CZ	3:I:28:ILE:HG13	2.54	0.43
1:B:2773:TRP:NE1	1:B:2777:GLU:OE2	2.51	0.43
1:B:3496:PHE:CE2	1:B:3555:ALA:HB3	2.53	0.43
1:B:3496:PHE:HE2	1:B:3555:ALA:HB3	1.83	0.43
1:B:4888:CYS:HB3	1:B:4891:CYS:SG	2.58	0.43
1:C:1829:LEU:HG	1:C:1912:TYR:CE2	2.53	0.43
1:C:1896:MET:HG2	1:C:1896:MET:O	2.18	0.43
1:C:2087:LEU:O	1:C:2091:GLN:HG2	2.18	0.43
1:C:2988:ARG:HD2	1:C:2990:LEU:O	2.19	0.43
1:D:3840:PHE:CE1	1:D:3874:THR:HG23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2224:ASN:O	1:A:2227:VAL:HG23	2.19	0.43
1:A:4888:CYS:HB3	1:A:4891:CYS:SG	2.58	0.43
2:G:25:VAL:HG12	2:G:104:LEU:HA	1.99	0.43
3:I:83:GLU:O	3:I:87:ARG:HG2	2.18	0.43
3:J:17:PHE:CZ	3:J:28:ILE:HG13	2.54	0.43
1:B:3499:LYS:CE	1:B:3564:LYS:NZ	2.81	0.43
1:B:3661:VAL:HG23	1:B:3666:GLN:HG2	2.00	0.43
1:C:931:TYR:HA	1:C:934:GLN:HB2	2.01	0.43
1:C:3109:PHE:O	1:C:3165:ALA:HB2	2.18	0.43
1:D:1896:MET:O	1:D:1896:MET:HG2	2.18	0.43
1:D:3483:PRO:O	1:D:3486:GLN:HB2	2.18	0.43
1:D:3794:ALA:HB2	1:D:3868:VAL:HG11	2.00	0.43
1:A:76:ARG:HH11	1:A:80:GLU:HG3	1.82	0.43
1:A:2082:ARG:HG3	1:A:3687:LEU:HD22	2.01	0.43
1:A:2759:PRO:O	1:A:2762:LEU:N	2.51	0.43
1:A:3763:ILE:HD11	1:A:3838:ASP:O	2.18	0.43
1:A:4584:PHE:O	1:A:4587:ILE:HG22	2.18	0.43
3:K:83:GLU:O	3:K:87:ARG:HG2	2.18	0.43
1:B:3370:TYR:HB3	1:B:3465:LEU:HD12	1.99	0.43
1:B:3545:GLU:HG2	1:B:3546:LYS:N	2.32	0.43
1:C:2255:LEU:O	1:C:3810:ARG:NH1	2.47	0.43
1:C:2716:LYS:HG3	1:C:2717:LEU:HD22	2.00	0.43
1:C:2759:PRO:O	1:C:2762:LEU:N	2.51	0.43
1:D:1051:ARG:HA	1:D:1054:VAL:HG12	2.00	0.43
1:D:2759:PRO:HD3	1:D:2821:TYR:HB2	2.01	0.43
1:D:3109:PHE:O	1:D:3165:ALA:HB2	2.18	0.43
1:D:3496:PHE:HE2	1:D:3555:ALA:HB3	1.83	0.43
1:A:935:MET:O	1:A:939:THR:OG1	2.31	0.43
1:A:2258:ARG:HB3	1:A:2260:PRO:HD2	2.00	0.43
1:A:3483:PRO:O	1:A:3486:GLN:HB2	2.18	0.43
3:I:21:ASP:OD1	3:I:22:LYS:N	2.51	0.43
3:J:83:GLU:O	3:J:87:ARG:HG2	2.18	0.43
1:B:1091:GLU:HB3	1:B:1094:TYR:CD2	2.53	0.43
1:B:2716:LYS:HG3	1:B:2717:LEU:HD22	2.00	0.43
1:B:3035:ILE:O	1:B:3039:THR:HG23	2.19	0.43
1:C:2736:LYS:HD2	1:C:2757:MET:SD	2.59	0.43
1:C:3323:MET:HE1	1:C:3326:LEU:HD22	2.01	0.43
1:C:4162:LYS:HD2	1:C:4203:ALA:HB1	2.01	0.43
1:C:4606:VAL:HA	1:C:4609:LYS:HE2	2.01	0.43
1:D:758:CYS:HB3	1:D:819:TYR:CE2	2.53	0.43
1:D:1091:GLU:HB3	1:D:1094:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1829:LEU:HG	1:D:1912:TYR:CE2	2.53	0.43
1:D:2176:VAL:HG22	1:D:2220:TYR:CZ	2.53	0.43
1:D:2596:VAL:HG21	1:D:2610:LEU:HD11	1.99	0.43
1:D:2884:LYS:O	1:D:2887:GLU:HG3	2.18	0.43
1:D:3470:LEU:HD12	1:D:3471:LYS:HD3	2.01	0.43
1:A:514:PHE:CD2	1:A:526:TRP:HB2	2.54	0.43
1:A:3331:ALA:HA	1:A:3334:VAL:HG22	2.01	0.43
1:A:3496:PHE:CE2	1:A:3555:ALA:HB3	2.53	0.43
1:A:3496:PHE:HE2	1:A:3555:ALA:HB3	1.83	0.43
3:J:61:ASN:OD1	3:J:62:GLY:N	2.49	0.43
3:L:17:PHE:CZ	3:L:28:ILE:HG13	2.54	0.43
1:B:115:TYR:CD1	1:B:175:VAL:HG22	2.53	0.43
1:B:330:THR:HG23	1:B:366:VAL:HG22	2.01	0.43
1:B:514:PHE:CD2	1:B:526:TRP:HB2	2.54	0.43
1:B:3312:PRO:HA	1:B:3376:PHE:HZ	1.82	0.43
1:B:4569:GLU:HB3	1:B:4570:PRO:HD3	2.00	0.43
1:C:514:PHE:CD2	1:C:526:TRP:HB2	2.54	0.43
1:C:1298:ASP:OD1	1:C:1299:ILE:N	2.52	0.43
1:C:2224:ASN:O	1:C:2227:VAL:HG23	2.19	0.43
1:C:3308:ASN:OD1	1:C:3437:SER:CB	2.61	0.43
1:C:4921:PHE:HE2	1:C:4940:VAL:HG11	1.84	0.43
1:D:150:GLN:NE2	1:D:158:CYS:SG	2.72	0.43
1:D:1966:ARG:NH2	1:D:3605:MET:O	2.52	0.43
1:D:2082:ARG:HG3	1:D:3687:LEU:HD22	2.00	0.43
1:D:2911:GLU:HG2	1:D:2912:LEU:HD23	1.99	0.43
1:D:2988:ARG:HD2	1:D:2990:LEU:O	2.19	0.43
1:D:3221:LEU:C	1:D:3223:GLU:H	2.22	0.43
1:D:3426:ASN:HD22	1:D:3426:ASN:HA	1.63	0.43
1:D:3606:ALA:HA	1:D:3607:PRO:HD3	1.86	0.43
1:D:3661:VAL:HG23	1:D:3666:GLN:HG2	2.00	0.43
1:D:4660:PHE:C	1:D:4660:PHE:CD2	2.92	0.43
1:D:4752:THR:HG23	1:D:4753:LEU:HD12	2.00	0.43
1:D:4792:PHE:HB3	1:D:4843:ARG:NH2	2.33	0.43
1:A:3488:LEU:HA	1:A:3491:LEU:HD23	2.01	0.43
1:A:4113:THR:HA	1:A:4116:GLN:HB2	2.01	0.43
1:A:4753:LEU:HD23	1:B:4773:LEU:HD13	2.00	0.43
1:B:766:ILE:HB	1:B:779:PHE:HB2	2.01	0.43
1:B:3109:PHE:O	1:B:3165:ALA:HB2	2.18	0.43
1:B:4113:THR:HA	1:B:4116:GLN:HB2	2.01	0.43
1:C:1091:GLU:HB3	1:C:1094:TYR:HD2	1.84	0.43
1:C:1966:ARG:NH2	1:C:3605:MET:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2422:ILE:HD11	1:D:189:GLU:OE2	2.19	0.43
1:C:3174:HIS:ND1	1:C:3175:LEU:HG	2.33	0.43
1:C:3522:PRO:O	1:C:3525:ARG:HG2	2.19	0.43
1:C:3661:VAL:HG23	1:C:3666:GLN:HG2	2.00	0.43
1:C:4903:HIS:H	1:D:4183:LYS:CD	2.27	0.43
1:D:674:TYR:CD2	1:D:815:PRO:HB3	2.54	0.43
1:D:3545:GLU:HG2	1:D:3546:LYS:N	2.32	0.43
1:A:766:ILE:HB	1:A:779:PHE:HB2	2.01	0.43
1:A:3794:ALA:HB2	1:A:3868:VAL:HG11	2.00	0.43
1:A:4023:LEU:HD12	1:A:4026:LEU:HD23	2.01	0.43
1:A:4660:PHE:C	1:A:4660:PHE:CD2	2.92	0.43
1:A:4752:THR:HG23	1:A:4753:LEU:HD12	2.00	0.43
3:L:83:GLU:O	3:L:87:ARG:HG2	2.18	0.43
1:B:1966:ARG:NH2	1:B:3605:MET:O	2.52	0.43
1:B:2224:ASN:O	1:B:2227:VAL:HG23	2.19	0.43
1:B:3794:ALA:HB2	1:B:3868:VAL:HG11	2.00	0.43
1:B:4555:ILE:HD12	1:B:4555:ILE:HA	1.79	0.43
1:B:4770:THR:HG23	1:B:4862:ILE:HG12	2.00	0.43
1:B:4792:PHE:HB3	1:B:4843:ARG:NH2	2.33	0.43
1:B:4921:PHE:HE2	1:B:4940:VAL:HG11	1.84	0.43
1:C:1559:ARG:HD2	1:C:1565:PRO:HD3	2.00	0.43
1:C:4061:SER:O	1:C:4064:GLU:HG3	2.19	0.43
1:D:995:MET:HE3	1:D:995:MET:HB3	1.87	0.43
1:D:2087:LEU:O	1:D:2091:GLN:HG2	2.18	0.43
1:D:3763:ILE:HD11	1:D:3838:ASP:O	2.18	0.43
1:A:330:THR:HG23	1:A:366:VAL:HG22	2.01	0.42
1:A:3307:ILE:HD12	1:A:3375:ARG:HD3	2.00	0.42
1:A:4606:VAL:HA	1:A:4609:LYS:HE2	2.01	0.42
1:B:3071:THR:HG23	1:B:3094:ILE:HD12	2.01	0.42
1:B:3482:ALA:O	1:B:3486:GLN:HG2	2.19	0.42
1:B:3522:PRO:O	1:B:3525:ARG:HG2	2.19	0.42
1:B:4023:LEU:HD12	1:B:4026:LEU:HD23	2.01	0.42
1:B:4606:VAL:HA	1:B:4609:LYS:HE2	2.01	0.42
1:B:4625:ASP:OD1	1:B:4625:ASP:N	2.43	0.42
1:B:4863:GLN:NE2	1:C:4860:ALA:HB2	2.34	0.42
1:B:4903:HIS:H	1:C:4183:LYS:HD2	1.84	0.42
1:C:3483:PRO:O	1:C:3486:GLN:HB2	2.18	0.42
1:C:4569:GLU:HB3	1:C:4570:PRO:HD3	2.00	0.42
1:C:4770:THR:HG23	1:C:4862:ILE:HG12	2.00	0.42
1:D:76:ARG:HH11	1:D:80:GLU:HG3	1.82	0.42
1:D:766:ILE:HB	1:D:779:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1559:ARG:HD2	1:D:1565:PRO:HD3	2.01	0.42
1:D:3035:ILE:O	1:D:3039:THR:HG23	2.18	0.42
1:A:1943:ARG:O	1:A:1946:GLU:HG2	2.19	0.42
1:A:2988:ARG:HD2	1:A:2990:LEU:O	2.19	0.42
1:A:3035:ILE:O	1:A:3039:THR:HG23	2.19	0.42
1:A:4792:PHE:HB3	1:A:4843:ARG:NH2	2.33	0.42
3:J:77:MET:O	3:J:79:ASP:N	2.47	0.42
3:K:17:PHE:CZ	3:K:28:ILE:HG13	2.54	0.42
1:B:674:TYR:CD2	1:B:815:PRO:HB3	2.54	0.42
1:B:718:VAL:HG23	1:B:793:SER:HB3	2.01	0.42
1:B:739:ARG:HD2	1:B:739:ARG:HA	1.81	0.42
1:B:2193:VAL:HG11	1:B:2227:VAL:HG11	2.00	0.42
1:B:3366:LEU:HG	1:B:3370:TYR:CD1	2.53	0.42
1:C:514:PHE:HD2	1:C:526:TRP:HB2	1.83	0.42
1:C:718:VAL:HG23	1:C:793:SER:HB3	2.01	0.42
1:C:1898:LEU:HD13	1:C:1902:VAL:HG12	2.01	0.42
1:C:2759:PRO:HD3	1:C:2821:TYR:HB2	2.01	0.42
1:C:4555:ILE:HD12	1:C:4555:ILE:HA	1.79	0.42
1:D:2736:LYS:HD2	1:D:2757:MET:SD	2.59	0.42
1:D:3071:THR:HG23	1:D:3094:ILE:HD12	2.02	0.42
1:D:3307:ILE:HD12	1:D:3375:ARG:HD3	2.00	0.42
1:A:938:GLU:O	1:A:942:THR:HG23	2.20	0.42
1:A:1298:ASP:OD1	1:A:1299:ILE:N	2.52	0.42
1:A:1427:TYR:HB2	1:A:1563:VAL:HG11	2.02	0.42
1:A:2641:SER:HB3	1:A:2676:LEU:HD21	2.01	0.42
1:A:4203:ALA:HA	1:A:4206:ILE:HG12	2.00	0.42
1:B:1051:ARG:HA	1:B:1054:VAL:HG12	2.00	0.42
1:B:1559:ARG:HD2	1:B:1565:PRO:HD3	2.00	0.42
1:C:674:TYR:CD2	1:C:815:PRO:HB3	2.54	0.42
1:C:3470:LEU:HD12	1:C:3471:LYS:HD3	2.00	0.42
1:C:4113:THR:HA	1:C:4116:GLN:HB2	2.01	0.42
1:D:2224:ASN:O	1:D:2227:VAL:HG23	2.19	0.42
1:D:2258:ARG:HB3	1:D:2260:PRO:HD2	2.00	0.42
1:D:2872:VAL:HG22	1:D:2873:PRO:HD2	2.02	0.42
1:D:3496:PHE:CE2	1:D:3555:ALA:HB3	2.53	0.42
1:D:3496:PHE:HE2	1:D:3552:LEU:O	2.00	0.42
1:D:4569:GLU:HB3	1:D:4570:PRO:HD3	2.00	0.42
1:D:4888:CYS:HB3	1:D:4891:CYS:SG	2.58	0.42
1:A:931:TYR:HA	1:A:934:GLN:HB2	2.01	0.42
1:A:931:TYR:O	1:A:935:MET:HG2	2.19	0.42
3:K:101:ILE:HD12	3:K:137:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3214:LEU:CD2	1:B:3242:LEU:HD21	2.49	0.42
1:B:3338:ASP:HA	1:B:3341:LYS:HD2	2.01	0.42
1:D:931:TYR:O	1:D:935:MET:HG2	2.19	0.42
1:D:1220:ASP:O	1:D:1223:THR:OG1	2.28	0.42
1:D:3331:ALA:HA	1:D:3334:VAL:HG22	2.01	0.42
1:D:3522:PRO:O	1:D:3525:ARG:HG2	2.19	0.42
1:D:4023:LEU:HD12	1:D:4026:LEU:HD23	2.01	0.42
1:A:897:LYS:HE2	5:A:5005:ATP:HN61	1.79	0.42
1:A:1966:ARG:NH2	1:A:3605:MET:O	2.52	0.42
1:A:3071:THR:HG23	1:A:3094:ILE:HD12	2.01	0.42
1:A:3089:GLY:O	1:A:3093:ILE:HG12	2.20	0.42
1:A:3427:ASN:CB	1:A:3463:THR:OG1	2.42	0.42
1:A:4921:PHE:HE2	1:A:4940:VAL:HG11	1.84	0.42
3:I:101:ILE:HD12	3:I:137:VAL:O	2.19	0.42
3:J:104:ALA:O	3:J:108:HIS:CD2	2.73	0.42
1:B:674:TYR:HE1	1:B:756:SER:HB3	1.84	0.42
1:B:675:TYR:CE1	1:B:790:PRO:HB3	2.55	0.42
1:B:896:ASN:HA	1:B:899:GLU:CD	2.40	0.42
1:B:931:TYR:HA	1:B:934:GLN:HB2	2.01	0.42
1:B:2119:LEU:HD21	1:B:2167:MET:HE1	2.01	0.42
1:B:2486:HIS:O	1:B:2490:VAL:HG22	2.20	0.42
1:B:2736:LYS:HD2	1:B:2757:MET:SD	2.59	0.42
1:B:3280:ILE:HG23	1:B:3299:LEU:HD21	2.02	0.42
1:B:3467:VAL:HB	1:B:3471:LYS:HZ3	1.84	0.42
1:B:3488:LEU:HA	1:B:3491:LEU:HD23	2.01	0.42
1:B:4660:PHE:C	1:B:4660:PHE:CD2	2.92	0.42
1:C:1051:ARG:HA	1:C:1054:VAL:HG12	2.01	0.42
1:C:2486:HIS:O	1:C:2490:VAL:HG22	2.20	0.42
1:C:2641:SER:HB3	1:C:2676:LEU:HD21	2.01	0.42
1:C:3496:PHE:CE2	1:C:3552:LEU:O	2.73	0.42
1:C:3763:ILE:HD11	1:C:3838:ASP:O	2.18	0.42
1:D:1298:ASP:OD1	1:D:1299:ILE:N	2.52	0.42
1:D:1898:LEU:HD13	1:D:1902:VAL:HG12	2.01	0.42
1:D:3214:LEU:CD2	1:D:3242:LEU:HD21	2.49	0.42
1:D:3488:LEU:HA	1:D:3491:LEU:HD23	2.01	0.42
1:A:2716:LYS:HG3	1:A:2717:LEU:HD22	2.00	0.42
1:A:3338:ASP:HA	1:A:3341:LYS:HD2	2.01	0.42
1:A:3496:PHE:CE2	1:A:3552:LEU:O	2.73	0.42
2:H:45:LYS:HE2	2:H:45:LYS:HB2	1.68	0.42
2:H:83:TYR:OH	1:D:1768:PHE:O	2.21	0.42
3:J:20:PHE:O	3:J:22:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1100:ARG:HB3	1:B:1236:TYR:CD1	2.55	0.42
1:B:1427:TYR:HB2	1:B:1563:VAL:HG11	2.02	0.42
1:B:3478:LEU:HD21	1:C:1233:GLN:HB3	2.01	0.42
1:C:330:THR:HG23	1:C:366:VAL:HG22	2.01	0.42
1:C:1100:ARG:HB3	1:C:1236:TYR:CD1	2.55	0.42
1:C:2828:MET:O	1:C:2894:LYS:HD3	2.19	0.42
1:C:3482:ALA:O	1:C:3486:GLN:HG2	2.19	0.42
1:C:4203:ALA:HA	1:C:4206:ILE:HG12	2.00	0.42
1:D:514:PHE:CD2	1:D:526:TRP:HB2	2.54	0.42
1:D:3089:GLY:O	1:D:3093:ILE:HG12	2.20	0.42
1:D:3308:ASN:OD1	1:D:3437:SER:CB	2.61	0.42
1:D:3393:GLU:CD	1:D:3537:ARG:HH22	2.23	0.42
1:D:3496:PHE:CE2	1:D:3552:LEU:O	2.73	0.42
1:D:4162:LYS:HD2	1:D:4203:ALA:HB1	2.00	0.42
1:D:4166:LYS:O	1:D:4170:ARG:HG3	2.20	0.42
1:A:1051:ARG:HA	1:A:1054:VAL:HG12	2.01	0.42
1:A:1897:LYS:HB2	1:A:1897:LYS:HE2	1.81	0.42
1:A:2789:ILE:HD13	1:A:2903:VAL:HB	2.02	0.42
1:A:3214:LEU:CD2	1:A:3242:LEU:HD21	2.49	0.42
1:A:3470:LEU:HD12	1:A:3471:LYS:HD3	2.01	0.42
1:A:3522:PRO:O	1:A:3525:ARG:HG2	2.19	0.42
1:A:4162:LYS:HD2	1:A:4203:ALA:HB1	2.01	0.42
1:B:931:TYR:O	1:B:935:MET:HG2	2.19	0.42
1:B:1785:ASP:N	1:B:1785:ASP:OD1	2.53	0.42
1:B:3324:GLU:HA	1:B:3327:LYS:HZ3	1.84	0.42
1:C:1446:ILE:HG12	1:C:1542:ALA:HB2	2.01	0.42
1:C:2580:LEU:HD23	1:C:2580:LEU:HA	1.81	0.42
1:C:2872:VAL:HG22	1:C:2873:PRO:HD2	2.02	0.42
1:C:3221:LEU:C	1:C:3223:GLU:H	2.22	0.42
1:C:3427:ASN:HD22	1:C:3463:THR:C	2.18	0.42
1:D:675:TYR:CE1	1:D:790:PRO:HB3	2.55	0.42
1:D:1446:ILE:HG12	1:D:1542:ALA:HB2	2.01	0.42
1:D:2119:LEU:HD21	1:D:2167:MET:HE1	2.01	0.42
1:D:4113:THR:HA	1:D:4116:GLN:HB2	2.01	0.42
1:D:4641:PRO:HG2	1:D:4647:LYS:HA	2.01	0.42
1:A:2736:LYS:HD2	1:A:2757:MET:SD	2.59	0.42
1:A:2828:MET:O	1:A:2894:LYS:HD3	2.20	0.42
3:I:77:MET:O	3:I:79:ASP:N	2.47	0.42
3:J:101:ILE:HD12	3:J:137:VAL:O	2.19	0.42
3:K:131:ILE:H	3:K:131:ILE:HG13	1.55	0.42
3:L:20:PHE:O	3:L:22:LYS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3089:GLY:O	1:B:3093:ILE:HG12	2.20	0.42
1:B:3427:ASN:HB2	1:B:3463:THR:HG1	1.77	0.42
1:B:3467:VAL:O	1:B:3470:LEU:HG	2.20	0.42
1:B:3496:PHE:CE2	1:B:3552:LEU:O	2.73	0.42
1:B:3855:GLN:NE2	1:B:3925:GLN:O	2.53	0.42
1:B:4061:SER:O	1:B:4064:GLU:HG3	2.19	0.42
1:B:4203:ALA:HA	1:B:4206:ILE:HG12	2.00	0.42
1:C:938:GLU:O	1:C:942:THR:HG23	2.20	0.42
1:C:3467:VAL:O	1:C:3470:LEU:HG	2.20	0.42
1:C:4166:LYS:O	1:C:4170:ARG:HG3	2.20	0.42
1:D:896:ASN:HA	1:D:899:GLU:CD	2.40	0.42
1:D:1729:MET:HE2	1:D:1930:ASP:HB2	2.02	0.42
1:D:1785:ASP:OD1	1:D:1785:ASP:N	2.53	0.42
1:D:3467:VAL:O	1:D:3470:LEU:HG	2.20	0.42
1:D:4091:ALA:O	1:D:4092:LYS:HB3	2.20	0.42
1:A:674:TYR:CD2	1:A:815:PRO:HB3	2.54	0.42
1:A:718:VAL:HG23	1:A:793:SER:HB3	2.01	0.42
1:A:1091:GLU:HB3	1:A:1094:TYR:HD2	1.84	0.42
1:A:1444:GLY:HA3	1:A:1487:MET:HA	2.02	0.42
1:A:1559:ARG:HD2	1:A:1565:PRO:HD3	2.00	0.42
1:A:3482:ALA:O	1:A:3486:GLN:HG2	2.19	0.42
1:B:1091:GLU:HB3	1:B:1094:TYR:HD2	1.84	0.42
1:B:1298:ASP:OD1	1:B:1299:ILE:N	2.52	0.42
1:B:2222:LEU:HD23	1:B:2222:LEU:HA	1.92	0.42
1:B:2708:THR:HB	1:B:2780:LYS:HB3	2.02	0.42
1:B:2828:MET:O	1:B:2894:LYS:HD3	2.20	0.42
1:B:2988:ARG:HD2	1:B:2990:LEU:O	2.19	0.42
1:B:4641:PRO:HG2	1:B:4647:LYS:HA	2.02	0.42
1:C:931:TYR:O	1:C:935:MET:HG2	2.20	0.42
1:C:3071:THR:HG23	1:C:3094:ILE:HD12	2.01	0.42
1:C:3331:ALA:HA	1:C:3334:VAL:HG22	2.01	0.42
1:C:3596:LYS:HD2	1:C:3597:ARG:NH1	2.35	0.42
1:D:330:THR:HG23	1:D:366:VAL:HG22	2.01	0.42
1:D:938:GLU:O	1:D:942:THR:HG23	2.20	0.42
1:D:1943:ARG:O	1:D:1946:GLU:HG2	2.19	0.42
1:D:1959:ALA:HA	1:D:1962:THR:HG22	2.01	0.42
1:D:2716:LYS:HG3	1:D:2717:LEU:HD22	2.00	0.42
1:D:2759:PRO:O	1:D:2762:LEU:N	2.51	0.42
1:A:674:TYR:HE1	1:A:756:SER:HB3	1.83	0.42
1:A:1100:ARG:HB3	1:A:1236:TYR:CD1	2.55	0.42
1:A:1966:ARG:NE	1:A:3602:CYS:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4091:ALA:O	1:A:4092:LYS:HB3	2.20	0.42
1:A:4092:LYS:HA	1:A:4129:PHE:CE1	2.55	0.42
2:F:90:GLY:HA2	1:B:638:PRO:HD3	2.01	0.42
3:L:93:PHE:HE2	3:L:101:ILE:HG23	1.85	0.42
1:B:1196:ASP:N	1:B:1196:ASP:OD1	2.53	0.42
1:B:2759:PRO:HD3	1:B:2821:TYR:HB2	2.01	0.42
1:B:3331:ALA:HA	1:B:3334:VAL:HG22	2.01	0.42
1:B:3466:ILE:H	1:B:3466:ILE:HD12	1.85	0.42
1:B:4092:LYS:HA	1:B:4129:PHE:CE1	2.55	0.42
1:B:4859:LEU:HD12	1:B:4859:LEU:HA	1.94	0.42
1:C:896:ASN:HA	1:C:899:GLU:CD	2.40	0.42
1:C:1419:PHE:O	1:C:1423:THR:HB	2.20	0.42
1:C:2258:ARG:HB3	1:C:2260:PRO:HD2	2.00	0.42
1:C:2344:LEU:HD22	1:C:2434:GLY:HA3	2.02	0.42
1:C:3495:ARG:NH1	1:C:3500:ASP:OD2	2.53	0.42
1:C:4023:LEU:HD12	1:C:4026:LEU:HD23	2.01	0.42
1:C:4091:ALA:O	1:C:4092:LYS:HB3	2.20	0.42
1:D:1091:GLU:HB3	1:D:1094:TYR:HD2	1.84	0.42
1:D:1419:PHE:O	1:D:1423:THR:HB	2.20	0.42
1:D:1444:GLY:HA3	1:D:1487:MET:HA	2.02	0.42
1:D:2690:GLU:HB2	1:D:2692:GLN:NE2	2.35	0.42
1:D:3022:PHE:CD2	1:D:3029:ILE:HD13	2.53	0.42
1:D:3596:LYS:HD2	1:D:3597:ARG:NH1	2.35	0.42
1:A:489:PHE:CD2	1:A:494:MET:HG3	2.55	0.41
1:A:675:TYR:CE1	1:A:790:PRO:HB3	2.55	0.41
3:I:104:ALA:O	3:I:108:HIS:CD2	2.73	0.41
3:L:101:ILE:HD12	3:L:137:VAL:O	2.19	0.41
3:L:104:ALA:O	3:L:108:HIS:CD2	2.73	0.41
1:B:489:PHE:CD2	1:B:494:MET:HG3	2.55	0.41
1:B:680:ASP:OD2	1:B:801:ARG:NE	2.53	0.41
1:B:1419:PHE:O	1:B:1423:THR:HB	2.20	0.41
1:B:2641:SER:HB3	1:B:2676:LEU:HD21	2.01	0.41
1:B:3215:MET:HA	1:B:3215:MET:CE	2.50	0.41
1:B:3396:PHE:HE1	1:B:3474:LEU:HD23	1.85	0.41
1:C:489:PHE:CD2	1:C:494:MET:HG3	2.55	0.41
1:C:674:TYR:HE1	1:C:756:SER:HB3	1.84	0.41
1:C:766:ILE:HB	1:C:779:PHE:HB2	2.01	0.41
1:C:3378:ASP:OD1	1:C:3379:TYR:N	2.53	0.41
1:C:3466:ILE:H	1:C:3466:ILE:HD12	1.85	0.41
1:D:169:ARG:NE	1:D:179:ASP:OD2	2.39	0.41
1:D:1100:ARG:HB3	1:D:1236:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2486:HIS:O	1:D:2490:VAL:HG22	2.20	0.41
1:D:2828:MET:O	1:D:2894:LYS:HD3	2.19	0.41
1:D:3495:ARG:NH1	1:D:3500:ASP:OD2	2.53	0.41
1:A:1196:ASP:OD1	1:A:1196:ASP:N	2.53	0.41
1:A:2690:GLU:HB2	1:A:2692:GLN:NE2	2.35	0.41
2:G:3:VAL:HG11	2:G:62:GLU:HG3	2.02	0.41
3:I:101:ILE:HD11	3:I:139:TYR:CD1	2.55	0.41
3:I:123:ASP:O	3:I:127:ARG:HD3	2.21	0.41
3:K:20:PHE:O	3:K:22:LYS:HB2	2.20	0.41
3:K:101:ILE:HD11	3:K:139:TYR:CD1	2.55	0.41
3:L:38:ARG:HD2	3:L:43:ASN:HA	2.03	0.41
1:B:1943:ARG:O	1:B:1946:GLU:HG2	2.19	0.41
1:B:2720:PHE:CE1	1:B:2896:LEU:HD23	2.55	0.41
1:B:2757:MET:HE2	1:B:2757:MET:HB2	1.61	0.41
1:B:3606:ALA:HA	1:B:3607:PRO:HD3	1.86	0.41
1:B:3890:TRP:CD2	1:C:76:ARG:HD3	2.55	0.41
1:B:4091:ALA:O	1:B:4092:LYS:HB3	2.20	0.41
1:C:614:LEU:HD22	1:C:632:ILE:HG12	2.02	0.41
1:C:1785:ASP:OD1	1:C:1785:ASP:N	2.53	0.41
1:C:3214:LEU:CD2	1:C:3242:LEU:HD21	2.49	0.41
1:C:4137:GLU:O	1:C:4918:TYR:OH	2.32	0.41
1:C:4191:ASN:OD1	1:C:4608:ARG:NH1	2.52	0.41
1:C:4641:PRO:HG2	1:C:4647:LYS:HA	2.01	0.41
1:D:1972:GLN:O	1:D:1975:MET:HG3	2.21	0.41
1:D:2247:VAL:HG11	1:D:2257:LEU:HD21	2.03	0.41
1:D:3323:MET:HE1	1:D:3326:LEU:HD22	2.02	0.41
1:D:3338:ASP:HA	1:D:3341:LYS:HD2	2.01	0.41
1:D:3482:ALA:O	1:D:3486:GLN:HG2	2.20	0.41
1:A:614:LEU:HD22	1:A:632:ILE:HG12	2.02	0.41
1:A:1768:PHE:O	2:E:83:TYR:OH	2.24	0.41
1:A:2759:PRO:HD3	1:A:2821:TYR:HB2	2.01	0.41
1:A:3297:LYS:HB3	1:A:3297:LYS:HE3	1.34	0.41
1:A:3505:VAL:CG2	1:A:3552:LEU:HD13	2.50	0.41
1:A:4061:SER:O	1:A:4064:GLU:HG3	2.19	0.41
1:A:4191:ASN:OD1	1:A:4608:ARG:NH1	2.52	0.41
1:A:4660:PHE:O	1:A:4660:PHE:HD2	2.04	0.41
3:J:101:ILE:HD11	3:J:139:TYR:CD1	2.55	0.41
3:L:4:GLN:OE1	3:L:4:GLN:N	2.53	0.41
1:B:614:LEU:HD22	1:B:632:ILE:HG12	2.02	0.41
1:B:938:GLU:O	1:B:942:THR:HG23	2.20	0.41
1:B:3221:LEU:C	1:B:3223:GLU:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3296:MET:HE2	1:B:3296:MET:HB2	1.95	0.41
1:B:3378:ASP:OD1	1:B:3379:TYR:N	2.53	0.41
1:B:3495:ARG:NH1	1:B:3500:ASP:OD2	2.53	0.41
1:B:3505:VAL:CG2	1:B:3552:LEU:HD13	2.50	0.41
1:C:675:TYR:CE1	1:C:790:PRO:HB3	2.55	0.41
1:C:3022:PHE:CD2	1:C:3029:ILE:HD13	2.53	0.41
1:D:698:ALA:HB3	1:D:789:PHE:CE1	2.56	0.41
1:D:2332:GLY:O	1:D:2336:ARG:HG3	2.21	0.41
1:D:2344:LEU:HD22	1:D:2434:GLY:HA3	2.02	0.41
1:D:2641:SER:HB3	1:D:2676:LEU:HD21	2.01	0.41
1:D:2724:TYR:HB3	1:D:2775:ILE:HD13	2.02	0.41
1:D:3378:ASP:OD1	1:D:3379:TYR:N	2.53	0.41
1:D:4921:PHE:HE2	1:D:4940:VAL:HG11	1.84	0.41
1:A:612:ASP:OD1	1:A:1656:HIS:ND1	2.54	0.41
1:A:1898:LEU:HD13	1:A:1902:VAL:HG12	2.01	0.41
1:A:2119:LEU:HD21	1:A:2167:MET:HE1	2.01	0.41
1:A:2235:ARG:HG2	1:A:2297:ARG:NH1	2.31	0.41
1:A:2332:GLY:O	1:A:2336:ARG:HG3	2.20	0.41
1:A:2872:VAL:HG22	1:A:2873:PRO:HD2	2.02	0.41
1:A:2917:ILE:HD11	1:A:2999:LYS:HB3	2.03	0.41
1:A:3215:MET:HA	1:A:3215:MET:CE	2.51	0.41
1:A:3378:ASP:OD1	1:A:3379:TYR:N	2.53	0.41
1:A:3596:LYS:HD2	1:A:3597:ARG:NH1	2.35	0.41
1:A:3975:GLN:O	1:A:3979:VAL:HG23	2.20	0.41
2:G:43:ARG:HA	1:C:1682:GLU:OE2	2.20	0.41
3:I:93:PHE:HE2	3:I:101:ILE:HG23	1.85	0.41
3:K:123:ASP:O	3:K:127:ARG:HD3	2.21	0.41
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.92	0.41
1:B:1898:LEU:HD13	1:B:1902:VAL:HG12	2.01	0.41
1:B:2872:VAL:HG22	1:B:2873:PRO:HD2	2.02	0.41
1:B:3470:LEU:HD12	1:B:3471:LYS:HD3	2.01	0.41
1:C:1444:GLY:HA3	1:C:1487:MET:HA	2.02	0.41
1:C:1959:ALA:HA	1:C:1962:THR:HG22	2.01	0.41
1:C:1972:GLN:O	1:C:1975:MET:HG3	2.21	0.41
1:C:2119:LEU:HD21	1:C:2167:MET:HE1	2.01	0.41
1:C:2708:THR:HB	1:C:2780:LYS:HB3	2.03	0.41
1:C:3215:MET:CE	1:C:3215:MET:HA	2.51	0.41
1:C:3280:ILE:HG23	1:C:3299:LEU:HD21	2.02	0.41
1:C:3338:ASP:HA	1:C:3341:LYS:HD2	2.01	0.41
1:C:3396:PHE:HE1	1:C:3474:LEU:HD23	1.86	0.41
1:C:3855:GLN:NE2	1:C:3925:GLN:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:SER:HA	1:D:555:LEU:HD13	2.02	0.41
1:A:713:TRP:CZ2	1:A:1251:LEU:HD21	2.55	0.41
1:A:896:ASN:HA	1:A:899:GLU:CD	2.40	0.41
1:A:1959:ALA:HA	1:A:1962:THR:HG22	2.01	0.41
1:A:2486:HIS:O	1:A:2490:VAL:HG22	2.20	0.41
1:A:2720:PHE:CE1	1:A:2896:LEU:HD23	2.56	0.41
2:H:3:VAL:HG11	2:H:62:GLU:HG3	2.02	0.41
3:I:38:ARG:HD2	3:I:43:ASN:HA	2.02	0.41
1:B:1929:SER:HG	1:B:3620:PHE:HD2	1.68	0.41
1:B:2789:ILE:HD13	1:B:2903:VAL:HB	2.02	0.41
1:B:2856:LYS:HD3	1:B:2859:GLU:OE2	2.21	0.41
1:B:4166:LYS:O	1:B:4170:ARG:HG3	2.20	0.41
1:C:680:ASP:OD2	1:C:801:ARG:NE	2.53	0.41
1:C:1943:ARG:O	1:C:1946:GLU:HG2	2.19	0.41
1:C:2332:GLY:O	1:C:2336:ARG:HG3	2.20	0.41
1:C:3488:LEU:HA	1:C:3491:LEU:HD23	2.01	0.41
1:D:612:ASP:OD1	1:D:1656:HIS:ND1	2.54	0.41
1:D:1427:TYR:HB2	1:D:1563:VAL:HG11	2.02	0.41
1:D:4660:PHE:O	1:D:4660:PHE:HD2	2.03	0.41
1:A:162:ILE:O	1:A:163:HIS:ND1	2.54	0.41
1:A:2934:ASP:O	1:A:2938:GLN:HG2	2.21	0.41
2:F:3:VAL:HG11	2:F:62:GLU:HG3	2.03	0.41
3:K:4:GLN:OE1	3:K:4:GLN:N	2.53	0.41
1:B:1972:GLN:O	1:B:1975:MET:HG3	2.21	0.41
1:B:2697:SER:O	1:B:2699:GLY:N	2.48	0.41
1:B:2893:LEU:HD13	1:B:2896:LEU:HD12	2.03	0.41
1:B:3596:LYS:HD2	1:B:3597:ARG:NH1	2.35	0.41
1:C:612:ASP:OD1	1:C:1656:HIS:ND1	2.54	0.41
1:C:1711:LEU:HB3	1:C:1831:MET:SD	2.61	0.41
1:C:2247:VAL:HG11	1:C:2257:LEU:HD21	2.03	0.41
1:C:2856:LYS:HD3	1:C:2859:GLU:OE2	2.21	0.41
1:C:3393:GLU:CD	1:C:3537:ARG:HH22	2.23	0.41
1:C:4107:GLU:OE1	1:C:4149:TYR:OH	2.23	0.41
1:D:614:LEU:HD22	1:D:632:ILE:HG12	2.02	0.41
1:D:674:TYR:HE1	1:D:756:SER:HB3	1.83	0.41
1:D:1196:ASP:OD1	1:D:1196:ASP:N	2.53	0.41
1:D:2154:VAL:HG13	1:D:2158:HIS:CD2	2.56	0.41
1:D:4509:VAL:CG1	1:D:4579:HIS:HB2	2.51	0.41
1:D:4721:TYR:OH	1:D:4745:ASP:OD1	2.31	0.41
1:A:252:HIS:C	1:A:257:ARG:HH12	2.24	0.41
1:A:967:PRO:HB2	1:A:969:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1785:ASP:OD1	1:A:1785:ASP:N	2.53	0.41
1:A:2261:ASP:O	1:A:2265:VAL:HG23	2.21	0.41
1:A:2708:THR:HB	1:A:2780:LYS:HB3	2.03	0.41
1:A:3280:ILE:HG23	1:A:3299:LEU:HD21	2.02	0.41
1:A:3488:LEU:HA	1:A:3491:LEU:CD2	2.51	0.41
1:A:4166:LYS:O	1:A:4170:ARG:HG3	2.20	0.41
1:A:4509:VAL:CG1	1:A:4579:HIS:HB2	2.51	0.41
2:E:3:VAL:HG11	2:E:62:GLU:HG3	2.03	0.41
3:J:1:MET:O	3:J:1:MET:SD	2.79	0.41
3:J:4:GLN:OE1	3:J:4:GLN:N	2.53	0.41
3:K:93:PHE:HE2	3:K:101:ILE:HG23	1.85	0.41
1:B:612:ASP:OD1	1:B:1656:HIS:ND1	2.54	0.41
1:B:2247:VAL:HG11	1:B:2257:LEU:HD21	2.03	0.41
1:C:2760:TYR:CE1	1:C:2768:LYS:HG2	2.56	0.41
1:C:3975:GLN:O	1:C:3979:VAL:HG23	2.21	0.41
1:C:4092:LYS:HA	1:C:4129:PHE:CE1	2.55	0.41
1:C:4172:PHE:CZ	1:C:4189:PHE:HA	2.56	0.41
1:D:3397:ARG:NH2	1:D:3550:ARG:HD2	2.24	0.41
1:A:1929:SER:HG	1:A:3620:PHE:HD2	1.67	0.41
1:A:2241:ASP:OD2	1:A:2297:ARG:NH2	2.54	0.41
1:A:2247:VAL:HG11	1:A:2257:LEU:HD21	2.03	0.41
1:A:2255:LEU:O	1:A:3810:ARG:NH1	2.47	0.41
1:A:3152:ARG:HA	1:A:3155:LEU:HD12	2.03	0.41
1:A:3396:PHE:HE1	1:A:3474:LEU:HD23	1.86	0.41
1:A:3466:ILE:H	1:A:3466:ILE:HD12	1.85	0.41
1:A:3495:ARG:NH1	1:A:3500:ASP:OD2	2.53	0.41
3:L:1:MET:SD	3:L:1:MET:O	2.79	0.41
1:B:1446:ILE:HG12	1:B:1542:ALA:HB2	2.01	0.41
1:B:1711:LEU:HB3	1:B:1831:MET:SD	2.61	0.41
1:B:2241:ASP:OD2	1:B:2297:ARG:NH2	2.54	0.41
1:B:3312:PRO:HA	1:B:3376:PHE:CZ	2.56	0.41
1:B:3393:GLU:CD	1:B:3537:ARG:HH22	2.23	0.41
1:B:3890:TRP:CE3	1:C:76:ARG:HD3	2.55	0.41
1:B:4753:LEU:CD1	1:C:4769:LEU:HB3	2.50	0.41
1:C:1914:CYS:SG	1:C:2091:GLN:NE2	2.78	0.41
1:C:2488:LEU:HD11	1:C:2548:LEU:HD13	2.03	0.41
1:C:2893:LEU:HD13	1:C:2896:LEU:HD12	2.03	0.41
1:C:4660:PHE:C	1:C:4660:PHE:CD2	2.92	0.41
1:D:162:ILE:O	1:D:163:HIS:ND1	2.54	0.41
1:D:252:HIS:C	1:D:257:ARG:HH12	2.24	0.41
1:D:661:LEU:HD13	1:D:673:TRP:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1711:LEU:HB3	1:D:1831:MET:SD	2.61	0.41
1:D:2488:LEU:HD11	1:D:2548:LEU:HD13	2.03	0.41
1:D:2917:ILE:HD11	1:D:2999:LYS:HB3	2.03	0.41
1:D:2984:SER:O	1:D:3001:LYS:NZ	2.32	0.41
1:D:3499:LYS:CE	1:D:3564:LYS:NZ	2.81	0.41
1:D:3505:VAL:CG2	1:D:3552:LEU:HD13	2.50	0.41
1:A:229:ILE:HG22	1:A:288:HIS:CD2	2.56	0.41
1:A:552:SER:HA	1:A:555:LEU:HD13	2.02	0.41
1:A:661:LEU:HD13	1:A:673:TRP:CD1	2.56	0.41
1:A:680:ASP:OD2	1:A:801:ARG:NE	2.53	0.41
1:A:698:ALA:HB3	1:A:789:PHE:CE1	2.56	0.41
1:A:739:ARG:HD2	1:A:739:ARG:HA	1.81	0.41
1:A:1972:GLN:O	1:A:1975:MET:HG3	2.21	0.41
1:A:2154:VAL:HG13	1:A:2158:HIS:CD2	2.56	0.41
1:A:2724:TYR:HB3	1:A:2775:ILE:HD13	2.02	0.41
1:A:2760:TYR:CE1	1:A:2768:LYS:HG2	2.56	0.41
1:A:3221:LEU:C	1:A:3223:GLU:H	2.22	0.41
1:A:3323:MET:HE1	1:A:3326:LEU:HD22	2.02	0.41
1:A:3393:GLU:CD	1:A:3537:ARG:HH22	2.23	0.41
1:A:3467:VAL:O	1:A:3470:LEU:HG	2.20	0.41
1:A:3855:GLN:NE2	1:A:3925:GLN:O	2.53	0.41
3:K:104:ALA:O	3:K:108:HIS:CD2	2.73	0.41
3:L:6:THR:HG1	3:L:9:GLN:CD	2.17	0.41
3:L:101:ILE:HD11	3:L:139:TYR:CD1	2.55	0.41
3:L:123:ASP:O	3:L:127:ARG:HD3	2.21	0.41
1:B:252:HIS:C	1:B:257:ARG:HH12	2.24	0.41
1:B:698:ALA:HB3	1:B:789:PHE:CE1	2.56	0.41
1:B:713:TRP:CZ2	1:B:1251:LEU:HD21	2.55	0.41
1:B:1267:HIS:HB3	1:B:1287:GLN:NE2	2.36	0.41
1:B:1444:GLY:HA3	1:B:1487:MET:HA	2.02	0.41
1:B:1914:CYS:SG	1:B:2091:GLN:NE2	2.78	0.41
1:B:2645:PHE:HB2	1:B:2672:VAL:HG11	2.03	0.41
1:B:2934:ASP:O	1:B:2938:GLN:HG2	2.21	0.41
1:B:3152:ARG:HA	1:B:3155:LEU:HD12	2.03	0.41
1:B:3427:ASN:HD22	1:B:3463:THR:C	2.18	0.41
1:B:3488:LEU:HA	1:B:3491:LEU:CD2	2.51	0.41
1:B:3493:LYS:HZ3	1:B:3558:LEU:HB3	1.84	0.41
1:B:3534:LEU:HA	1:B:3535:PRO:HD3	1.97	0.41
1:C:147:VAL:HG21	1:C:192:LEU:HD23	2.03	0.41
1:C:229:ILE:HG22	1:C:288:HIS:CD2	2.56	0.41
1:C:252:HIS:C	1:C:257:ARG:HH12	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:698:ALA:HB3	1:C:789:PHE:CE1	2.56	0.41
1:C:1196:ASP:N	1:C:1196:ASP:OD1	2.53	0.41
1:C:1267:HIS:HB3	1:C:1287:GLN:NE2	2.36	0.41
1:C:1427:TYR:HB2	1:C:1563:VAL:HG11	2.02	0.41
1:C:2261:ASP:O	1:C:2265:VAL:HG23	2.21	0.41
1:C:2720:PHE:CE1	1:C:2896:LEU:HD23	2.55	0.41
1:C:2789:ILE:HD13	1:C:2903:VAL:HB	2.02	0.41
1:C:2930:ILE:HD12	1:C:3003:MET:HE2	2.02	0.41
1:C:3089:GLY:O	1:C:3093:ILE:HG12	2.20	0.41
1:D:21:VAL:HG23	1:D:215:ALA:HB3	2.03	0.41
1:D:111:ARG:HA	1:D:111:ARG:HD3	1.69	0.41
1:D:147:VAL:HG21	1:D:192:LEU:HD23	2.03	0.41
1:D:192:LEU:O	1:D:210:THR:HG22	2.21	0.41
1:D:489:PHE:CD2	1:D:494:MET:HG3	2.55	0.41
1:D:648:LEU:HD23	1:D:648:LEU:HA	1.94	0.41
1:D:718:VAL:HG23	1:D:793:SER:HB3	2.01	0.41
1:D:1267:HIS:HB3	1:D:1287:GLN:NE2	2.36	0.41
1:D:1843:LEU:HD23	1:D:1843:LEU:HA	1.95	0.41
1:D:2708:THR:HB	1:D:2780:LYS:HB3	2.02	0.41
1:D:2720:PHE:CE1	1:D:2896:LEU:HD23	2.56	0.41
1:D:2856:LYS:HD3	1:D:2859:GLU:OE2	2.21	0.41
1:D:3102:LEU:HB2	1:D:3103:PRO:HD3	2.03	0.41
1:D:3159:LEU:HD12	1:D:3159:LEU:HA	1.95	0.41
1:D:3396:PHE:HE1	1:D:3474:LEU:HD23	1.85	0.41
1:D:3488:LEU:HA	1:D:3491:LEU:CD2	2.51	0.41
1:D:4061:SER:O	1:D:4064:GLU:HG3	2.19	0.41
1:A:1419:PHE:O	1:A:1423:THR:HB	2.20	0.41
1:A:1728:PRO:HD3	1:A:1757:LEU:HG	2.03	0.41
1:A:3102:LEU:HB2	1:A:3103:PRO:HD3	2.03	0.41
1:A:3398:MET:O	1:A:3402:VAL:HG23	2.21	0.41
1:A:4649:VAL:HA	1:A:4652:LYS:HG2	2.03	0.41
3:I:45:THR:N	3:I:48:GLU:HB2	2.36	0.41
3:J:45:THR:N	3:J:48:GLU:HB2	2.36	0.41
3:K:45:THR:N	3:K:48:GLU:HB2	2.36	0.41
1:B:150:GLN:NE2	1:B:158:CYS:SG	2.72	0.41
1:B:808:HIS:CG	1:B:832:LEU:HD23	2.56	0.41
1:B:877:HIS:O	1:B:880:ARG:HD3	2.21	0.41
1:B:2261:ASP:O	1:B:2265:VAL:HG23	2.21	0.41
1:B:2655:LYS:O	1:B:2958:GLN:NE2	2.54	0.41
1:B:2724:TYR:HB3	1:B:2775:ILE:HD13	2.02	0.41
1:C:192:LEU:O	1:C:210:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3333:VAL:HA	1:C:3336:GLU:CD	2.42	0.41
1:D:877:HIS:O	1:D:880:ARG:HD3	2.21	0.41
1:D:1728:PRO:HD3	1:D:1757:LEU:HG	2.03	0.41
1:D:2255:LEU:O	1:D:3810:ARG:NH1	2.47	0.41
1:D:2261:ASP:O	1:D:2265:VAL:HG23	2.21	0.41
1:D:2760:TYR:CE1	1:D:2768:LYS:HG2	2.56	0.41
1:D:3427:ASN:HD22	1:D:3463:THR:C	2.18	0.41
1:D:4092:LYS:HA	1:D:4129:PHE:CE1	2.55	0.41
1:D:4832:GLU:HG2	1:D:4833:ASP:H	1.86	0.41
1:A:192:LEU:O	1:A:210:THR:HG22	2.21	0.40
1:A:808:HIS:CG	1:A:832:LEU:HD23	2.56	0.40
1:A:2419:ILE:HA	1:A:2422:ILE:HD12	2.03	0.40
1:A:2837:LEU:HD22	1:A:2897:GLN:NE2	2.37	0.40
1:A:3493:LYS:HZ2	1:A:3558:LEU:CD1	2.34	0.40
1:A:4641:PRO:HG2	1:A:4647:LYS:HA	2.01	0.40
2:G:88:HIS:CD2	2:G:89:PRO:HD2	2.56	0.40
3:I:20:PHE:O	3:I:22:LYS:HB2	2.20	0.40
3:I:141:GLU:HA	3:I:144:GLN:NE2	2.36	0.40
3:L:22:LYS:HA	3:L:22:LYS:HD2	1.81	0.40
1:B:349:MET:CE	1:B:349:MET:HA	2.51	0.40
1:B:552:SER:HA	1:B:555:LEU:HD13	2.02	0.40
1:B:1959:ALA:HA	1:B:1962:THR:HG22	2.01	0.40
1:B:2332:GLY:O	1:B:2336:ARG:HG3	2.21	0.40
1:B:2930:ILE:HD12	1:B:3003:MET:HE2	2.03	0.40
1:B:3102:LEU:HB2	1:B:3103:PRO:HD3	2.03	0.40
1:B:3333:VAL:HA	1:B:3336:GLU:CD	2.41	0.40
1:B:4191:ASN:OD1	1:B:4608:ARG:NH1	2.52	0.40
1:B:4660:PHE:O	1:B:4660:PHE:HD2	2.04	0.40
1:C:21:VAL:HG23	1:C:215:ALA:HB3	2.03	0.40
1:C:967:PRO:HB2	1:C:969:ASN:OD1	2.21	0.40
1:C:2826:ILE:HD12	1:D:1501:ASN:ND2	2.35	0.40
1:C:3152:ARG:HA	1:C:3155:LEU:HD12	2.03	0.40
1:C:3315:LEU:HA	1:C:3319:PHE:HB2	2.04	0.40
1:C:3423:ASN:O	1:C:3425:ILE:CD1	2.46	0.40
1:C:3478:LEU:HD21	1:D:1233:GLN:CB	2.46	0.40
1:C:4509:VAL:CG1	1:C:4579:HIS:HB2	2.51	0.40
1:C:4678:ASP:OD1	1:C:4678:ASP:N	2.55	0.40
1:D:310:GLU:OE1	1:D:310:GLU:N	2.31	0.40
1:D:897:LYS:HE2	5:D:5005:ATP:HN61	1.79	0.40
1:D:2241:ASP:OD2	1:D:2297:ARG:NH2	2.54	0.40
1:D:3215:MET:HA	1:D:3215:MET:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4650:LYS:HG2	1:D:4670:LEU:HD22	2.03	0.40
1:A:23:GLN:HG2	1:A:36:CYS:SG	2.61	0.40
1:A:147:VAL:HG21	1:A:192:LEU:HD23	2.03	0.40
1:A:2763:LEU:O	1:A:2768:LYS:HE2	2.22	0.40
1:A:4176:VAL:HA	1:A:4180:GLY:HA3	2.03	0.40
2:E:88:HIS:CD2	2:E:89:PRO:HD2	2.56	0.40
3:I:1:MET:O	3:I:1:MET:SD	2.79	0.40
3:J:123:ASP:O	3:J:127:ARG:HD3	2.21	0.40
3:L:45:THR:N	3:L:48:GLU:HB2	2.36	0.40
1:B:23:GLN:HG2	1:B:36:CYS:SG	2.61	0.40
1:B:3975:GLN:O	1:B:3979:VAL:HG23	2.21	0.40
1:B:4172:PHE:CZ	1:B:4189:PHE:HA	2.56	0.40
1:C:552:SER:HA	1:C:555:LEU:HD13	2.02	0.40
1:C:2426:LEU:HG	1:D:143:LEU:HD13	2.03	0.40
1:C:2724:TYR:HB3	1:C:2775:ILE:HD13	2.02	0.40
1:C:2917:ILE:HD11	1:C:2999:LYS:HB3	2.03	0.40
1:C:2934:ASP:O	1:C:2938:GLN:HG2	2.21	0.40
1:D:967:PRO:HB2	1:D:969:ASN:OD1	2.21	0.40
1:D:3152:ARG:HA	1:D:3155:LEU:HD12	2.03	0.40
1:D:3505:VAL:HG23	1:D:3552:LEU:CD1	2.52	0.40
1:D:4172:PHE:CZ	1:D:4189:PHE:HA	2.56	0.40
1:A:911:ASN:OD1	1:A:912:LYS:N	2.55	0.40
1:A:992:GLN:O	1:A:996:VAL:HG23	2.22	0.40
1:A:2645:PHE:HB2	1:A:2672:VAL:HG11	2.03	0.40
1:A:2893:LEU:HD13	1:A:2896:LEU:HD12	2.03	0.40
1:A:3122:ILE:O	1:A:3123:LEU:HD22	2.22	0.40
1:A:4832:GLU:HG2	1:A:4833:ASP:H	1.86	0.40
1:B:229:ILE:HG22	1:B:288:HIS:CD2	2.56	0.40
1:B:967:PRO:HB2	1:B:969:ASN:OD1	2.21	0.40
1:B:2904:SER:HB2	1:B:2908:LYS:HZ3	1.87	0.40
1:B:3315:LEU:HA	1:B:3319:PHE:HB2	2.04	0.40
1:B:3505:VAL:HG23	1:B:3552:LEU:CD1	2.51	0.40
1:B:4509:VAL:CG1	1:B:4579:HIS:HB2	2.51	0.40
1:B:4832:GLU:HG2	1:B:4833:ASP:H	1.86	0.40
1:C:111:ARG:HD3	1:C:111:ARG:HA	1.69	0.40
1:C:2407:HIS:CE1	1:C:2408:LEU:HG	2.56	0.40
1:C:2763:LEU:O	1:C:2768:LYS:HE2	2.22	0.40
1:C:2837:LEU:HD22	1:C:2897:GLN:NE2	2.36	0.40
1:C:3312:PRO:HA	1:C:3376:PHE:CZ	2.56	0.40
1:C:3505:VAL:CG2	1:C:3552:LEU:HD13	2.50	0.40
1:C:4650:LYS:HG2	1:C:4670:LEU:HD22	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2655:LYS:O	1:D:2958:GLN:NE2	2.54	0.40
1:D:2893:LEU:HD13	1:D:2896:LEU:HD12	2.03	0.40
1:D:3329:LYS:O	1:D:3333:VAL:HG23	2.21	0.40
1:D:4649:VAL:HA	1:D:4652:LYS:HG2	2.03	0.40
1:A:1446:ILE:HG12	1:A:1542:ALA:HB2	2.01	0.40
1:A:3505:VAL:HG23	1:A:3552:LEU:CD1	2.52	0.40
1:A:4172:PHE:CZ	1:A:4189:PHE:HA	2.56	0.40
1:A:4678:ASP:OD1	1:A:4678:ASP:N	2.55	0.40
3:J:38:ARG:HD2	3:J:43:ASN:HA	2.02	0.40
3:J:93:PHE:HE2	3:J:101:ILE:HG23	1.85	0.40
3:L:67:PRO:HB2	1:D:2202:TYR:CZ	2.57	0.40
3:L:121:GLU:HG2	3:L:122:VAL:H	1.87	0.40
1:B:1792:ILE:HD11	1:B:1838:ASP:HB3	2.04	0.40
1:B:1897:LYS:HB2	1:B:1897:LYS:HE2	1.80	0.40
1:B:2760:TYR:CE1	1:B:2768:LYS:HG2	2.56	0.40
1:B:4600:PHE:HB2	1:B:4643:ASN:HB3	2.04	0.40
1:B:4650:LYS:HG2	1:B:4670:LEU:HD22	2.03	0.40
1:C:495:ILE:H	1:C:495:ILE:HD12	1.87	0.40
1:C:969:ASN:OD1	1:C:970:TYR:N	2.55	0.40
1:C:1220:ASP:O	1:C:1223:THR:OG1	2.28	0.40
1:C:1415:ASP:OD1	1:C:1415:ASP:N	2.55	0.40
1:C:3102:LEU:HB2	1:C:3103:PRO:HD3	2.03	0.40
1:C:3122:ILE:O	1:C:3123:LEU:HD22	2.22	0.40
1:C:3505:VAL:HG23	1:C:3552:LEU:CD1	2.52	0.40
1:D:349:MET:HA	1:D:349:MET:CE	2.51	0.40
1:D:765:SER:HA	1:D:779:PHE:O	2.21	0.40
1:D:1139:GLY:HA3	1:D:1156:TRP:CE3	2.56	0.40
1:D:1792:ILE:HD11	1:D:1838:ASP:HB3	2.04	0.40
1:D:2407:HIS:CE1	1:D:2408:LEU:HG	2.56	0.40
1:D:2487:LEU:HA	1:D:2490:VAL:HG22	2.04	0.40
1:D:2757:MET:HE2	1:D:2757:MET:HB2	1.62	0.40
1:D:2837:LEU:HD22	1:D:2897:GLN:NE2	2.36	0.40
1:D:3280:ILE:HG23	1:D:3299:LEU:HD21	2.02	0.40
1:D:3509:ILE:CD1	1:D:3552:LEU:CD2	2.95	0.40
1:A:638:PRO:HD3	2:E:90:GLY:HA2	2.04	0.40
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.94	0.40
1:A:1711:LEU:HB3	1:A:1831:MET:SD	2.61	0.40
1:A:2635:GLU:OE2	1:A:2680:TYR:OH	2.35	0.40
1:A:2856:LYS:HD3	1:A:2859:GLU:OE2	2.21	0.40
1:A:4847:ASP:OD2	1:D:4818:TYR:OH	2.29	0.40
3:K:1:MET:O	3:K:1:MET:SD	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:141:GLU:HA	3:L:144:GLN:NE2	2.36	0.40
1:B:992:GLN:O	1:B:996:VAL:HG23	2.22	0.40
1:B:1988:CYS:HA	1:B:1989:PRO:HD3	1.97	0.40
1:B:2419:ILE:HA	1:B:2422:ILE:HD12	2.03	0.40
1:B:3320:LEU:CD2	1:B:3321:PRO:HD3	2.51	0.40
1:B:3366:LEU:HG	1:B:3370:TYR:CE1	2.57	0.40
1:B:4176:VAL:HA	1:B:4180:GLY:HA3	2.03	0.40
1:C:877:HIS:O	1:C:880:ARG:HD3	2.21	0.40
1:C:1139:GLY:HA3	1:C:1156:TRP:CE3	2.56	0.40
1:C:1792:ILE:HD11	1:C:1838:ASP:HB3	2.04	0.40
1:C:2241:ASP:OD2	1:C:2297:ARG:NH2	2.54	0.40
1:C:2487:LEU:HA	1:C:2490:VAL:HG22	2.04	0.40
1:C:2496:LEU:HD23	1:C:2520:LEU:HD13	2.03	0.40
1:C:2655:LYS:O	1:C:2958:GLN:NE2	2.55	0.40
1:D:739:ARG:HA	1:D:739:ARG:HD2	1.81	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	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	51	80
1	B	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	51	80
1	C	4343/4967 (87%)	4192 (96%)	147 (3%)	4 (0%)	51	80
1	D	4343/4967 (87%)	4191 (96%)	148 (3%)	4 (0%)	51	80
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
3	J	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
3	K	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
3	L	136/149 (91%)	124 (91%)	12 (9%)	0	100	100
All	All	18336/20896 (88%)	17666 (96%)	654 (4%)	16 (0%)	54	80

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1495	SER
1	A	2358	SER
1	B	1495	SER
1	B	2358	SER
1	C	1495	SER
1	C	2358	SER
1	D	1495	SER
1	D	2358	SER
1	A	1955	ALA
1	B	1955	ALA
1	C	1955	ALA
1	D	1955	ALA
1	A	313	ASN
1	B	313	ASN
1	C	313	ASN
1	D	313	ASN

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	3836/4358 (88%)	3792 (99%)	44 (1%)	73	90
1	B	3836/4358 (88%)	3792 (99%)	44 (1%)	73	90
1	C	3836/4358 (88%)	3792 (99%)	44 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	3836/4358 (88%)	3792 (99%)	44 (1%)	73 90
2	E	88/89 (99%)	85 (97%)	3 (3%)	37 68
2	F	88/89 (99%)	85 (97%)	3 (3%)	37 68
2	G	88/89 (99%)	85 (97%)	3 (3%)	37 68
2	H	88/89 (99%)	85 (97%)	3 (3%)	37 68
3	I	119/127 (94%)	108 (91%)	11 (9%)	9 26
3	J	119/127 (94%)	108 (91%)	11 (9%)	9 26
3	K	119/127 (94%)	108 (91%)	11 (9%)	9 26
3	L	119/127 (94%)	108 (91%)	11 (9%)	9 26
All	All	16172/18296 (88%)	15940 (99%)	232 (1%)	68 86

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ARG
1	A	309	MET
1	A	343	ARG
1	A	349	MET
1	A	778	MET
1	A	880	ARG
1	A	912	LYS
1	A	995	MET
1	A	1022	GLN
1	A	1044	LYS
1	A	1494	MET
1	A	1975	MET
1	A	2054	LYS
1	A	2172	MET
1	A	2737	LEU
1	A	2757	MET
1	A	2760	TYR
1	A	2761	LYS
1	A	2838[A]	HIS
1	A	2838[B]	HIS
1	A	2847	ASN
1	A	2884	LYS
1	A	3018	ARG
1	A	3047	LYS
1	A	3150	ARG

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Mol	Chain	Res	Type
1	A	3190	ARG
1	A	3215	MET
1	A	3221	LEU
1	A	3231	MET
1	A	3235	MET
1	A	3281	LEU
1	A	3296	MET
1	A	3297	LYS
1	A	3381	ARG
1	A	3398	MET
1	A	3422	GLN
1	A	3461	MET
1	A	3719	MET
1	A	4660	PHE
1	A	4672	MET
1	A	4690	LYS
1	A	4925	LEU
1	A	4942	LYS
1	A	4951	PHE
2	E	4	GLU
2	E	50	ARG
2	E	86	THR
2	F	4	GLU
2	F	50	ARG
2	F	86	THR
2	G	4	GLU
2	G	50	ARG
2	G	86	THR
2	H	4	GLU
2	H	50	ARG
2	H	86	THR
3	I	15	GLU
3	I	22	LYS
3	I	75	ARG
3	I	76	LYS
3	I	77	MET
3	I	86	ILE
3	I	110	MET
3	I	118	THR
3	I	131	ILE
3	I	145	MET
3	I	146	MET

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Mol	Chain	Res	Type
3	J	15	GLU
3	J	22	LYS
3	J	75	ARG
3	J	76	LYS
3	J	77	MET
3	J	86	ILE
3	J	110	MET
3	J	118	THR
3	J	131	ILE
3	J	145	MET
3	J	146	MET
3	K	15	GLU
3	K	22	LYS
3	K	75	ARG
3	K	76	LYS
3	K	77	MET
3	K	86	ILE
3	K	110	MET
3	K	118	THR
3	K	131	ILE
3	K	145	MET
3	K	146	MET
3	L	15	GLU
3	L	22	LYS
3	L	75	ARG
3	L	76	LYS
3	L	77	MET
3	L	86	ILE
3	L	110	MET
3	L	118	THR
3	L	131	ILE
3	L	145	MET
3	L	146	MET
1	B	111	ARG
1	B	309	MET
1	B	343	ARG
1	B	349	MET
1	B	778	MET
1	B	880	ARG
1	B	912	LYS
1	B	995	MET
1	B	1022	GLN

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Mol	Chain	Res	Type
1	B	1044	LYS
1	B	1494	MET
1	B	1975	MET
1	B	2054	LYS
1	B	2172	MET
1	B	2737	LEU
1	B	2757	MET
1	B	2760	TYR
1	B	2761	LYS
1	B	2838[A]	HIS
1	B	2838[B]	HIS
1	B	2847	ASN
1	B	2884	LYS
1	B	3018	ARG
1	B	3047	LYS
1	B	3150	ARG
1	B	3190	ARG
1	B	3215	MET
1	B	3221	LEU
1	B	3231	MET
1	B	3235	MET
1	B	3281	LEU
1	B	3296	MET
1	B	3297	LYS
1	B	3381	ARG
1	B	3398	MET
1	B	3422	GLN
1	B	3461	MET
1	B	3719	MET
1	B	4660	PHE
1	B	4672	MET
1	B	4690	LYS
1	B	4925	LEU
1	B	4942	LYS
1	B	4951	PHE
1	C	111	ARG
1	C	309	MET
1	C	343	ARG
1	C	349	MET
1	C	778	MET
1	C	880	ARG
1	C	912	LYS

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Mol	Chain	Res	Type
1	C	995	MET
1	C	1022	GLN
1	C	1044	LYS
1	C	1494	MET
1	C	1975	MET
1	C	2054	LYS
1	C	2172	MET
1	C	2737	LEU
1	C	2757	MET
1	C	2760	TYR
1	C	2761	LYS
1	C	2838[A]	HIS
1	C	2838[B]	HIS
1	C	2847	ASN
1	C	2884	LYS
1	C	3018	ARG
1	C	3047	LYS
1	C	3150	ARG
1	C	3190	ARG
1	C	3215	MET
1	C	3221	LEU
1	C	3231	MET
1	C	3235	MET
1	C	3281	LEU
1	C	3296	MET
1	C	3297	LYS
1	C	3381	ARG
1	C	3398	MET
1	C	3422	GLN
1	C	3461	MET
1	C	3719	MET
1	C	4660	PHE
1	C	4672	MET
1	C	4690	LYS
1	C	4925	LEU
1	C	4942	LYS
1	C	4951	PHE
1	D	111	ARG
1	D	309	MET
1	D	343	ARG
1	D	349	MET
1	D	778	MET

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Mol	Chain	Res	Type
1	D	880	ARG
1	D	912	LYS
1	D	995	MET
1	D	1022	GLN
1	D	1044	LYS
1	D	1494	MET
1	D	1975	MET
1	D	2054	LYS
1	D	2172	MET
1	D	2737	LEU
1	D	2757	MET
1	D	2760	TYR
1	D	2761	LYS
1	D	2838[A]	HIS
1	D	2838[B]	HIS
1	D	2847	ASN
1	D	2884	LYS
1	D	3018	ARG
1	D	3047	LYS
1	D	3150	ARG
1	D	3190	ARG
1	D	3215	MET
1	D	3221	LEU
1	D	3231	MET
1	D	3235	MET
1	D	3281	LEU
1	D	3296	MET
1	D	3297	LYS
1	D	3381	ARG
1	D	3398	MET
1	D	3422	GLN
1	D	3461	MET
1	D	3719	MET
1	D	4660	PHE
1	D	4672	MET
1	D	4690	LYS
1	D	4925	LEU
1	D	4942	LYS
1	D	4951	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2754	GLN
1	A	3151	GLN
1	A	3256	ASN
1	A	3426	ASN
1	A	3563	GLN
3	I	108	HIS
3	J	108	HIS
3	K	108	HIS
3	L	108	HIS
1	B	2754	GLN
1	B	3151	GLN
1	B	3256	ASN
1	B	3426	ASN
1	B	3563	GLN
1	C	2754	GLN
1	C	3151	GLN
1	C	3256	ASN
1	C	3426	ASN
1	C	3563	GLN
1	D	2754	GLN
1	D	3151	GLN
1	D	3256	ASN
1	D	3426	ASN
1	D	3563	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	C	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
5	ATP	B	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
7	XAN	B	5004	-	8,12,12	1.56	1 (12%)	4,17,17	6.65	2 (50%)
7	XAN	D	5004	-	8,12,12	1.58	1 (12%)	4,17,17	6.59	2 (50%)
7	XAN	A	5004	-	8,12,12	1.57	1 (12%)	4,17,17	6.62	2 (50%)
5	ATP	A	5002	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	B	5002	-	26,33,33	0.60	0	31,52,52	0.76	2 (6%)
5	ATP	D	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
7	XAN	C	5004	-	8,12,12	1.57	1 (12%)	4,17,17	6.64	2 (50%)
5	ATP	C	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)
5	ATP	D	5002	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	A	5005	-	26,33,33	0.67	0	31,52,52	0.73	1 (3%)

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
5	ATP	C	5002	-	-	5/18/38/38	0/3/3/3
5	ATP	B	5005	-	-	4/18/38/38	0/3/3/3
7	XAN	B	5004	-	-	-	0/2/2/2
7	XAN	D	5004	-	-	-	0/2/2/2
7	XAN	A	5004	-	-	-	0/2/2/2
5	ATP	A	5002	-	-	5/18/38/38	0/3/3/3
5	ATP	B	5002	-	-	5/18/38/38	0/3/3/3
5	ATP	D	5005	-	-	4/18/38/38	0/3/3/3
7	XAN	C	5004	-	-	-	0/2/2/2
5	ATP	C	5005	-	-	4/18/38/38	0/3/3/3
5	ATP	D	5002	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	A	5005	-	-	4/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	5004	XAN	C6-N1	4.04	1.40	1.33
7	A	5004	XAN	C6-N1	4.01	1.40	1.33
7	C	5004	XAN	C6-N1	4.01	1.40	1.33
7	B	5004	XAN	C6-N1	3.98	1.40	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	5004	XAN	C2-N1-C6	11.41	124.78	115.14
7	C	5004	XAN	C2-N1-C6	11.41	124.77	115.14
7	A	5004	XAN	C2-N1-C6	11.37	124.74	115.14
7	D	5004	XAN	C2-N1-C6	11.31	124.69	115.14
7	B	5004	XAN	C5-C6-N1	-6.78	114.15	123.43
7	C	5004	XAN	C5-C6-N1	-6.77	114.17	123.43
7	A	5004	XAN	C5-C6-N1	-6.76	114.19	123.43
7	D	5004	XAN	C5-C6-N1	-6.74	114.21	123.43
5	B	5005	ATP	C5-C6-N6	2.34	123.90	120.35
5	C	5005	ATP	C5-C6-N6	2.33	123.89	120.35
5	D	5005	ATP	C5-C6-N6	2.32	123.88	120.35
5	A	5005	ATP	C5-C6-N6	2.31	123.87	120.35
5	D	5002	ATP	C5-C6-N6	2.31	123.86	120.35
5	A	5002	ATP	C5-C6-N6	2.30	123.85	120.35
5	B	5002	ATP	C5-C6-N6	2.30	123.85	120.35
5	C	5002	ATP	C5-C6-N6	2.27	123.81	120.35
5	C	5002	ATP	PB-O3B-PG	2.06	139.89	132.83
5	D	5002	ATP	PB-O3B-PG	2.06	139.88	132.83
5	A	5002	ATP	PB-O3B-PG	2.05	139.86	132.83
5	B	5002	ATP	PB-O3B-PG	2.05	139.85	132.83

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5002	ATP	C5'-O5'-PA-O1A
5	A	5005	ATP	PB-O3A-PA-O5'
5	A	5005	ATP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
5	B	5002	ATP	C5'-O5'-PA-O1A
5	B	5005	ATP	PB-O3A-PA-O5'
5	B	5005	ATP	C5'-O5'-PA-O1A
5	C	5002	ATP	C5'-O5'-PA-O1A
5	C	5005	ATP	PB-O3A-PA-O5'
5	C	5005	ATP	C5'-O5'-PA-O1A
5	D	5002	ATP	C5'-O5'-PA-O1A
5	D	5005	ATP	PB-O3A-PA-O5'
5	D	5005	ATP	C5'-O5'-PA-O1A
5	A	5002	ATP	C5'-O5'-PA-O3A
5	B	5002	ATP	C5'-O5'-PA-O3A
5	C	5002	ATP	C5'-O5'-PA-O3A
5	D	5002	ATP	C5'-O5'-PA-O3A
5	A	5002	ATP	C4'-C5'-O5'-PA
5	B	5002	ATP	C4'-C5'-O5'-PA
5	C	5002	ATP	C4'-C5'-O5'-PA
5	D	5002	ATP	C4'-C5'-O5'-PA
5	A	5002	ATP	C5'-O5'-PA-O2A
5	B	5002	ATP	C5'-O5'-PA-O2A
5	C	5002	ATP	C5'-O5'-PA-O2A
5	D	5002	ATP	C5'-O5'-PA-O2A
5	A	5005	ATP	C5'-O5'-PA-O3A
5	B	5005	ATP	C5'-O5'-PA-O3A
5	C	5005	ATP	C5'-O5'-PA-O3A
5	D	5005	ATP	C5'-O5'-PA-O3A
5	A	5002	ATP	O4'-C4'-C5'-O5'
5	A	5005	ATP	O4'-C4'-C5'-O5'
5	B	5002	ATP	O4'-C4'-C5'-O5'
5	B	5005	ATP	O4'-C4'-C5'-O5'
5	C	5002	ATP	O4'-C4'-C5'-O5'
5	C	5005	ATP	O4'-C4'-C5'-O5'
5	D	5002	ATP	O4'-C4'-C5'-O5'
5	D	5005	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	5002	ATP	3	0
5	B	5005	ATP	7	0
5	A	5002	ATP	3	0
5	B	5002	ATP	3	0

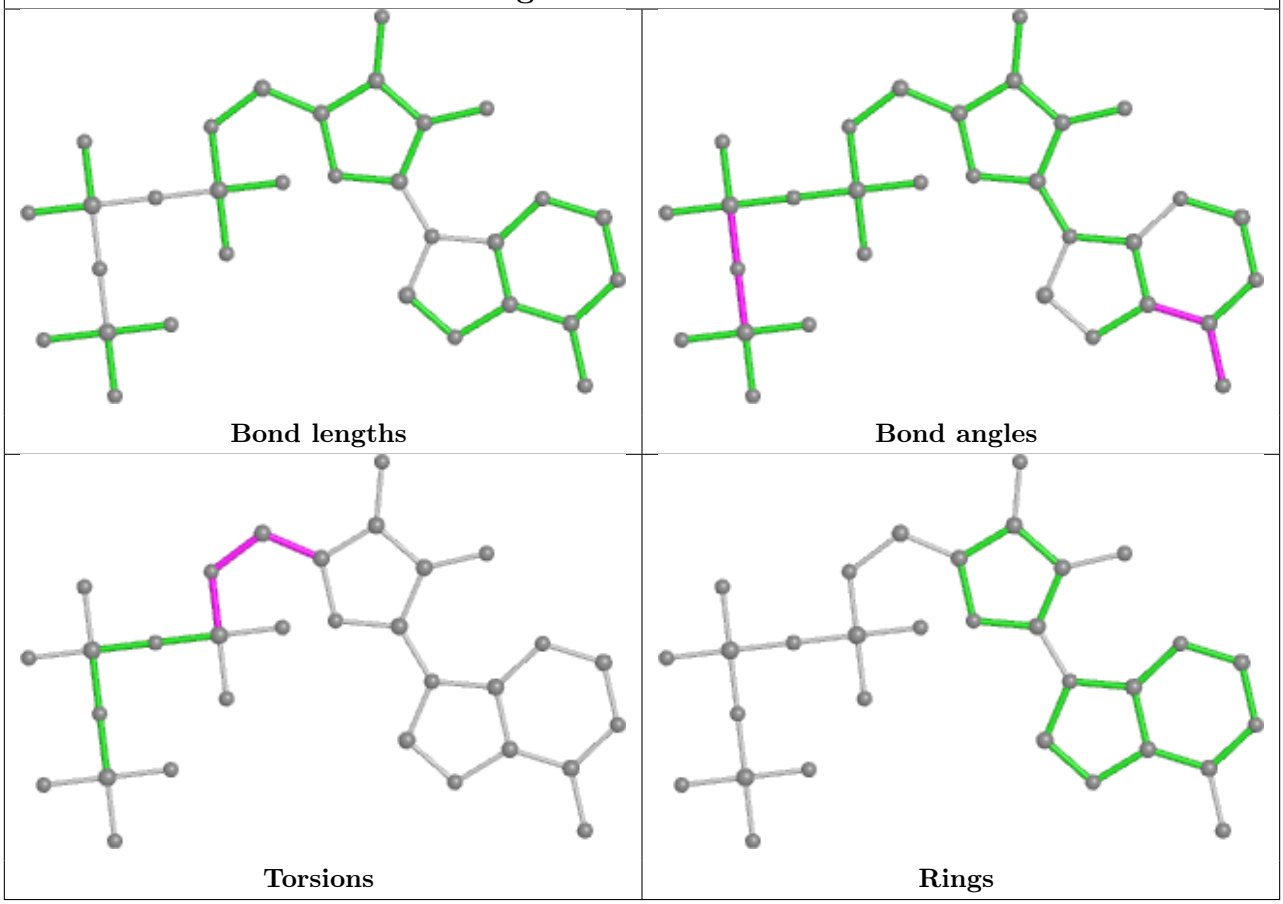
Continued on next page...

Continued from previous page...

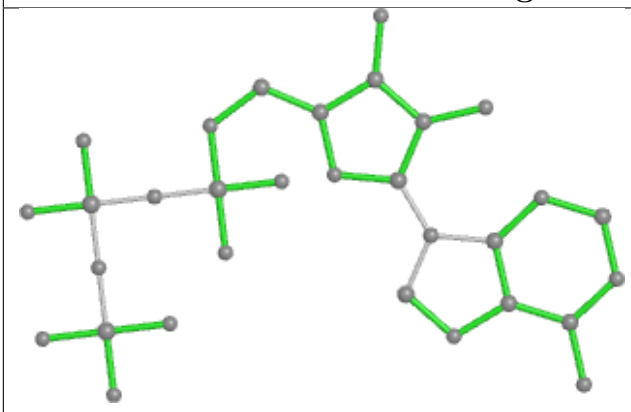
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5005	ATP	8	0
5	C	5005	ATP	7	0
5	D	5002	ATP	3	0
5	A	5005	ATP	8	0

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

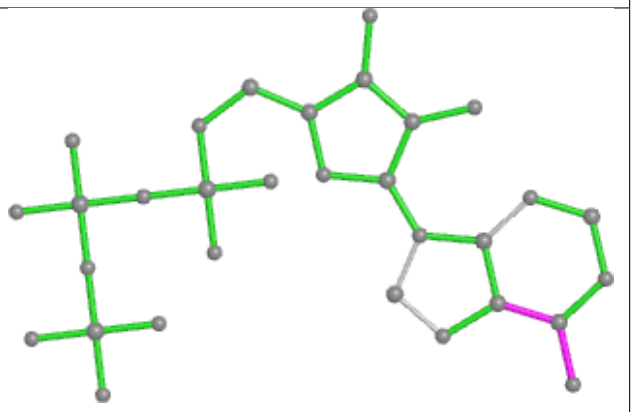
Ligand ATP C 5002



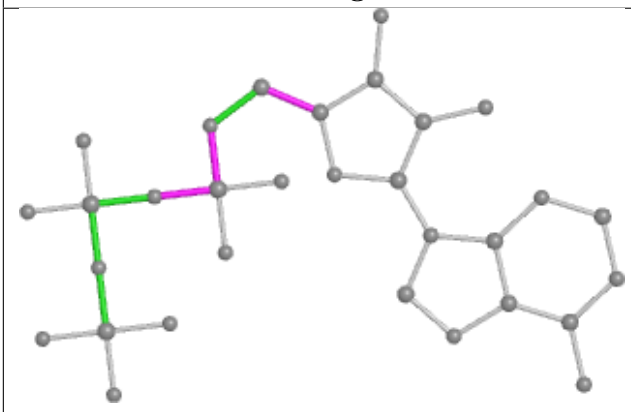
Ligand ATP B 5005



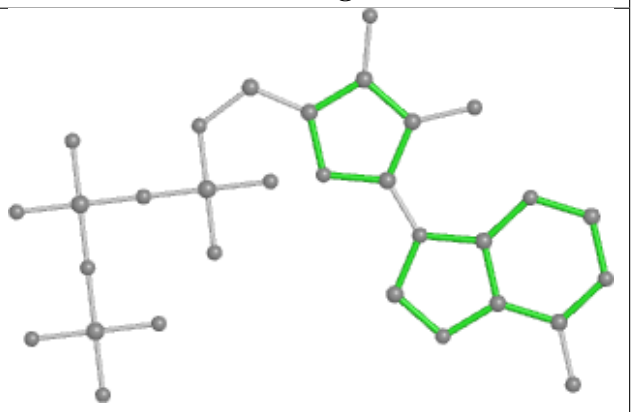
Bond lengths



Bond angles

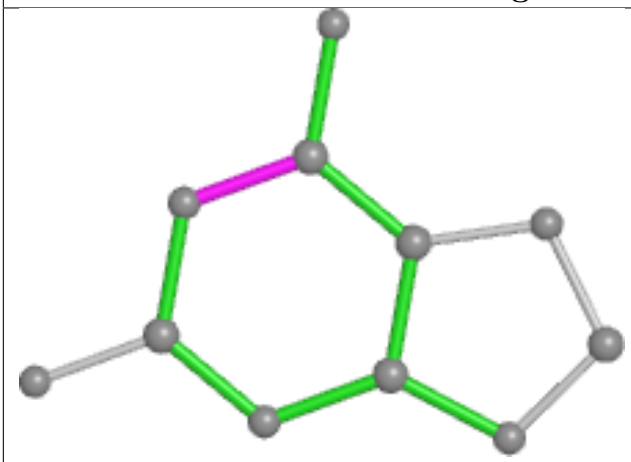


Torsions

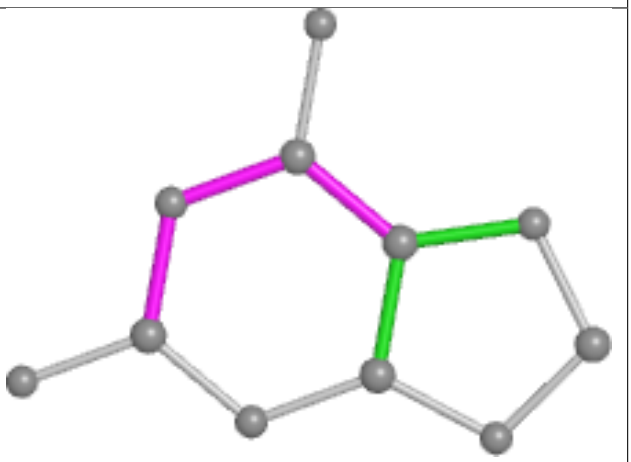


Rings

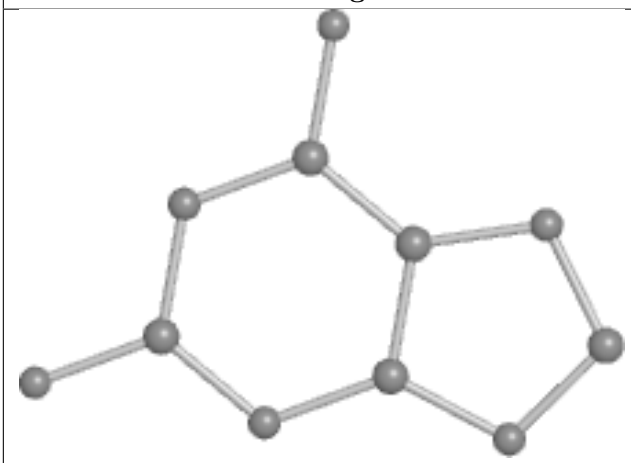
Ligand XAN B 5004



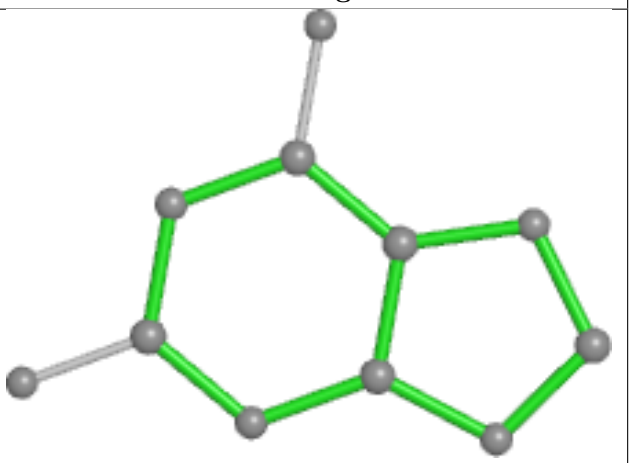
Bond lengths



Bond angles

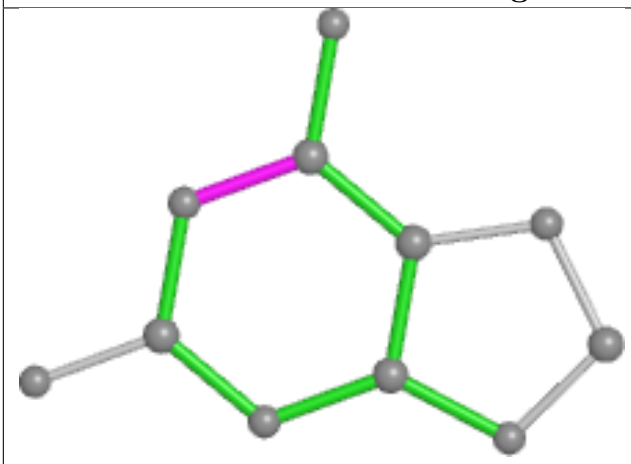


Torsions

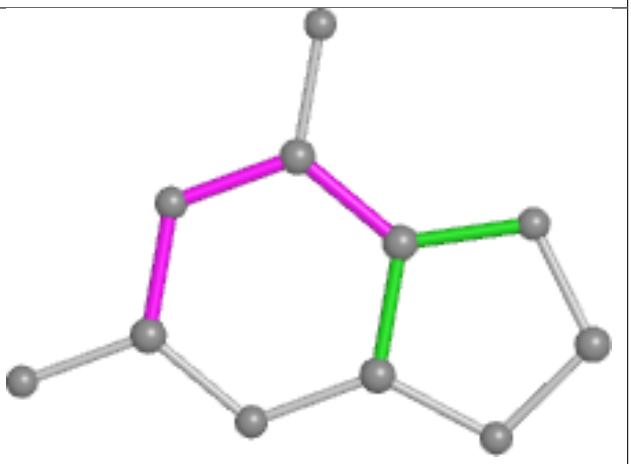


Rings

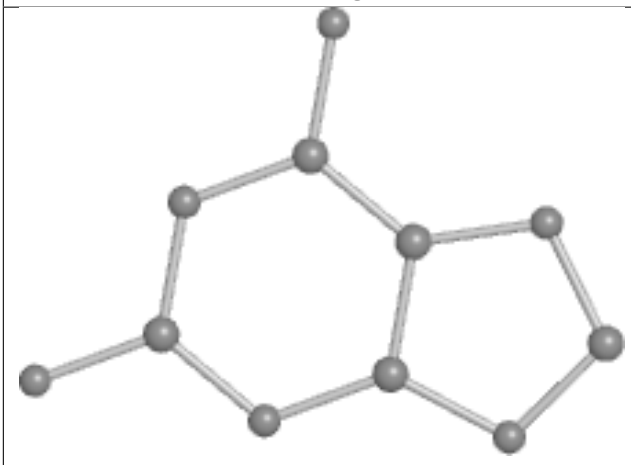
Ligand XAN D 5004



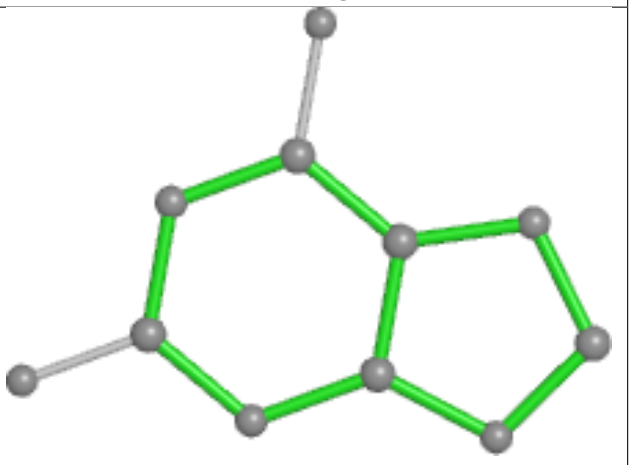
Bond lengths



Bond angles

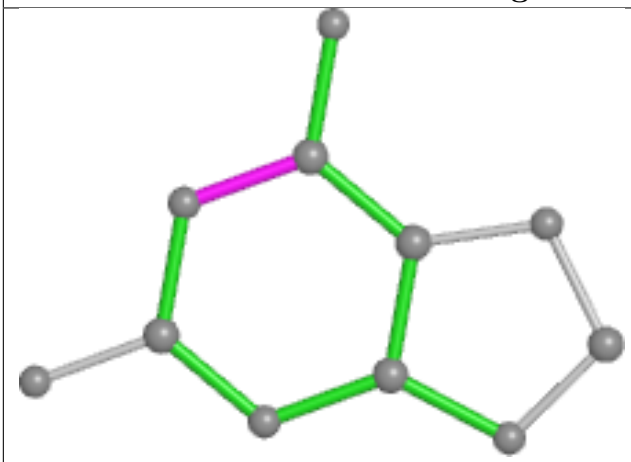


Torsions

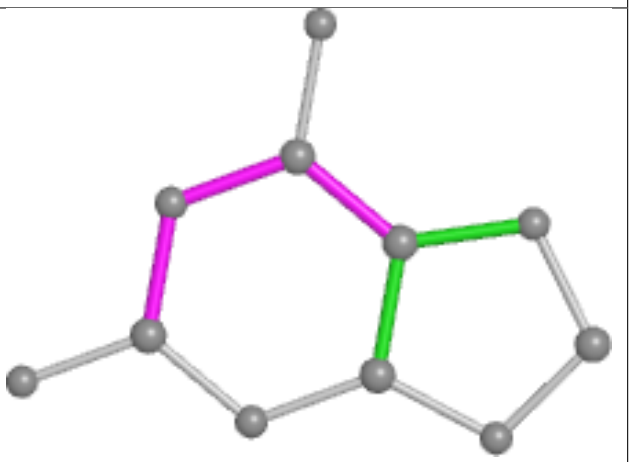


Rings

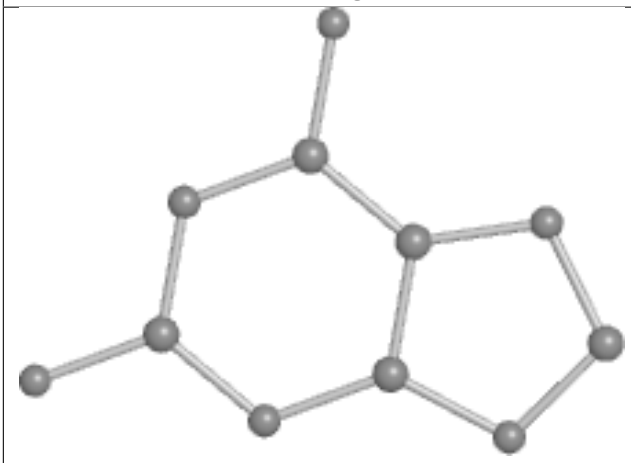
Ligand XAN A 5004



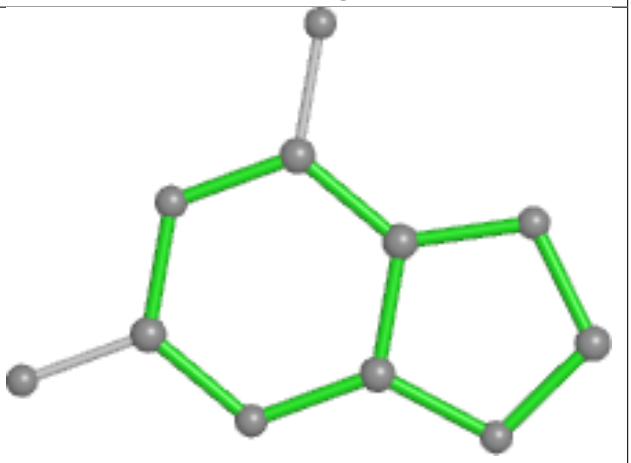
Bond lengths



Bond angles

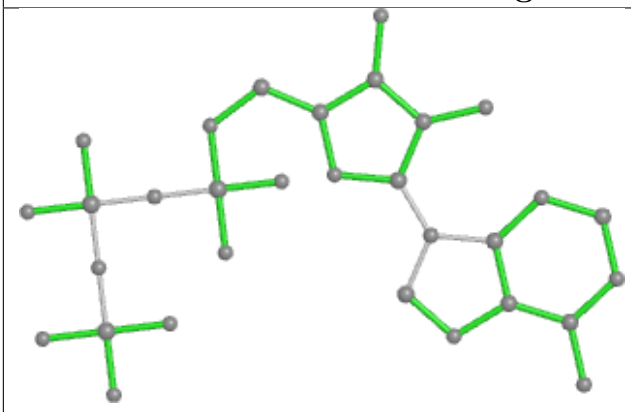


Torsions

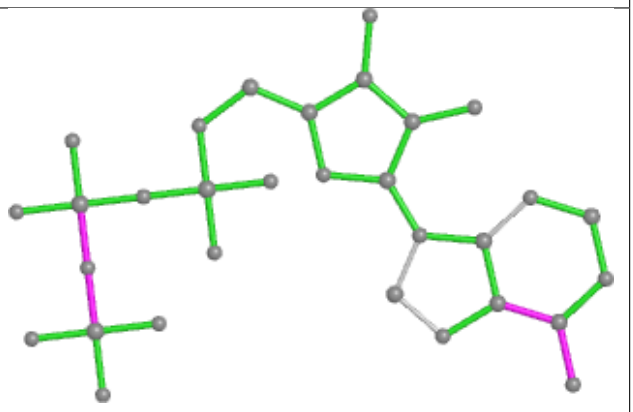


Rings

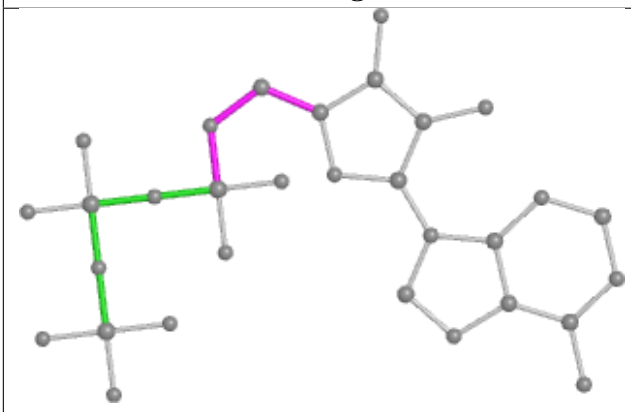
Ligand ATP A 5002



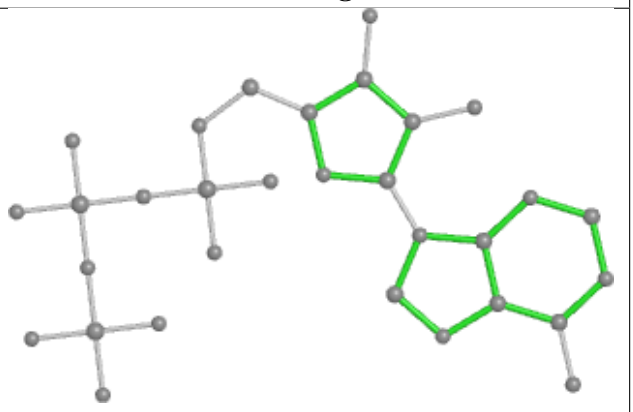
Bond lengths



Bond angles

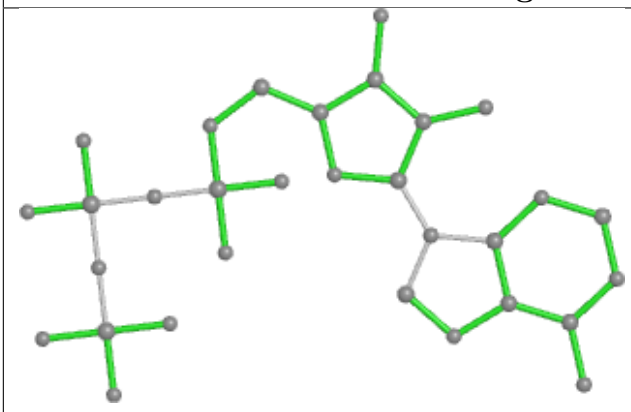


Torsions

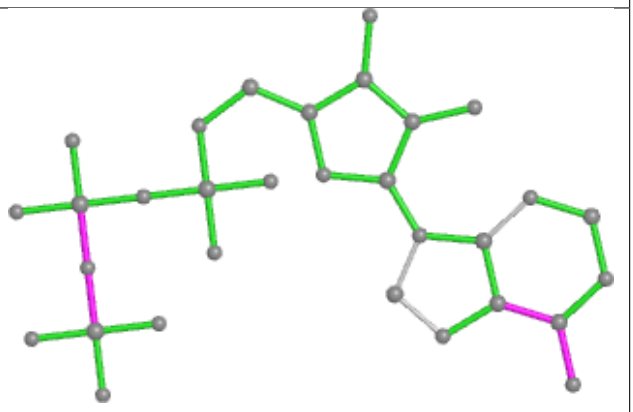


Rings

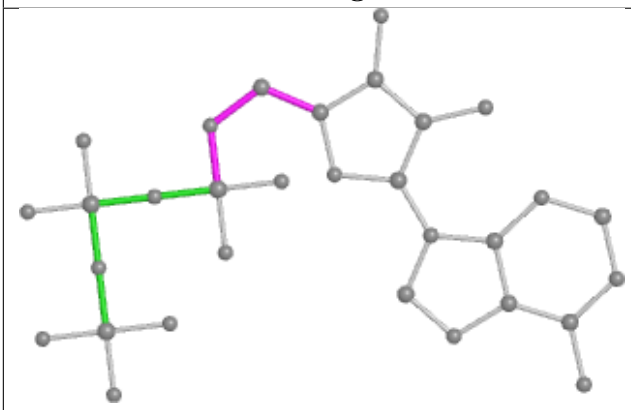
Ligand ATP B 5002



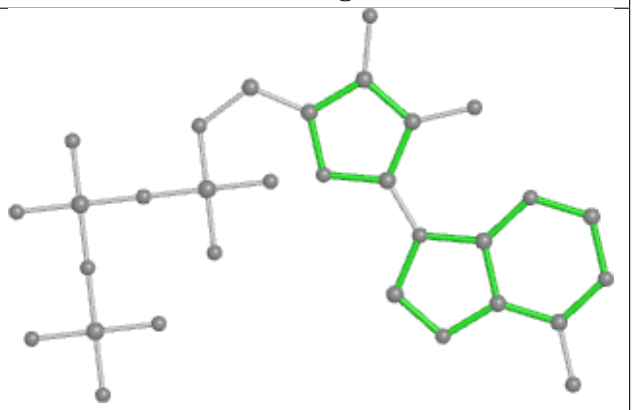
Bond lengths



Bond angles

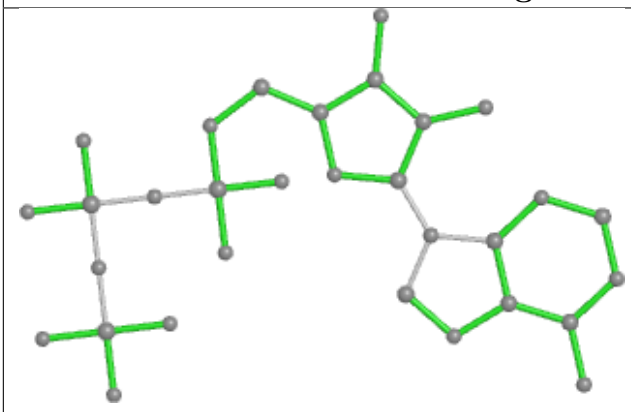


Torsions

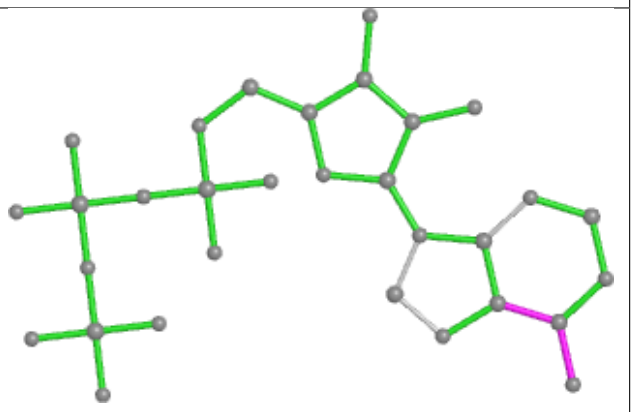


Rings

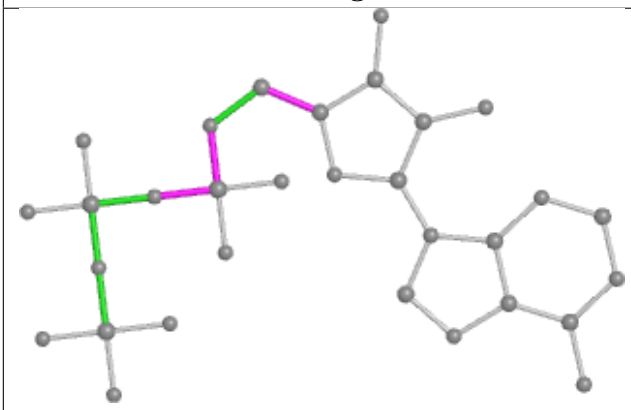
Ligand ATP D 5005



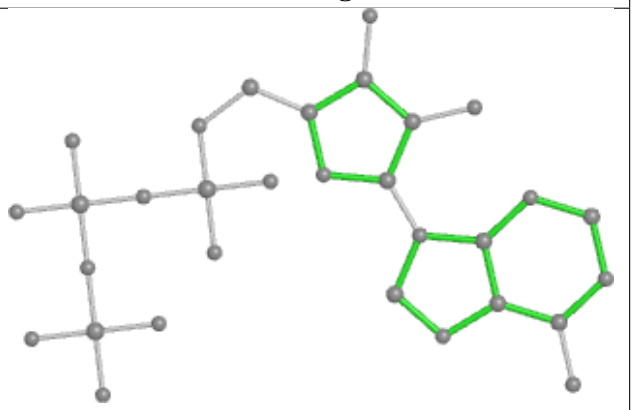
Bond lengths



Bond angles

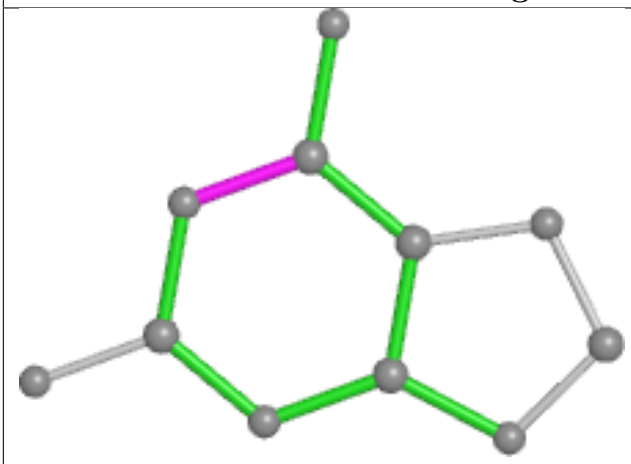


Torsions

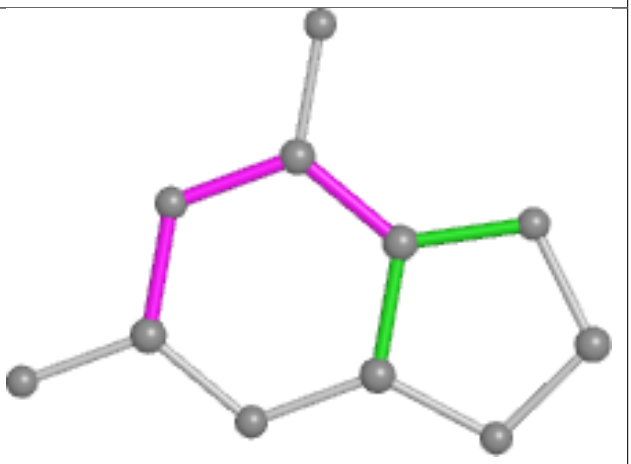


Rings

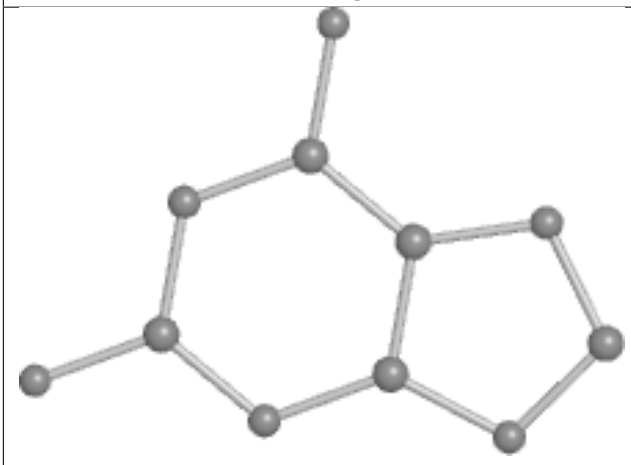
Ligand XAN C 5004



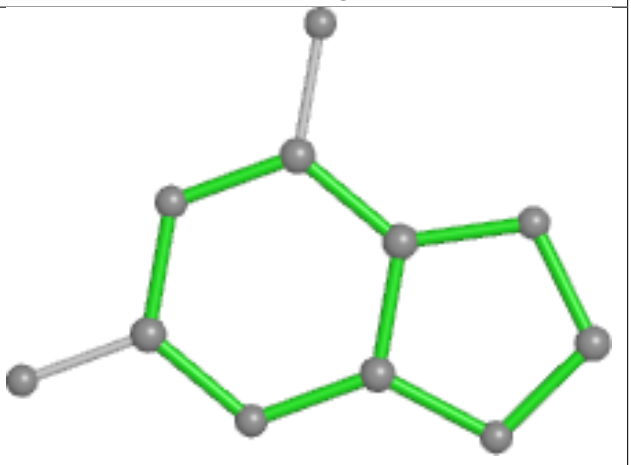
Bond lengths



Bond angles

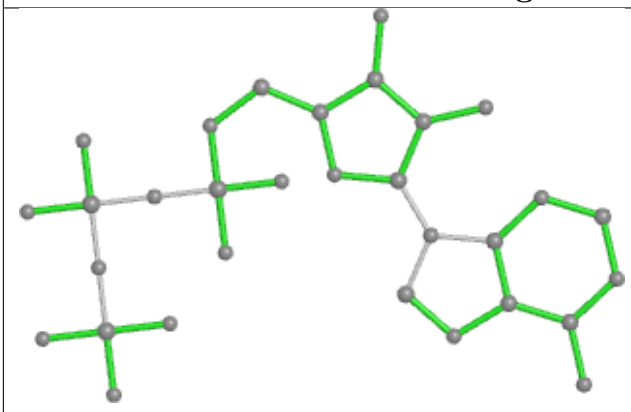


Torsions

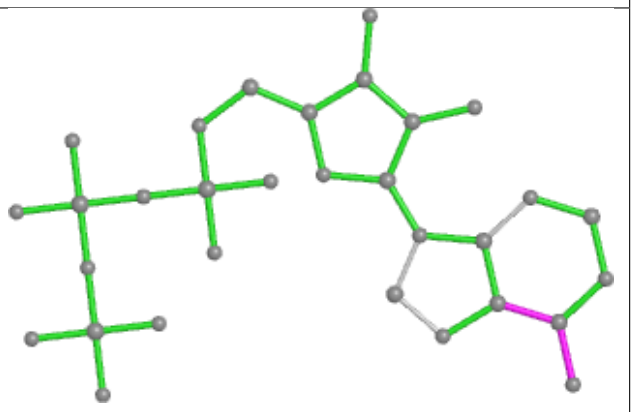


Rings

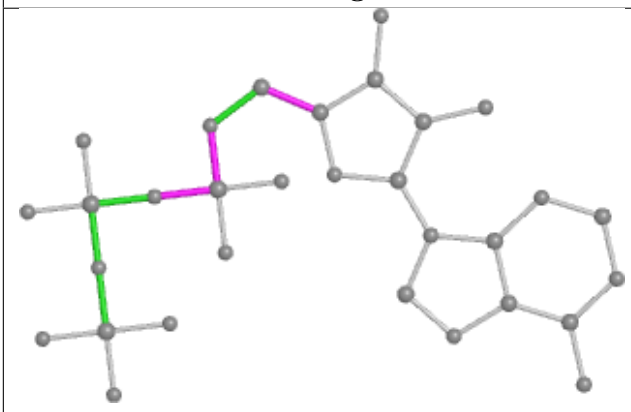
Ligand ATP C 5005



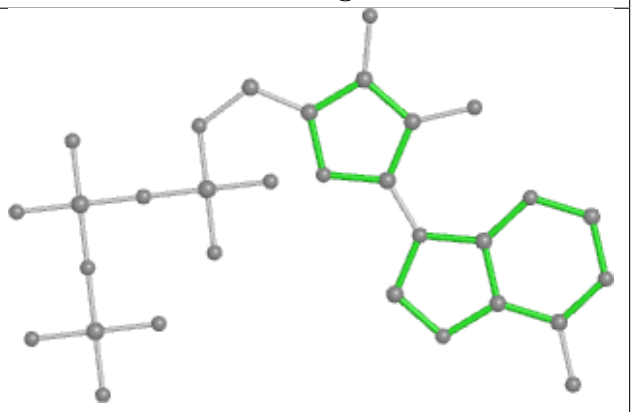
Bond lengths



Bond angles

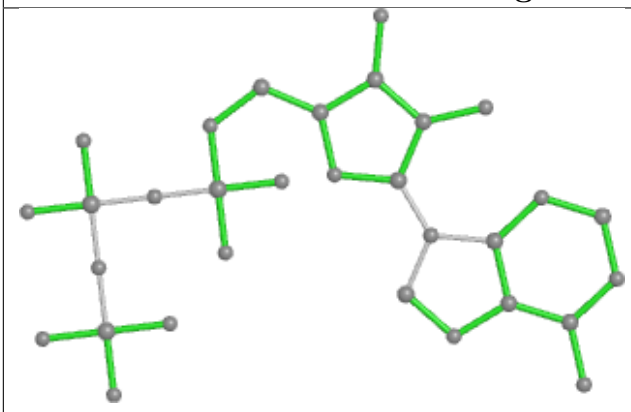


Torsions

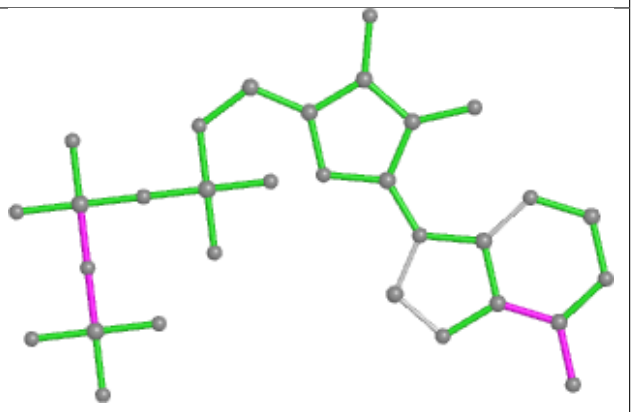


Rings

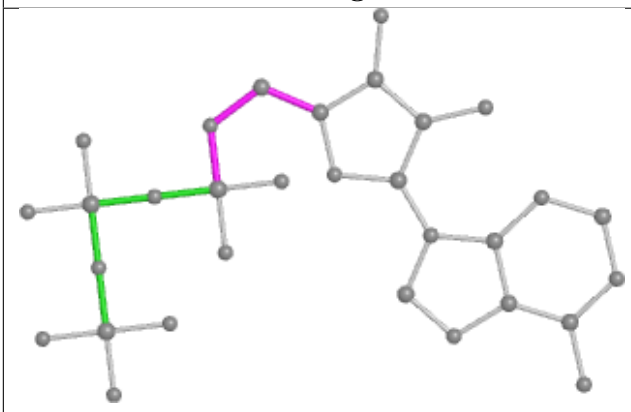
Ligand ATP D 5002



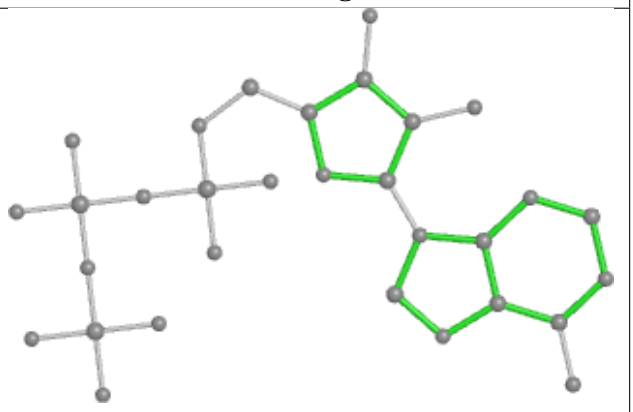
Bond lengths



Bond angles

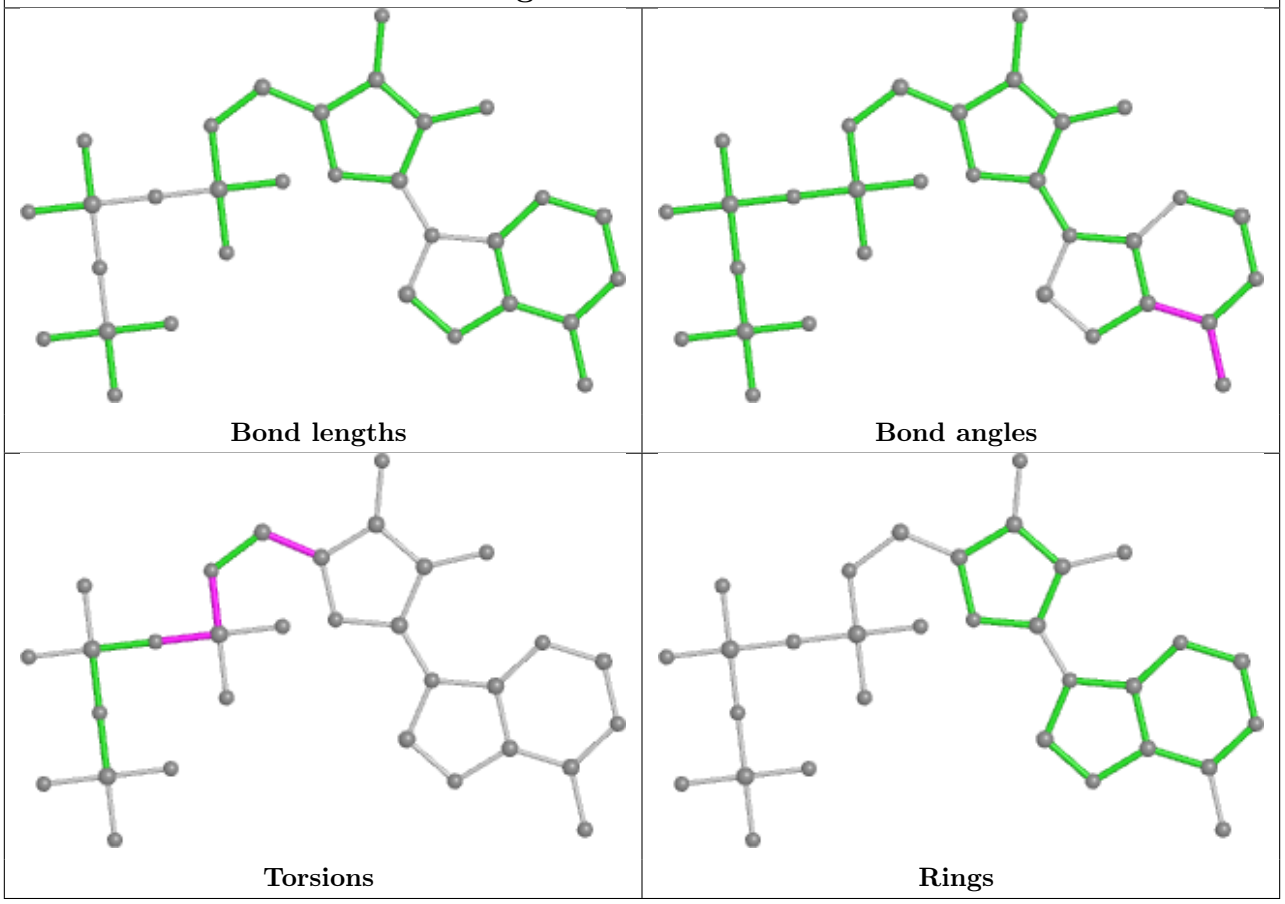


Torsions



Rings

Ligand ATP A 5005



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

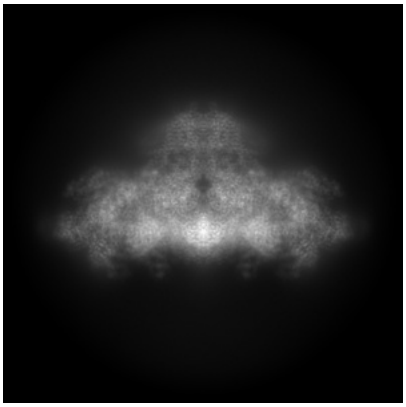
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26414. These allow visual inspection of the internal detail of the map and identification of artifacts.

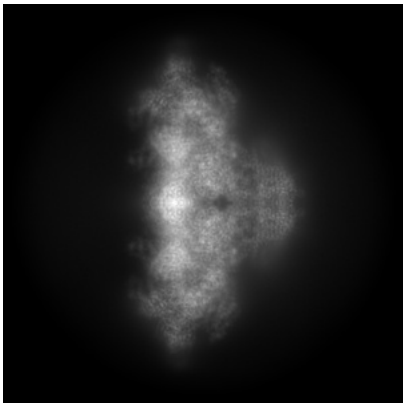
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

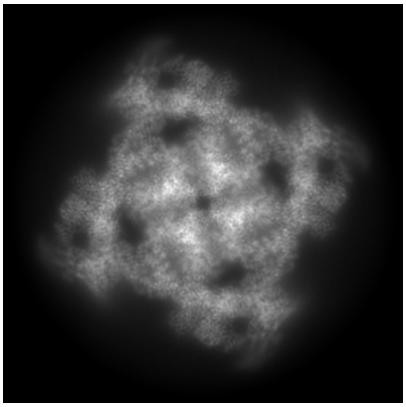
6.1.1 Primary map



X



Y

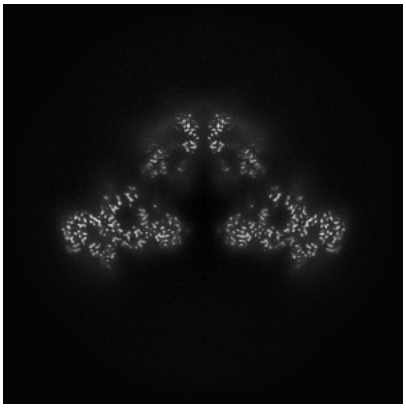


Z

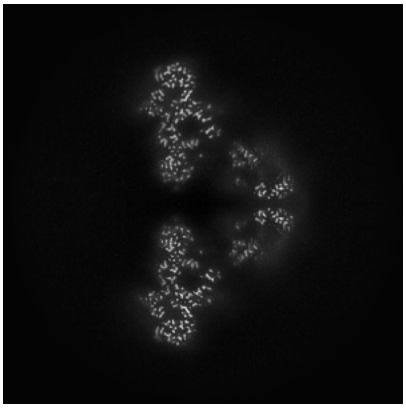
The images above show the map projected in three orthogonal directions.

6.2 Central slices

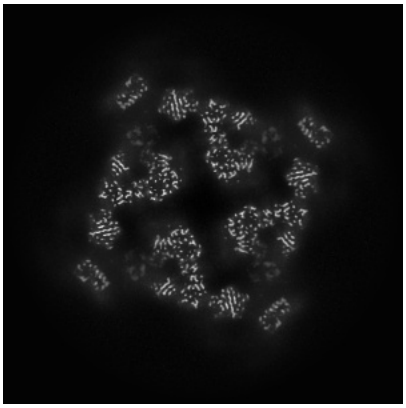
6.2.1 Primary map



X Index: 256



Y Index: 256

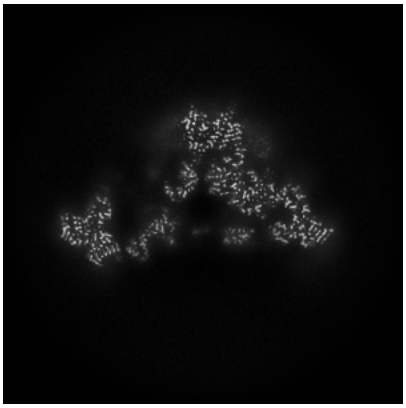


Z Index: 256

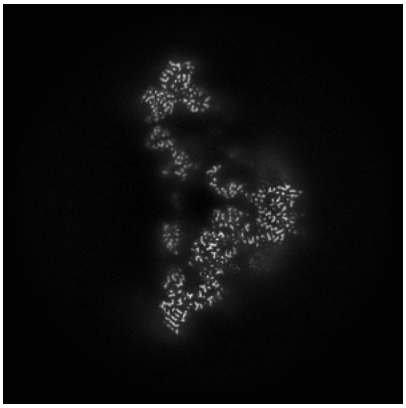
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

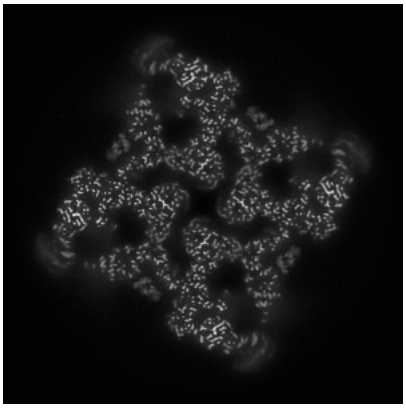
6.3.1 Primary map



X Index: 275



Y Index: 274

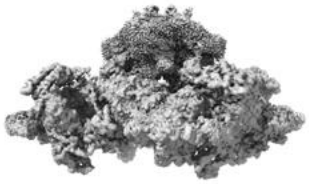


Z Index: 220

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

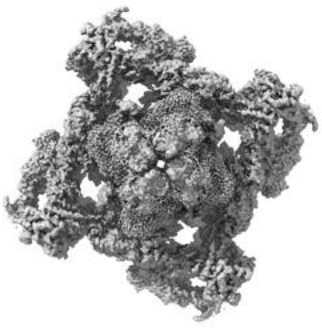
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

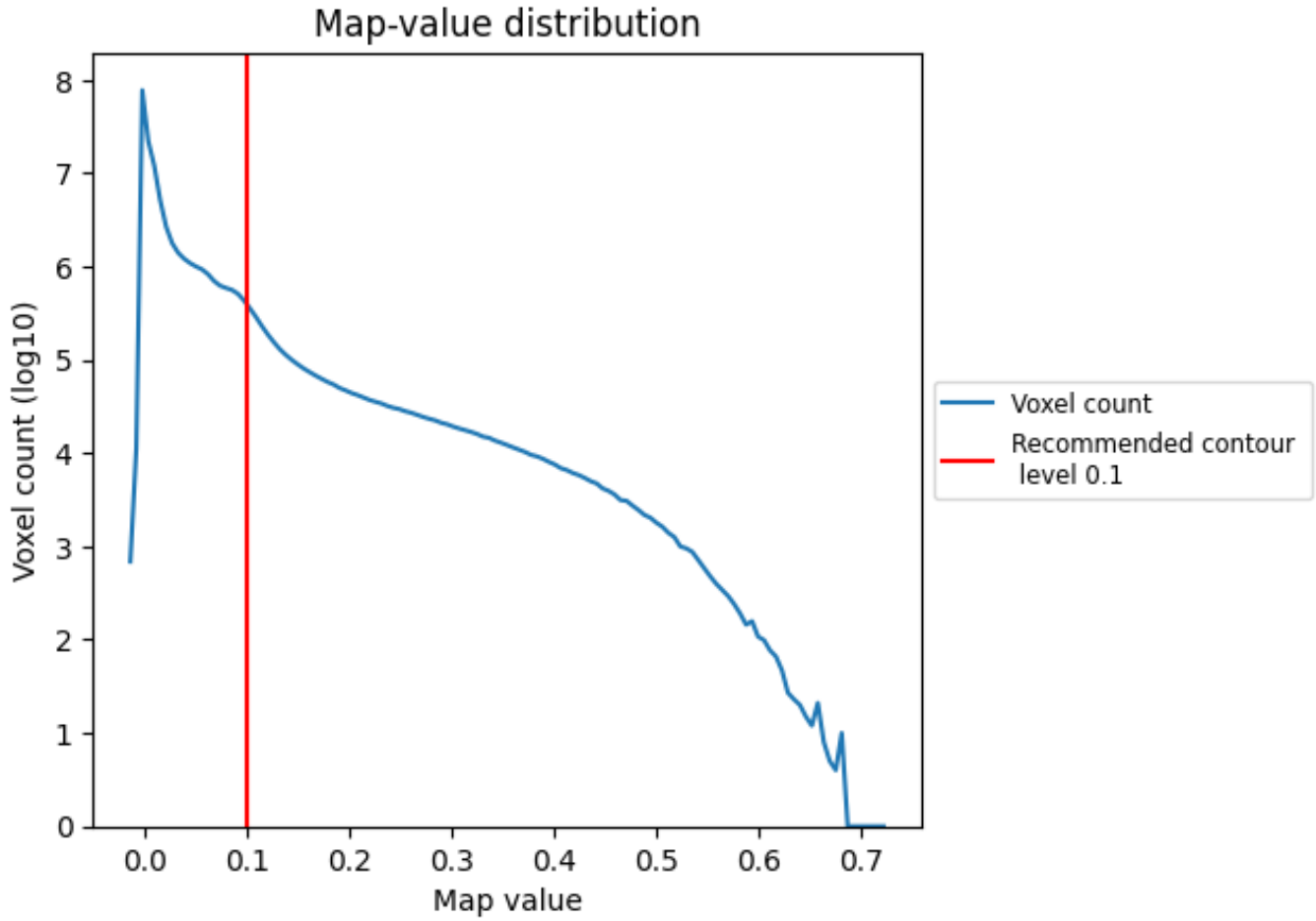
6.5 Mask visualisation (i)

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

7 Map analysis

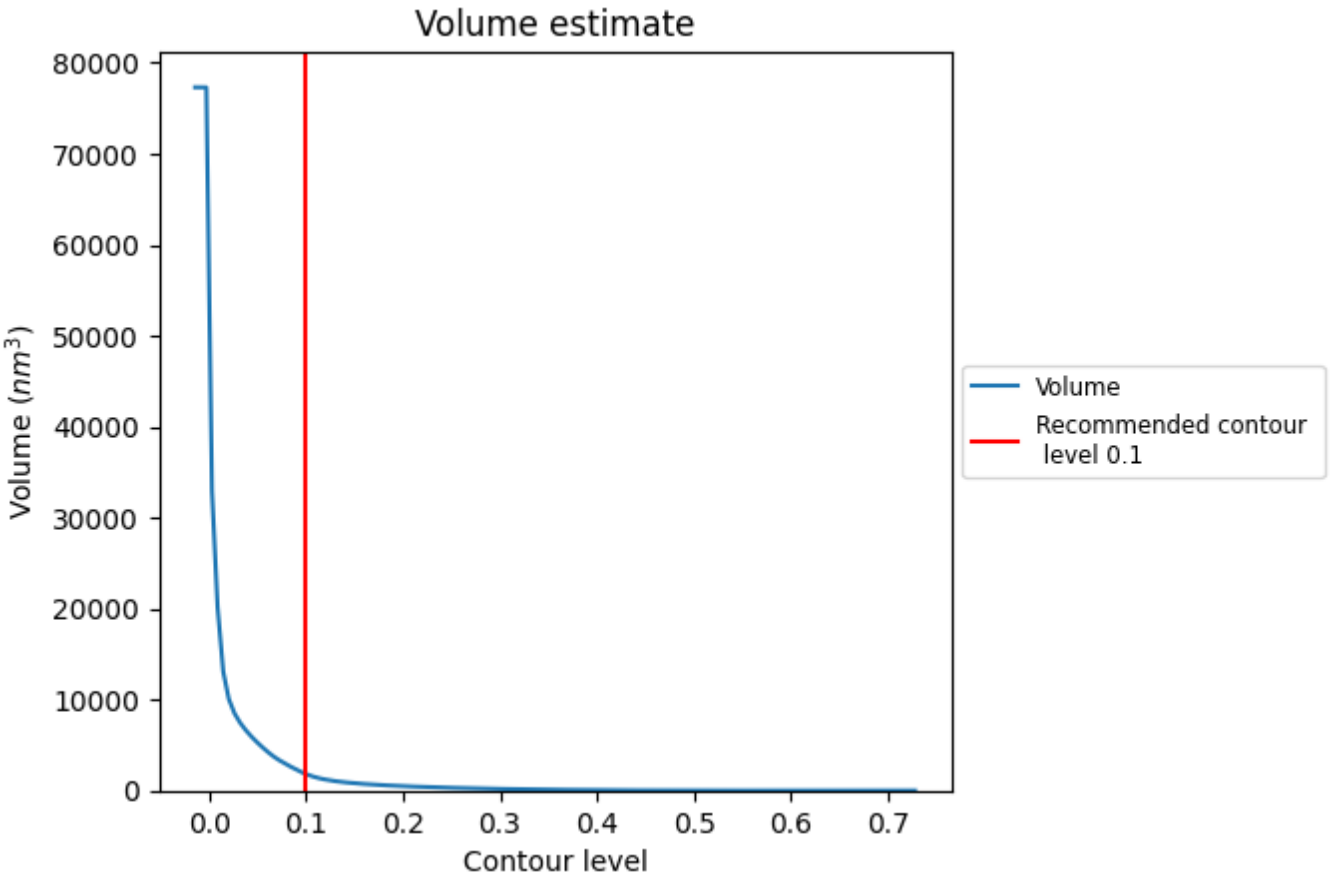
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

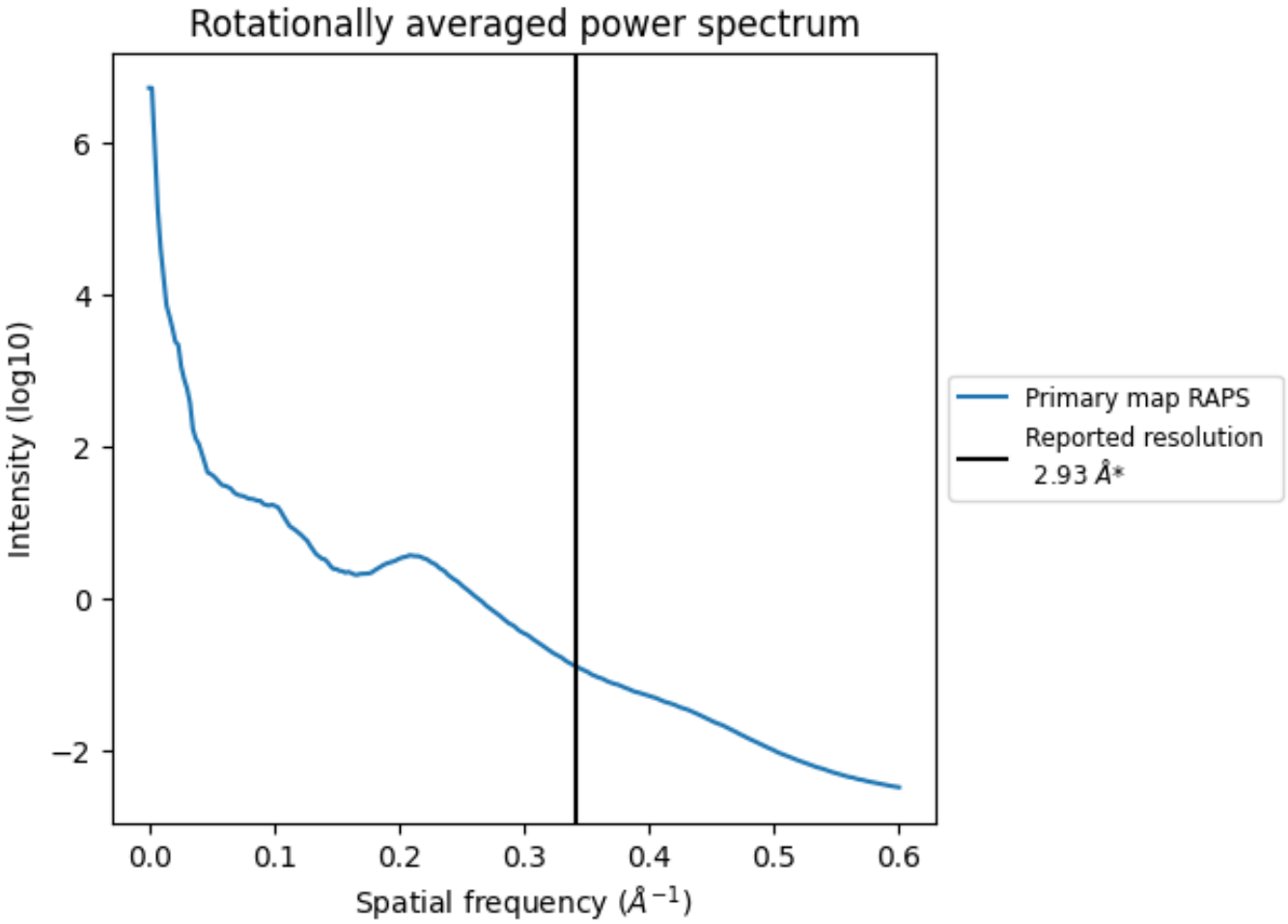
7.2 Volume estimate



The volume at the recommended contour level is 1824 nm^3; this corresponds to an approximate mass of 1648 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 0.341 $Å^{-1}$

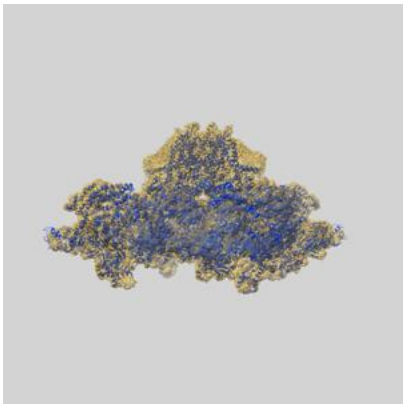
8 Fourier-Shell correlation

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

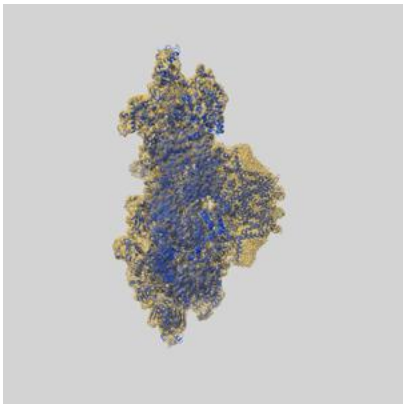
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26414 and PDB model 7UA4. Per-residue inclusion information can be found in section 3 on page 8.

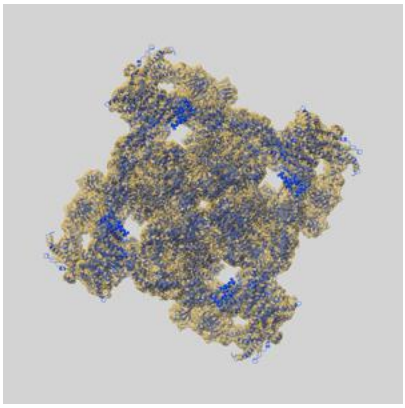
9.1 Map-model overlay



X



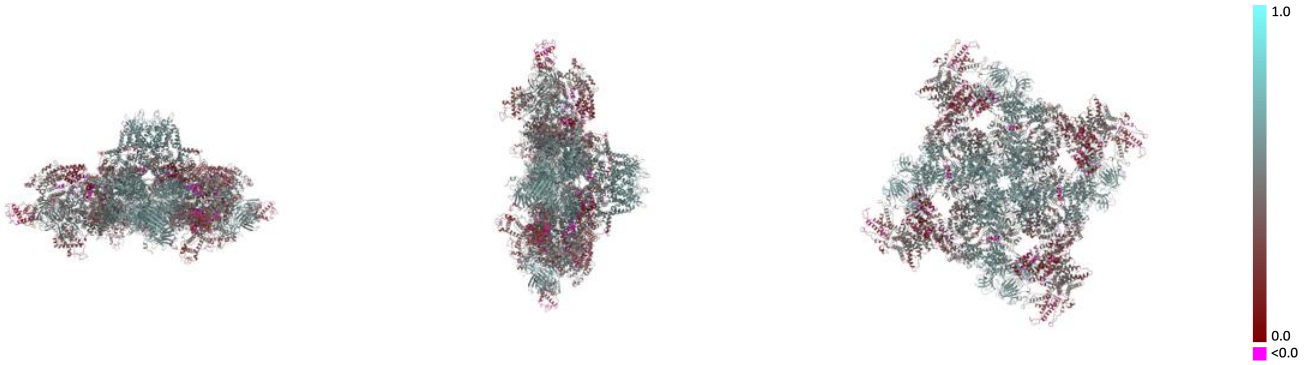
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

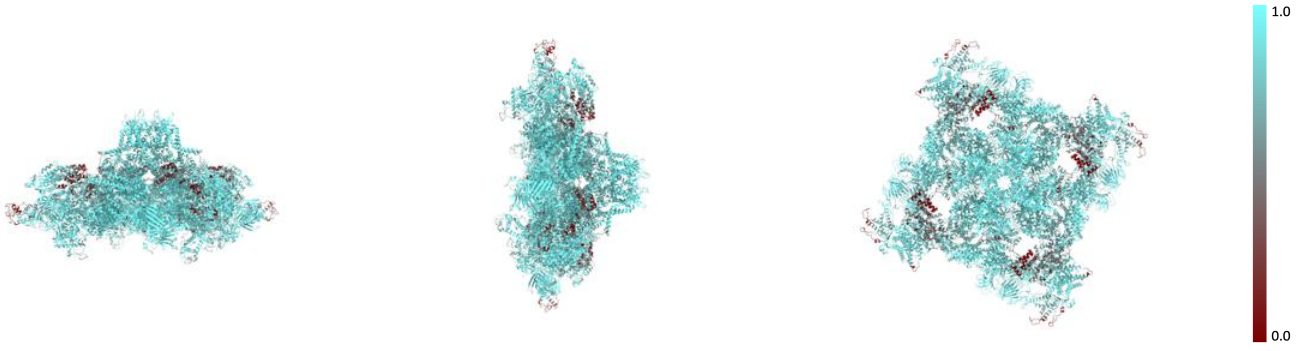
9.2 Q-score mapped to coordinate model



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.

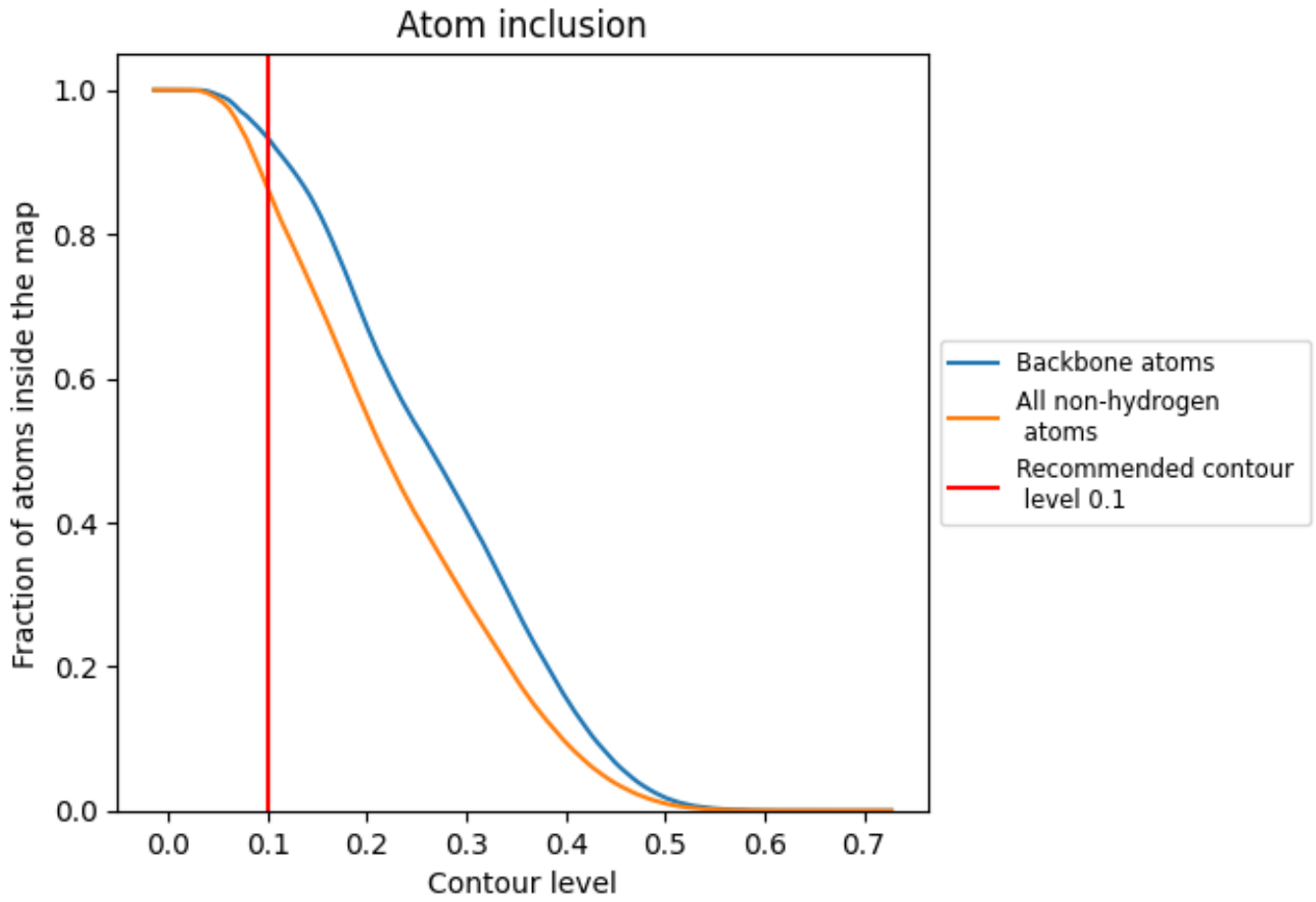
9.3 Atom inclusion mapped to coordinate model



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 86% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8634	0.4560
A	0.8680	0.4670
B	0.8670	0.4580
C	0.8662	0.4570
D	0.8664	0.4610
E	0.9665	0.5880
F	0.9715	0.5710
G	0.9715	0.5710
H	0.9690	0.5730
I	0.6903	0.2200
J	0.6639	0.2040
K	0.6876	0.2240
L	0.6648	0.2110