Full wwPDB EM Validation Report ⓘ

Jan 15, 2024 – 07:28 PM EST

PDB ID	:	8VK3
EMDB ID	:	EMD-43299
Title	:	Structure of mouse RyR1 in complex with S100A1 (EGTA-only dataset)
Authors	:	Weninger, G.; Marks, A.R.
Deposited on	:	2024-01-08
Resolution	:	3.21 Å(reported)

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

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

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

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

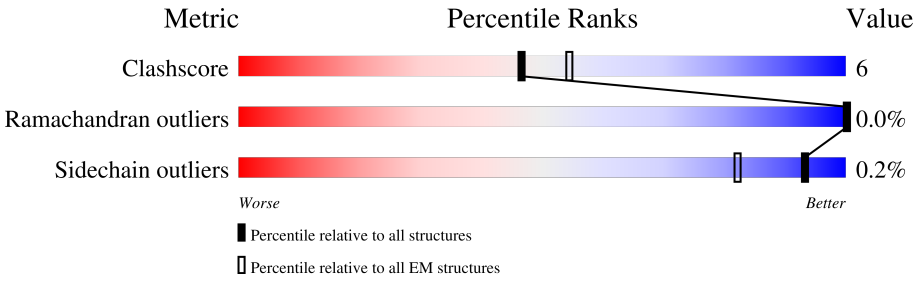
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.21 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	5035	15% 75% 12% 13%
1	B	5035	15% 75% 12% 13%
1	C	5035	15% 75% 12% 13%
1	D	5035	15% 75% 12% 13%
2	E	108	96%
2	F	108	94% 5%
2	G	108	92% 7%
2	H	108	94% 5%

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Mol	Chain	Length	Quality of chain
3	I	94	65% 48% 52%
3	J	94	66% 53% 45%
3	K	94	66% 47% 53%
3	L	94	67% 52% 46%
3	M	94	65% 45% 55%
3	N	94	66% 53% 45%
3	O	94	65% 45% 55%
3	P	94	67% 51% 47%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 148852 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4374	Total 34809	C 22140	N 5985	O 6447	S 237	1	0
1	D	4374	Total 34809	C 22140	N 5985	O 6447	S 237	1	0
1	B	4374	Total 34809	C 22140	N 5985	O 6447	S 237	1	0
1	C	4374	Total 34809	C 22140	N 5985	O 6447	S 237	1	0

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 829	C 526	N 145	O 155	S 3	0	0
2	H	107	Total 829	C 526	N 145	O 155	S 3	0	0
2	F	107	Total 829	C 526	N 145	O 155	S 3	0	0
2	G	107	Total 829	C 526	N 145	O 155	S 3	0	0

- Molecule 3 is a protein called Protein S100A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	93	Total 729	C 460	N 114	O 152	S 3	0	0
3	I	94	Total 737	C 465	N 115	O 153	S 4	0	0
3	K	94	Total 737	C 465	N 115	O 153	S 4	0	0
3	M	94	Total 737	C 465	N 115	O 153	S 4	0	0
3	O	94	Total 737	C 465	N 115	O 153	S 4	0	0

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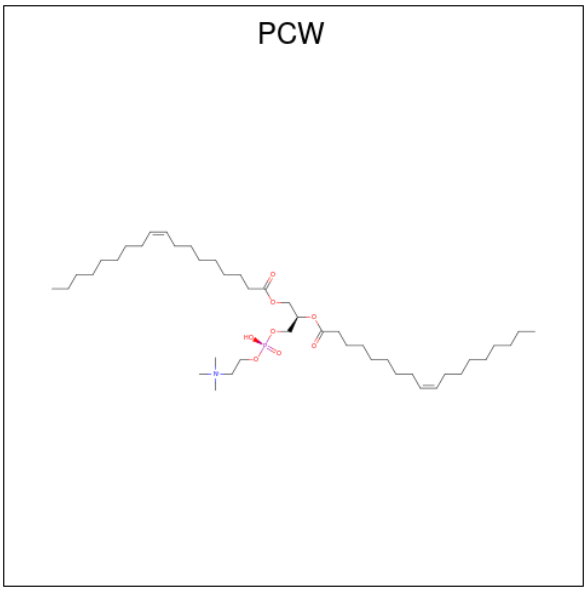
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
3	N	93	Total	C	N	O	S	0	0
			729	460	114	152	3		
3	P	93	Total	C	N	O	S	0	0
			729	460	114	152	3		

- 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	D	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	

- Molecule 5 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	

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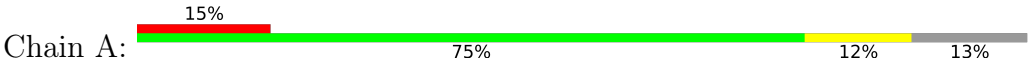
Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
5	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

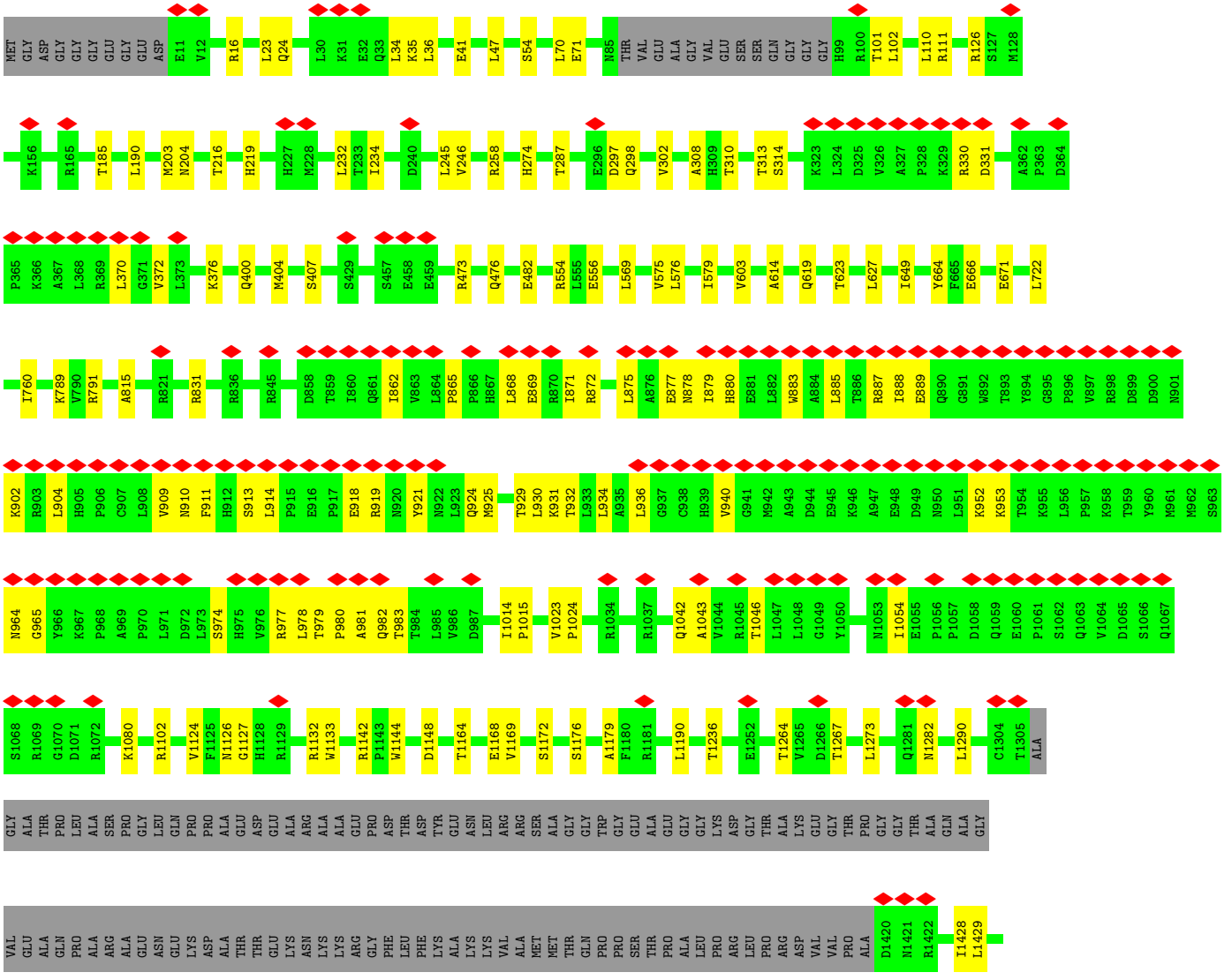
3 Residue-property plots (i)

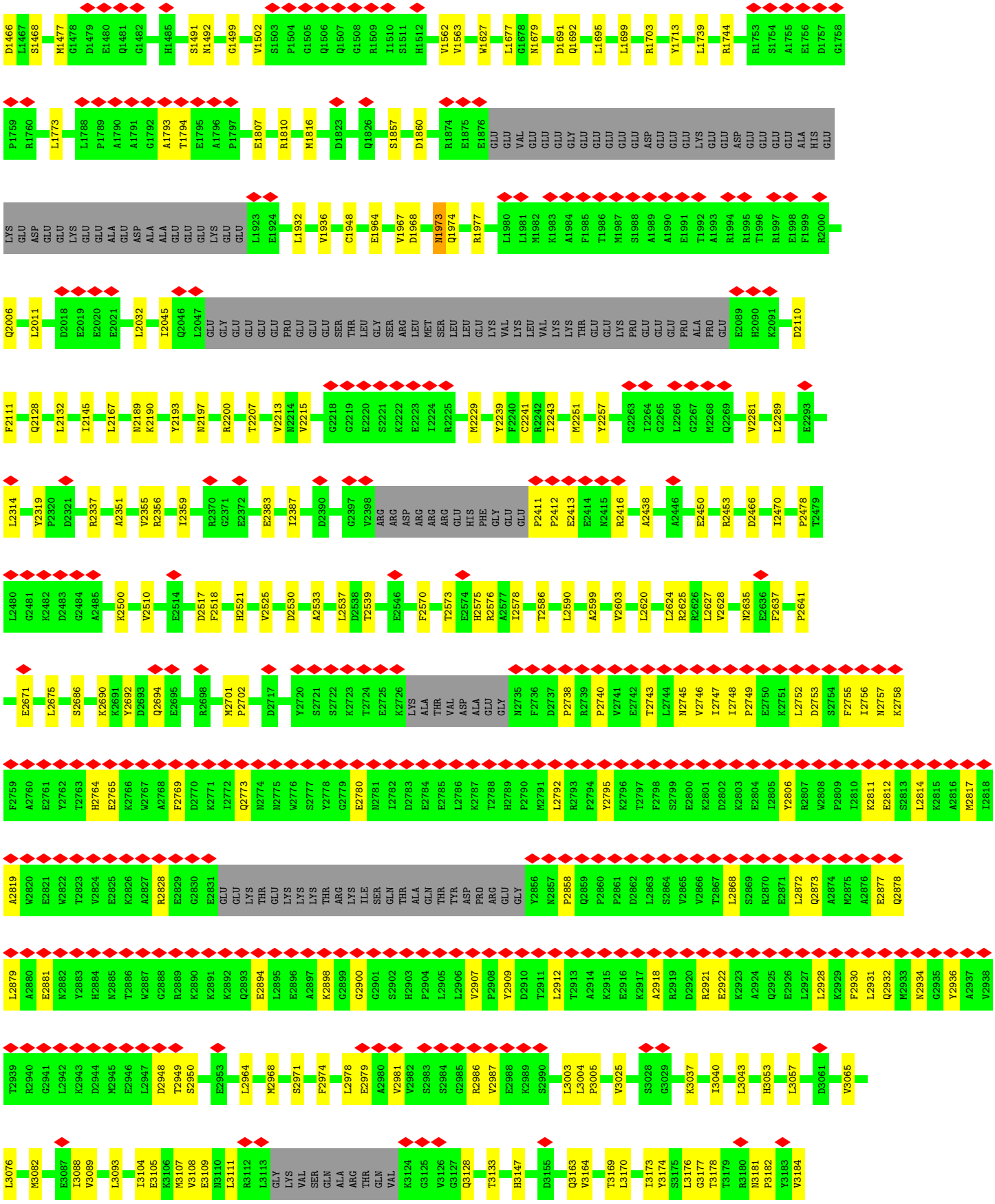
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

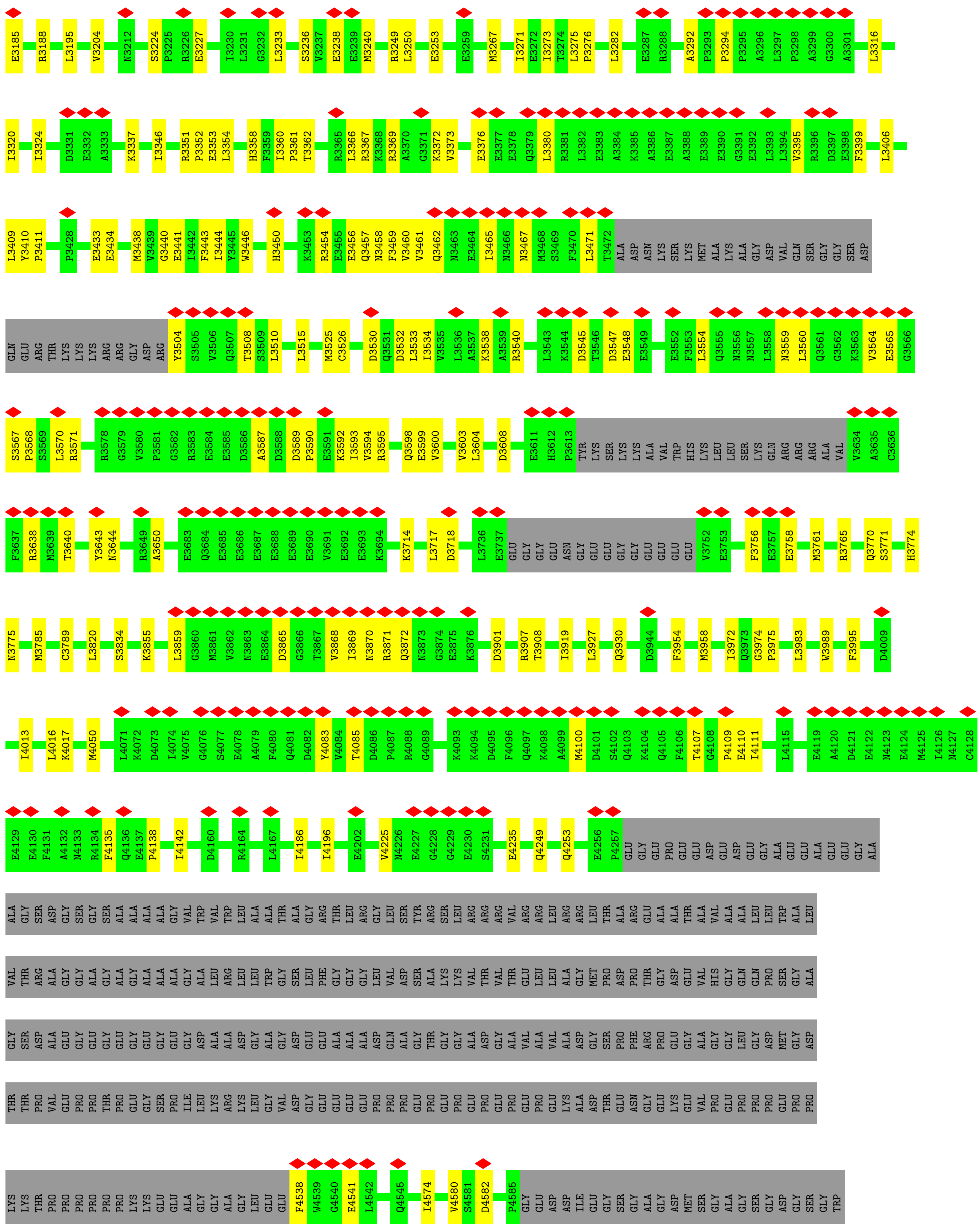
- Molecule 1: Ryanodine receptor 1

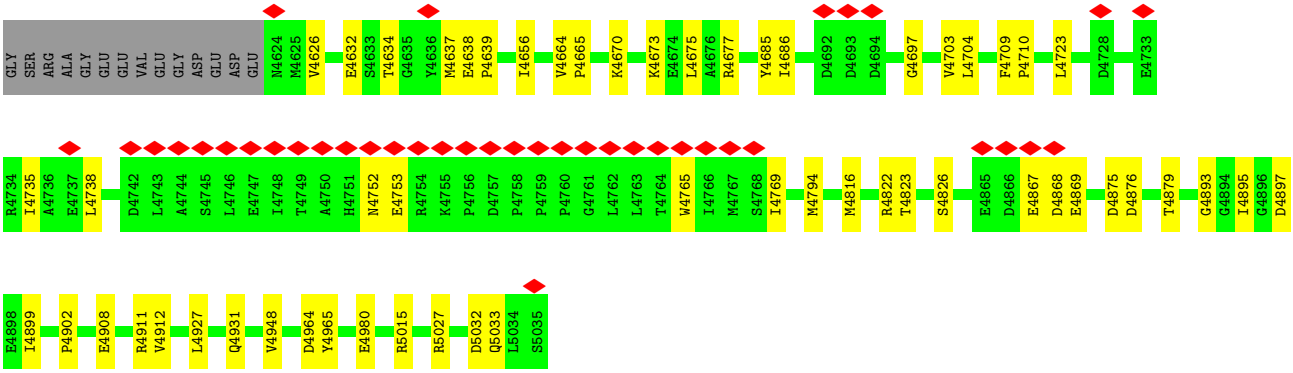
Chain A:





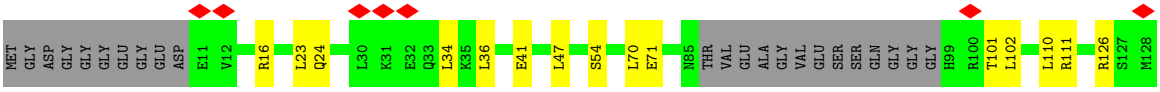


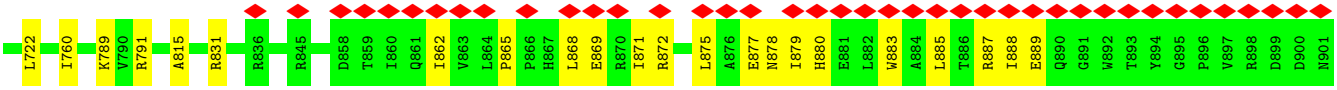

E3185 R3188 L3195 V3204 N3212 S3224 P3225 R3226 E3227 I3230 L3231 G3232 L3233 S3236 V3237 E3238 E3239 M3240 R3249 L3250 E3253 E3259 M3267 I3271 E3272 I3273 T3274 L3275 P3276 L3282 E3287 R3288 A3292 P3293 P3294 P3295 A3296 L3297 P3298 A3299 G3300 A3301 L3316
I3320 I3324 D3331 E3332 A3333 K3337 I3346 R3351 P3352 E3353 L3354 H3358 F3359 I3360 P3361 T3362 R3365 L3366 R3367 K3368 R3369 A3370 G3371 K3372 V3373 E3376 E3377 E3378 Q3379 L3380 R3381 L3382 E3383 A3384 K3385 A3386 E3387 A3388 E3389 E3390 G3391 E3392 L3393 L3394 V3395 R3396 D3397 E3398 F3399 L3406
L3409 Y3410 P3411 P3428 E3433 E3434 M3438 V3439 G3440 E3441 I3442 F3443 I3444 Y3445 W3446 H3450 K3453 R3454 E3455 E3456 Q3457 N3458 F3459 V3460 V3461 Q3462 N3463 E3464 I3465 N3466 N3467 M3468 S3469 F3470 L3471 T3472 ALA ASP ASN LYS SER LYS MET ALA LYS ALA GLY ASP VAL GLN SER GLY GLY SER ASP
GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3504 S3505 V3506 Q3507 T3508 S3509 L3510 L3515 M3525 C3526 D3530 Q3531 D3532 L3533 I3534 V3535 L3536 A3537 K3538 A3539 R3540 L3543 K3544 D3545 T3546 D3547 E3548 E3549 E3552 F3553 L3554 Q3555 N3556 N3557 L3558 N3559 L3560 Q3561 G3562 K3563 V3564 E3565 G3566
S3567 P3568 S3569 L3570 R3571 R3578 G3579 V3580 P3581 G3582 R3583 E3584 E3585 D3586 A3587 D3588 D3589 P3590 E3591 K3592 I3593 V3594 R3595 Q3598 E3599 V3600 V3603 L3604 D3608 E3611 H3612 P3613 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL V3634 A3635 C3636
F3637 R3638 M3639 T3640 Y3643 N3644 R3649 A3650 E3683 Q3684 E3685 E3686 E3687 E3688 E3689 E3690 V3691 E3692 E3693 K3694 K3714 L3717 D3718 L3736 E3737 GLU GLY GLY GLU ASN GLY GLU GLU GLY GLY GLU GLU GLU GLU V3752 E3753 F3756 E3757 E3758 M3761 R3765 Q3770 S3771 H3774
N3775 M3785 C3789 L3820 S3834 K3855 L3859 G3860 M3861 V3862 N3863 E3864 D3865 G3866 T3867 V3868 I3869 N3870 R3871 Q3872 N3873 G3874 E3875 K3876 D3901 R3907 T3908 I3919 L3927 Q3930 D3944 F3954 M3958 I3972 Q3973 G3974 P3975 L3983 W3989 F3995 D4009
I4013 L4016 K4017 M4050 L4071 K4072 D4073 I4074 V4075 G4076 S4077 E4078 A4079 F4080 Q4081 D4082 Y4083 V4084 T4085 D4086 P4087 R4088 G4089 K4093 K4094 D4095 F4096 Q4097 K4098 A4099 M4100 D4101 S4102 Q4103 K4104 Q4105 F4106 T4107 G4108 P4109 E4110 I4111 L4115 E4119 A4120 D4121 E4122 N4123 E4124 M4125 I4126 N4127 C4128
E4129 E4130 F4131 A4132 N4133 R4134 F4135 Q4136 E4137 P4138 I4142 D4160 R4164 L4167 I4186 I4196 E4202 V4225 N4226 E4227 G4228 G4229 E4230 S4231 E4235 Q4249 Q4253 E4256 P4257 GLU GLY GLU PRO GLU GLU ASP GLU ASP GLU GLY ALA GLU GLU ALA GLU GLU GLY ALA
ALA GLY SER ASP GLY SER GLY SER ALA ALA ALA ALA GLY VAL TRP VAL TRP LEU ALA ALA THR ALA GLY ARG THR LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA VAL ALA ALA LEU LEU TRP ALA LEU
VAL THR ARG ALA GLY GLY ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL ASP SER ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR GLY ASP GLU VAL HIS GLY GLN GLN PRO SER GLY ALA
GLY SER ASP ALA GLU GLY GLU GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA ASP GLY ALA GLY ASP GLU GLU ALA ALA ALA ASP GLN ALA GLY THR GLY GLY ALA ASP GLY ALA VAL ALA VAL ALA ASP GLY SER PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP
THR THR PRO VAL GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU PRO PRO PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP THR GLU ASN GLY GLU LYS GLU VAL PRO GLU PRO PRO PRO GLU PRO PRO
LYS LYS THR PRO PRO PRO PRO PRO LYS LYS GLU GLU ALA GLY GLY ALA GLY LEU GLU GLU F4538 W4539 G4540 E4541 L4542 Q4545 I4574 V4580 S4581 D4582 P4585 GLY GLU ASP ASP ILE GLU GLY SER GLY ALA GLY ASP MET SER GLY ALA GLY SER GLY ASP GLY SER GLY TRP

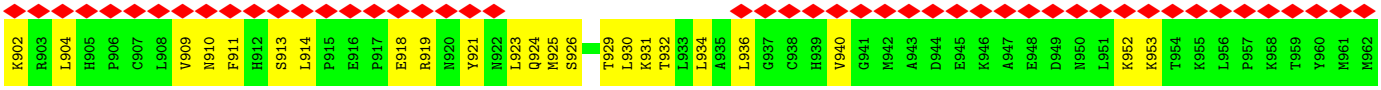


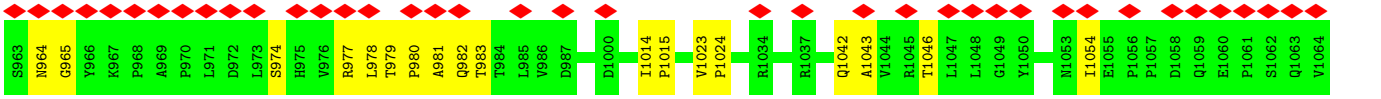
• Molecule 1: Ryanodine receptor 1

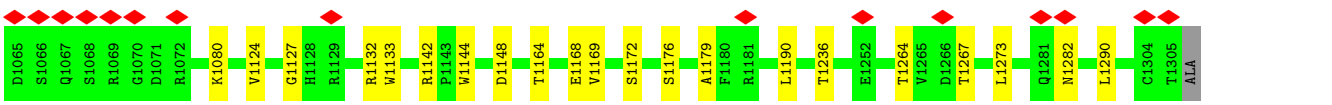
Chain D:

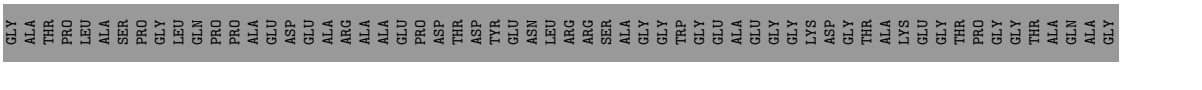


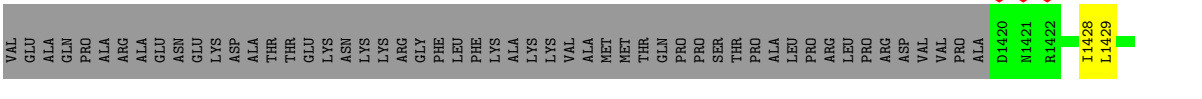


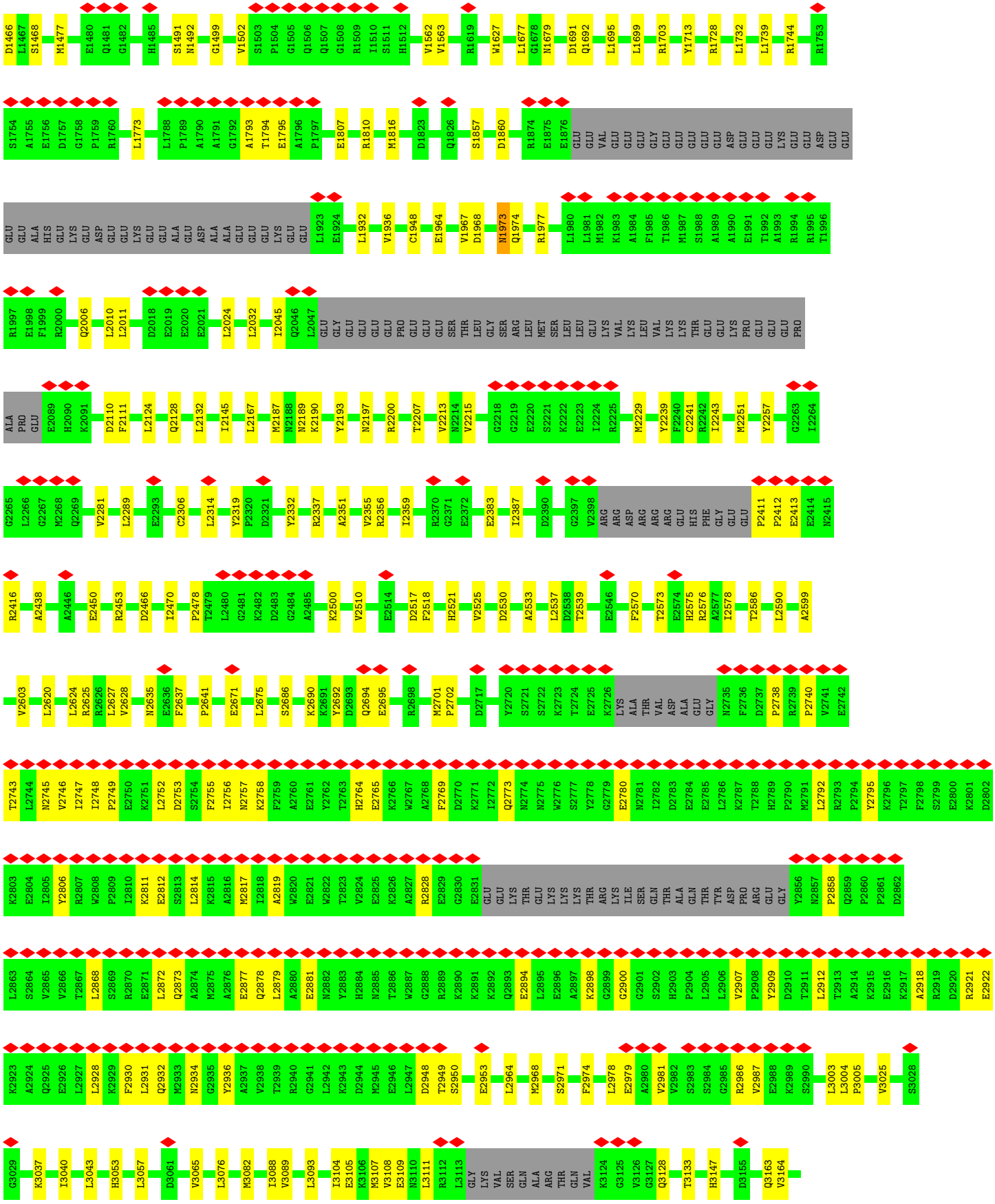








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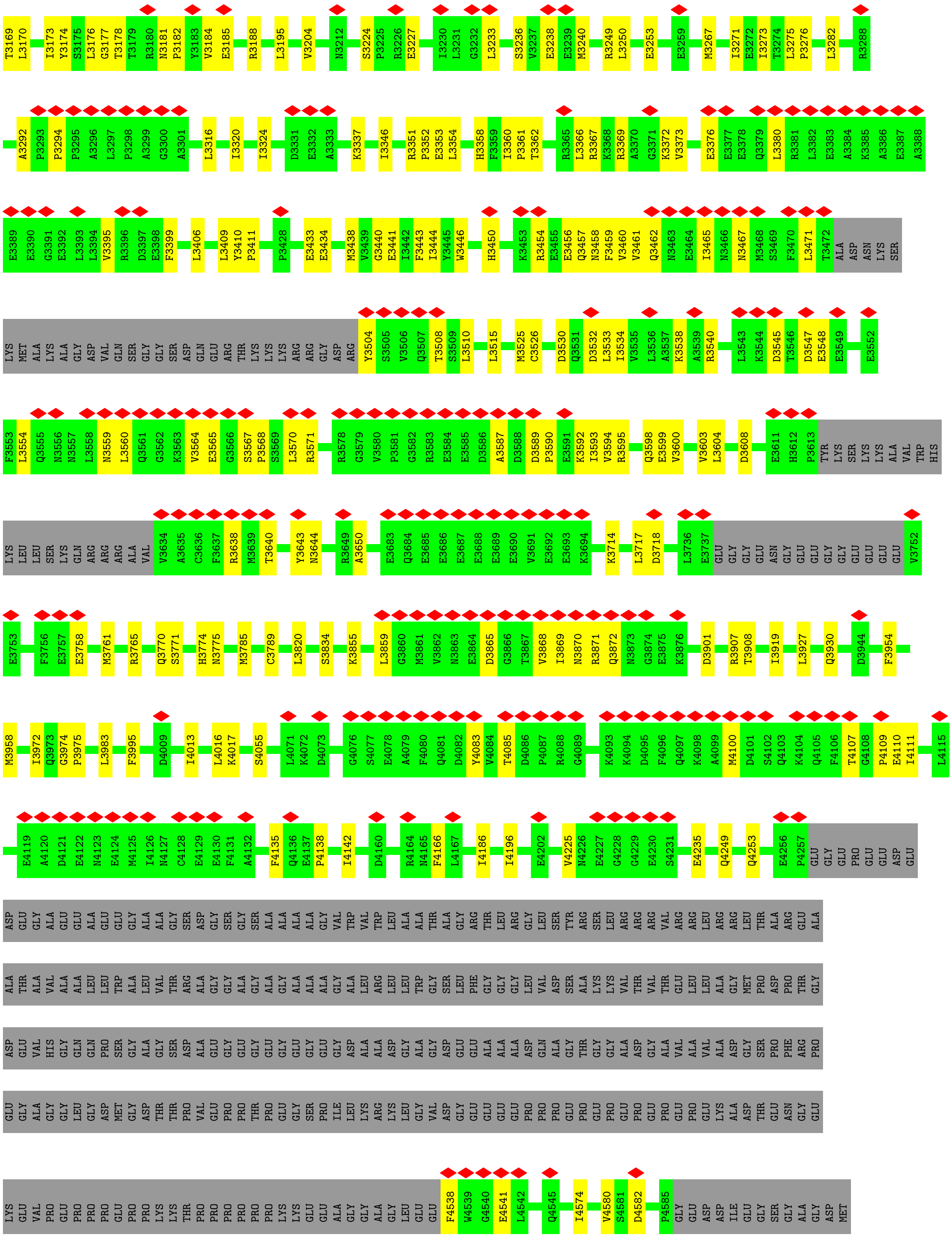
S1754 A1755 E1756 D1757 G1758 P1759 R1760 L1773 L1788 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 P1797 E1807 R1810 M1816 D1823 Q1826 S1857 D1860 R1874 E1875 E1876 GLU GLU VAL GLU GLU GLY GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU
GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU LYS GLU GLU L1923 E1924 L1932 V1936 C1948 E1964 V1967 D1968 N1973 Q1974 R1977 L1980 L1981 M1982 K1983 A1984 F1985 T1986 M1987 S1988 A1989 A1990 E1991 T1992 A1993 R1994 R1995 T1996
R1997 E1998 F1999 R2000 Q2006 L2010 L2011 D2018 E2019 E2020 E2021 L2024 L2032 I2045 Q2046 L2047 GLU GLY GLU GLU GLU PRO GLU GLU GLU SER THR LEU GLY SER ARG LEU MET SER LEU LEU GLU LYS VAL LYS LEU VAL LYS LYS THR GLU GLU LYS PRO GLU GLU GLU PRO
ALA PRO GLU E2089 H2090 K2091 D2110 F2111 L2124 Q2128 L2132 I2145 L2167 M2187 N2188 N2189 K2190 Y2193 N2197 R2200 T2207 V2213 N2214 V2215 G2218 G2219 E2220 S2221 K2222 E2223 I2224 R2225 M2229 Y2239 F2240 C2241 R2242 I2243 M2251 Y2257 G2263 I2264
G2265 L2266 G2267 M2268 Q2269 V2281 L2289 E2293 C2306 L2314 Y2319 P2320 D2321 Y2332 R2337 A2351 V2355 R2356 I2359 R2370 G2371 E2372 E2383 I2387 D2390 G2397 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 N2415
R2416 A2438 A2446 E2450 R2453 D2466 I2470 P2478 T2479 L2480 G2481 K2482 D2483 G2484 A2485 K2500 V2510 E2514 D2517 F2518 H2521 V2525 D2530 A2533 L2537 D2538 T2539 E2546 F2570 T2573 E2574 H2575 R2576 A2577 I2578 T2586 L2590 A2599
V2603 L2620 L2624 R2625 R2626 L2627 V2628 N2635 E2636 F2637 P2641 E2671 L2675 S2686 K2690 K2691 Y2692 D2693 Q2694 E2695 R2698 M2701 P2702 D2717 Y2720 S2721 S2722 K2723 T2724 E2725 K2726 LYS ALA THR VAL ASP ALA GLU GLY N2735 F2736 D2737 P2738 R2739 P2740 V2741 E2742
T2743 L2744 N2745 V2746 I2747 I2748 P2749 E2750 K2751 L2752 D2753 S2754 F2755 I2756 N2757 K2758 F2759 A2760 E2761 Y2762 T2763 H2764 E2765 K2766 W2767 A2768 F2769 D2770 K2771 I2772 Q2773 N2774 N2775 W2776 S2777 Y2778 G2779 E2780 N2781 I2782 D2783 E2784 E2785 L2786 K2787 T2788 H2789 P2790 M2791 L2792 R2793 P2794 Y2795 K2796 T2797 F2798 S2799 E2800 K2801 D2802
K2803 E2804 I2805 Y2806 R2807 W2808 P2809 I2810 K2811 E2812 S2813 L2814 K2815 A2816 M2817 I2818 A2819 W2820 E2821 W2822 T2823 V2824 E2825 K2826 A2827 R2828 E2829 G2830 E2831 GLU GLU LYS THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2856 N2857 P2858 Q2859 P2860 P2861 D2862
L2863 S2864 V2865 V2866 T2867 L2868 S2869 R2870 E2871 L2872 Q2873 A2874 M2875 A2876 E2877 Q2878 L2879 A2880 E2881 N2882 Y2883 H2884 N2885 T2886 W2887 G2888 R2889 K2890 K2891 K2892 Q2893 E2894 L2895 E2896 A2897 K2898 G2899 G2900 G2901 S2902 H2903 P2904 L2905 L2906 V2907 P2908 Y2909 D2910 T2911 L2912 T2913 A2914 K2915 E2916 K2917 A2918 R2919 D2920 R2921 E2922
K2923 A2924 Q2925 E2926 L2927 L2928 K2929 F2930 L2931 Q2932 M2933 N2934 G2935 Y2936 A2937 V2938 T2939 R2940 G2941 L2942 K2943 D2944 M2945 E2946 L2947 D2948 T2949 S2950 E2953 L2964 M2968 S2971 F2974 L2978 E2979 A2980 V2981 V2982 S2983 S2984 G2985 R2986 V2987 E2988 K2989 S2990 L3003 L3004 P3005 V3025 S3028
G3029 K3037 I3040 L3043 H3053 L3057 D3061 V3065 L3076 M3082 I3088 V3089 L3093 I3104 E3105 K3106 M3107 V3108 E3109 N3110 L3111 R3112 L3113 GLY LYS VAL SER GLN ALA ARG THR GLN VAL K3124 G3125 V3126 G3127 Q3128 T3133 H3147 D3155 Q3163 V3164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A3292 P3293 P3294 P3295 A3296 L3297 P3298 A3299 G3300 A3301 L3316 I3320 I3324 D3331 E3332 A3333 K3337 I3346 R3351 P3352 E3353 L3354 H3358 F3359 I3360 P3361 T3362 R3365 L3366 R3367 K3368 R3369 A3370 G3371 K3372 V3373 E3376 E3377 E3378 Q3379 L3380 R3381 L3382 E3383 A3384 K3385 A3386 E3387 A3388
E3389 E3390 G3391 E3392 L3393 L3394 V3395 R3396 D3397 E3398 F3399 L3406 L3409 Y3410 P3411 P3428 E3433 E3434 M3438 V3439 G3440 E3441 I3442 F3443 I3444 Y3445 W3446 H3450 K3453 R3454 E3455 E3456 Q3457 N3458 F3459 V3460 V3461 Q3462 N3463 E3464 I3465 N3466 N3467 M3468 S3469 F3470 L3471 T3472 ALA ASP ASN LYS SER
LYS MET ALA LYS ALA GLY ASP VAL GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3504 S3505 V3506 Q3507 T3508 S3509 L3510 L3515 M3525 C3526 D3530 Q3531 D3532 L3533 I3534 V3535 L3536 A3537 K3538 A3539 R3540 L3543 K3544 D3545 T3546 D3547 E3548 E3549 E3552
F3553 L3554 Q3555 N3556 N3557 L3558 N3559 L3560 Q3561 G3562 K3563 V3564 E3565 G3566 S3567 P3568 S3569 L3570 R3571 R3578 G3579 V3580 P3581 G3582 R3583 E3584 E3585 D3586 A3587 D3588 D3589 P3590 E3591 K3592 I3593 V3594 R3595 Q3598 E3599 V3600 V3603 L3604 D3608 E3611 H3612 P3613 TYR LYS SER LYS LYS ALA VAL TRP HIS
LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL V3634 A3635 C3636 F3637 R3638 M3639 T3640 Y3643 N3644 R3649 A3650 E3683 Q3684 E3685 E3686 E3687 E3688 E3689 E3690 V3691 E3692 E3693 K3694 K3714 L3717 D3718 L3736 E3737 GLU GLY GLY GLU ASN GLY GLU GLU GLY GLY GLU GLU GLU GLU V3752
E3753 F3756 E3757 E3758 M3761 R3765 Q3770 S3771 H3774 N3775 M3785 C3789 L3820 S3834 K3855 L3859 G3860 M3861 V3862 N3863 E3864 D3865 G3866 T3867 V3868 I3869 N3870 R3871 Q3872 N3873 G3874 E3875 K3876 D3901 R3907 T3908 I3919 L3927 Q3930 D3944 F3954
M3958 I3972 Q3973 G3974 P3975 L3983 F3995 D4009 I4013 L4016 K4017 S4055 L4071 K4072 D4073 G4076 S4077 E4078 A4079 F4080 Q4081 D4082 Y4083 V4084 T4085 D4086 P4087 R4088 G4089 K4093 K4094 D4095 F4096 Q4097 K4098 A4099 M4100 D4101 S4102 Q4103 K4104 Q4105 F4106 T4107 G4108 P4109 E4110 I4111 L4115
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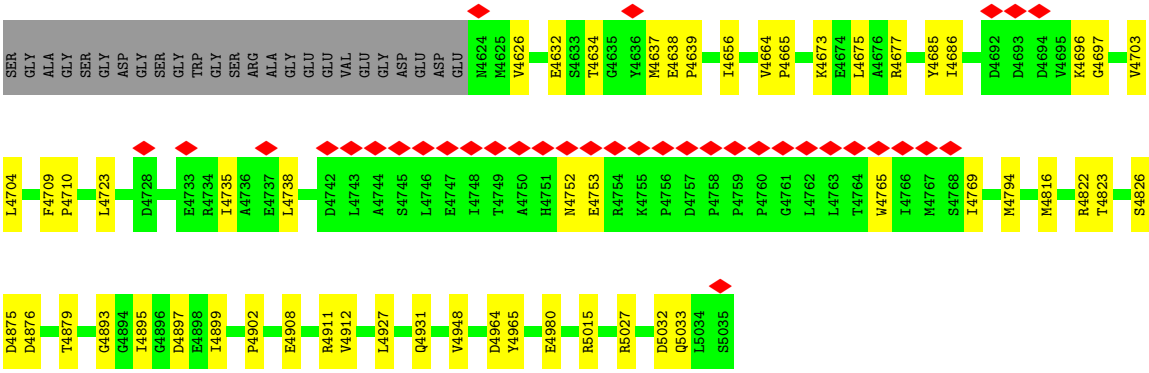
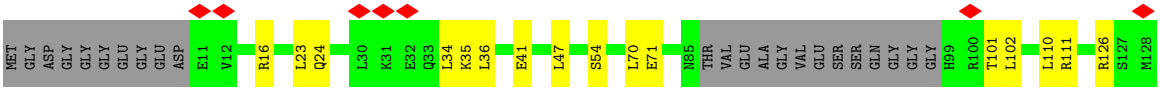
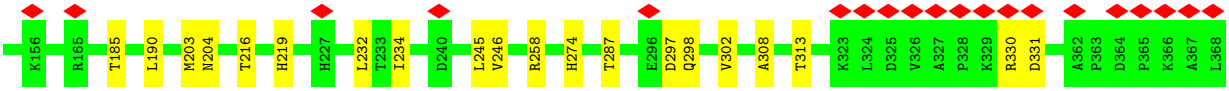
ASP GLU GLY ALA GLU GLU ALA GLU GLU GLY ALA ALA GLY SER ASP GLY SER GLY SER ALA ALA ALA ALA GLY VAL TRP VAL TRP LEU ALA ALA THR ALA GLY ARG THR LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA
ALA THR ALA VAL ALA ALA LEU LEU TRP ALA LEU VAL THR ARG ALA GLY GLY ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL ASP SER ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR GLY
ASP GLU VAL HIS GLY GLN GLN PRO SER GLY ALA GLY SER ASP ALA GLU GLY GLU GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA ASP GLY ALA GLY ASP GLU GLU ALA ALA ALA ASP GLN ALA GLY THR GLY GLY ALA ASP GLY ALA VAL ALA VAL ALA ASP GLY SER PRO PHE ARG PRO
GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO VAL GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU PRO PRO PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP THR GLU ASN GLY GLU
LYS GLU VAL PRO GLU PRO PRO PRO GLU PRO PRO LYS LYS THR PRO PRO PRO PRO PRO PRO LYS LYS GLU GLU ALA GLY GLY ALA GLY LEU GLU GLU F4538 W4539 G4540 E4541 L4542 Q4545 I4574 V4580 S4581 D4582 P4585 GLY GLU ASP ASP ILE GLU GLY SER GLY ALA GLY ASP MET

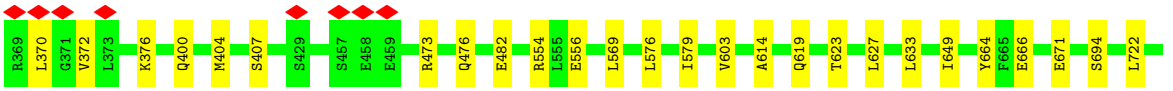


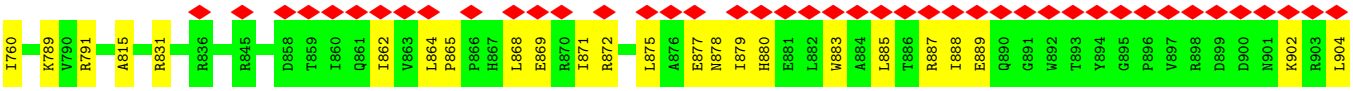
• Molecule 1: Ryanodine receptor 1

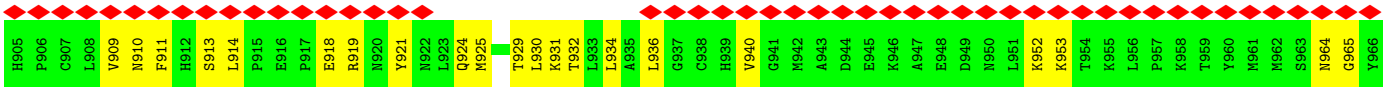
Chain B:

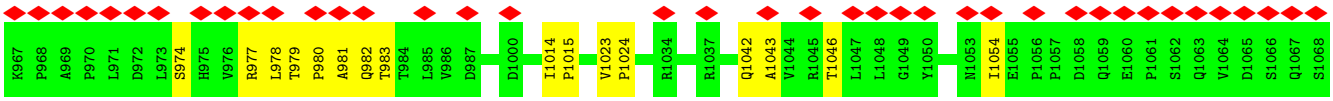


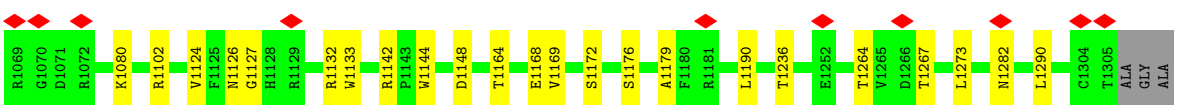


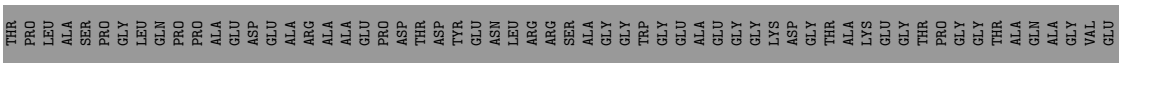


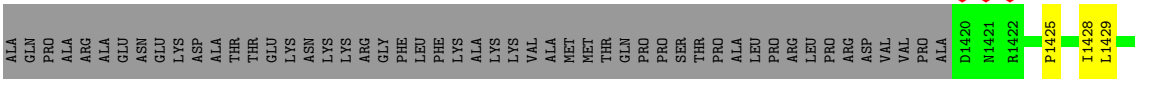


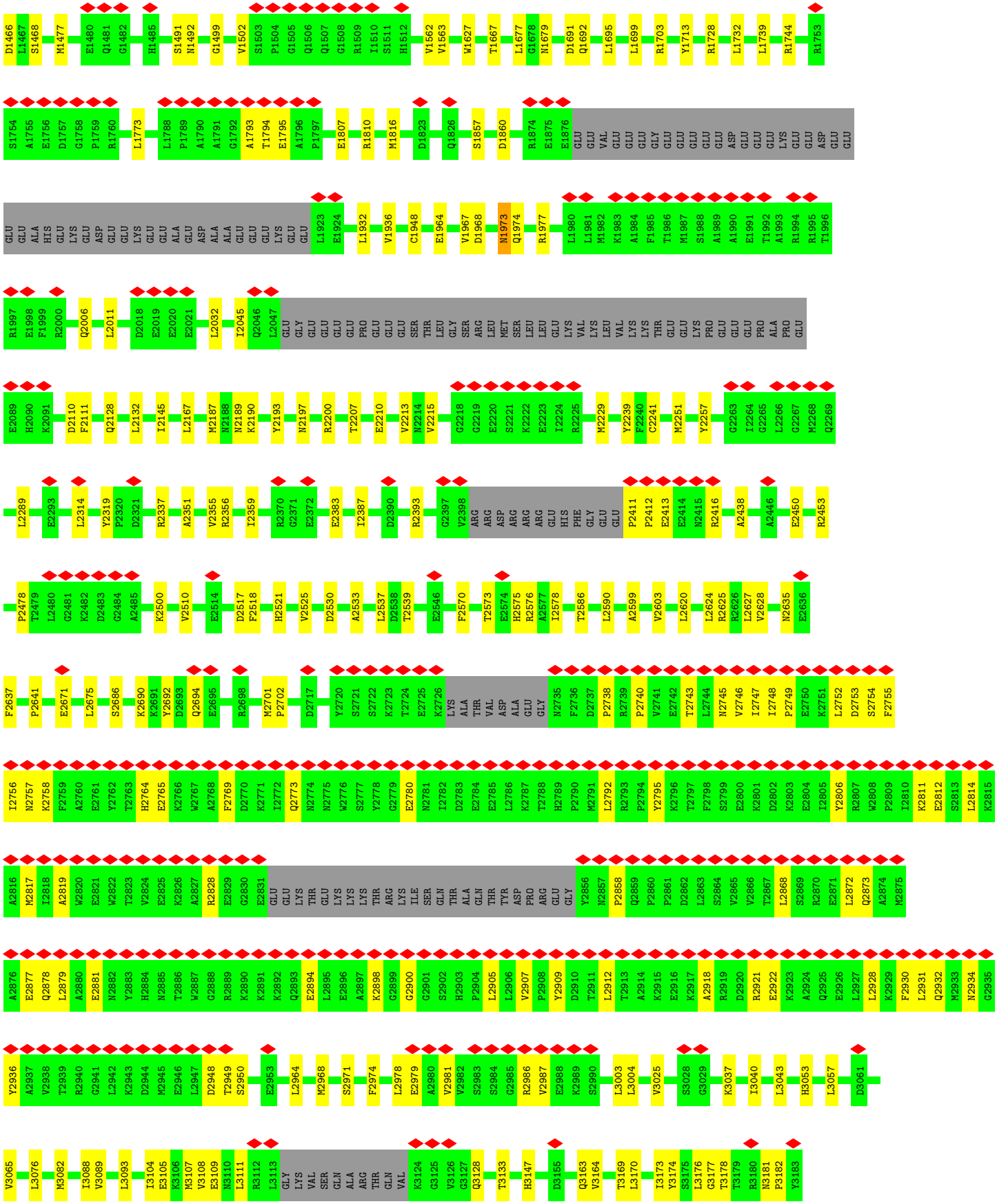








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S1754 A1755 E1756 D1757 G1758 P1759 R1760 L1773 L1788 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 P1797 E1807 R1810 M1816 D1823 Q1826 S1857 D1860 R1874 E1875 E1876 GLU GLU VAL GLU GLU GLU GLY GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU
GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU LYS GLU GLU L1923 E1924 L1932 V1936 C1948 E1964 V1967 D1968 N1973 Q1974 R1977 L1980 L1981 M1982 K1983 A1984 F1985 T1986 M1987 S1988 A1989 A1990 E1991 T1992 A1993 R1994 R1995 T1996
R1997 E1998 F1999 R2000 Q2006 L2011 D2018 E2019 E2020 E2021 L2032 I2045 Q2046 L2047 GLU GLY GLU GLU GLU PRO GLU GLU GLU SER THR LEU GLY SER ARG LEU MET SER LEU LEU GLU LYS VAL LYS LEU VAL LYS LYS THR GLU GLU LYS PRO GLU GLU GLU PRO ALA PRO GLU
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L2289 E2293 L2314 Y2319 P2320 D2321 R2337 A2351 V2355 R2356 I2359 R2370 G2371 E2372 E2383 I2387 D2390 R2393 G2397 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 N2415 R2416 A2438 A2446 E2450 R2453
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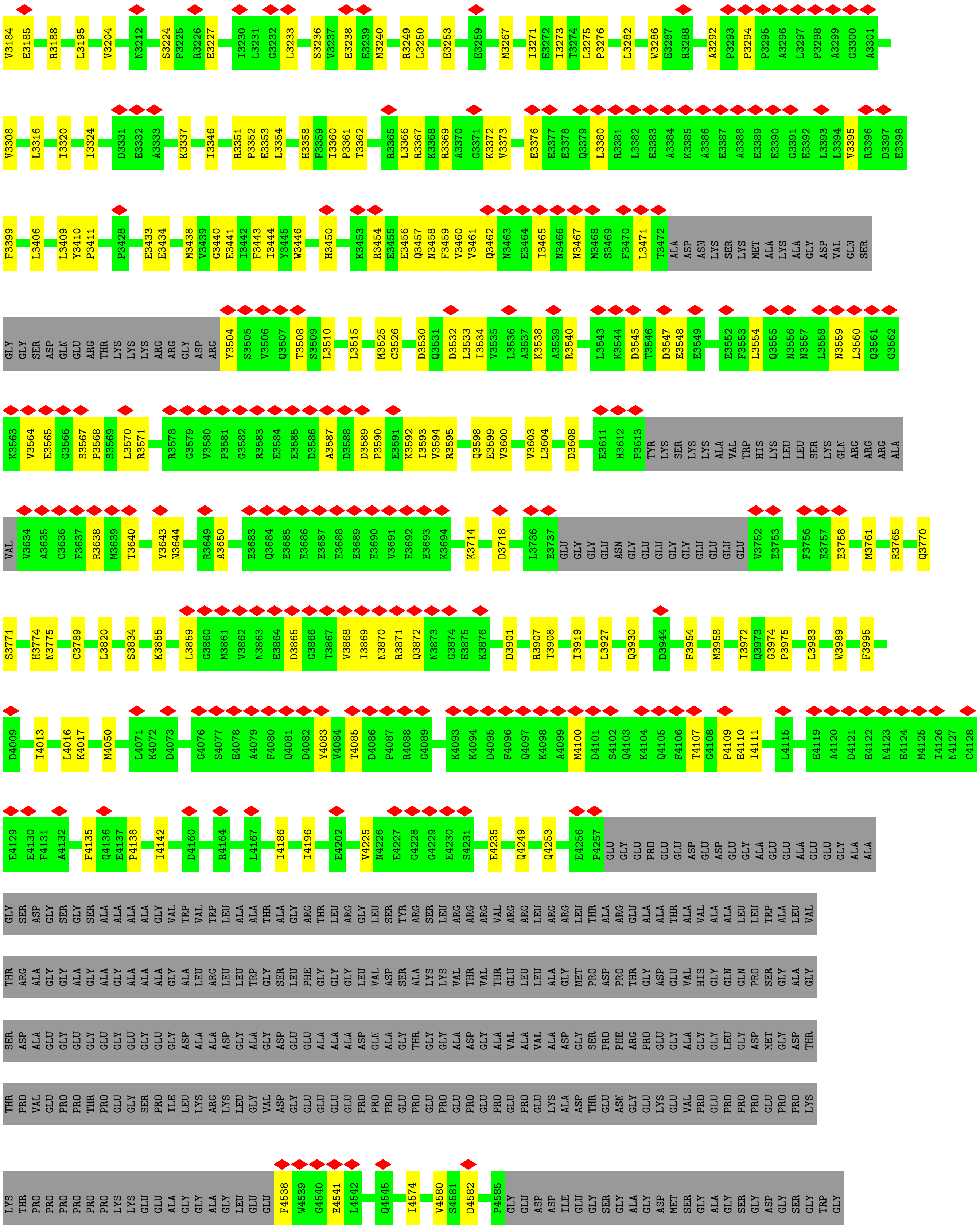
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GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG Y3504 S3505 V3506 Q3507 T3508 S3509 L3510 L3515 M3525 C3526 D3530 Q3531 D3532 L3533 I3534 V3535 L3536 A3537 K3538 A3539 R3540 L3543 K3544 D3545 T3546 D3547 E3548 E3549 E3552 F3553 L3554 Q3555 N3556 N3557 L3558 N3559 L3560 Q3561 G3562
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E4129 E4130 F4131 A4132 F4135 Q4136 E4137 P4138 I4142 D4160 R4164 L4167 I4186 I4196 E4202 V4225 N4226 E4227 G4228 G4229 E4230 S4231 E4235 Q4249 Q4253 E4256 P4257 GLU GLY GLU PRO GLU GLU ASP GLU ASP GLU GLY ALA GLU GLU ALA GLU GLU GLY ALA ALA
GLY SER ASP GLY SER GLY SER ALA ALA ALA ALA GLY VAL TRP VAL TRP LEU ALA ALA THR ALA GLY ARG THR LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG LEU THR ALA ARG GLU ALA ALA THR ALA VAL ALA ALA LEU LEU TRP ALA LEU VAL
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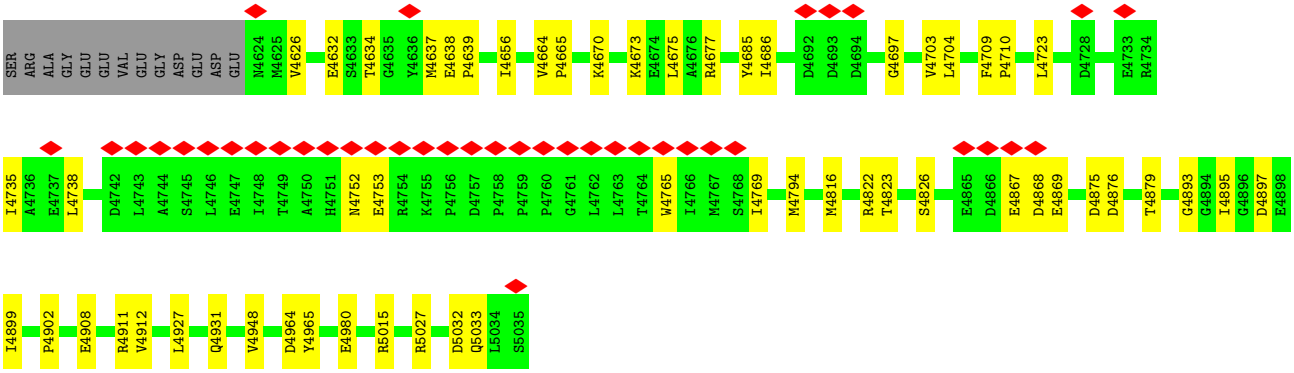
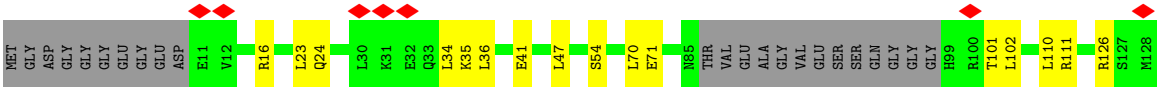
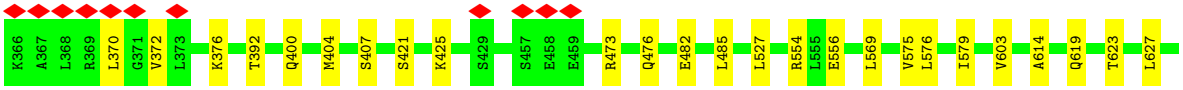
LYS THR PRO PRO PRO PRO PRO PRO LYS LYS GLU GLU ALA GLY GLY ALA GLY LEU GLU GLU F4538 W4539 G4540 E4541 L4542 Q4545 I4574 V4580 S4581 D4582 P4585 GLY GLU ASP ASP ILE GLU GLY SER GLY ALA GLY ASP MET SER GLY ALA GLY SER GLY ASP GLY SER GLY TRP GLY

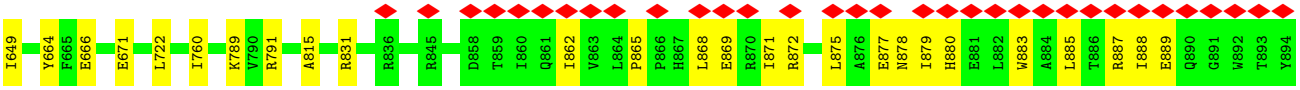


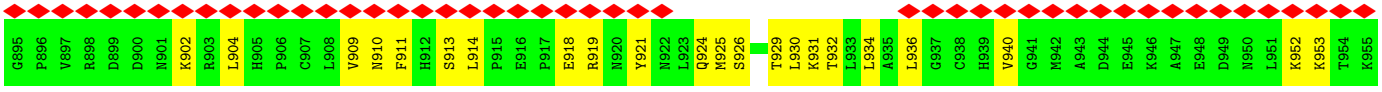
• Molecule 1: Ryanodine receptor 1

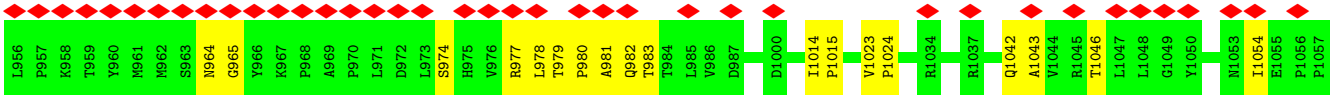
Chain C:

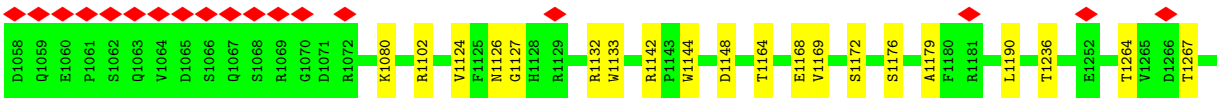


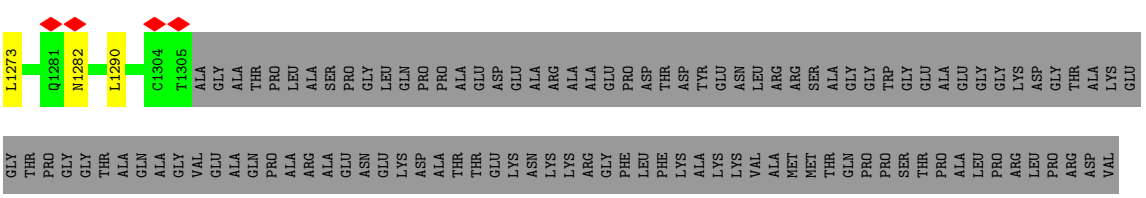


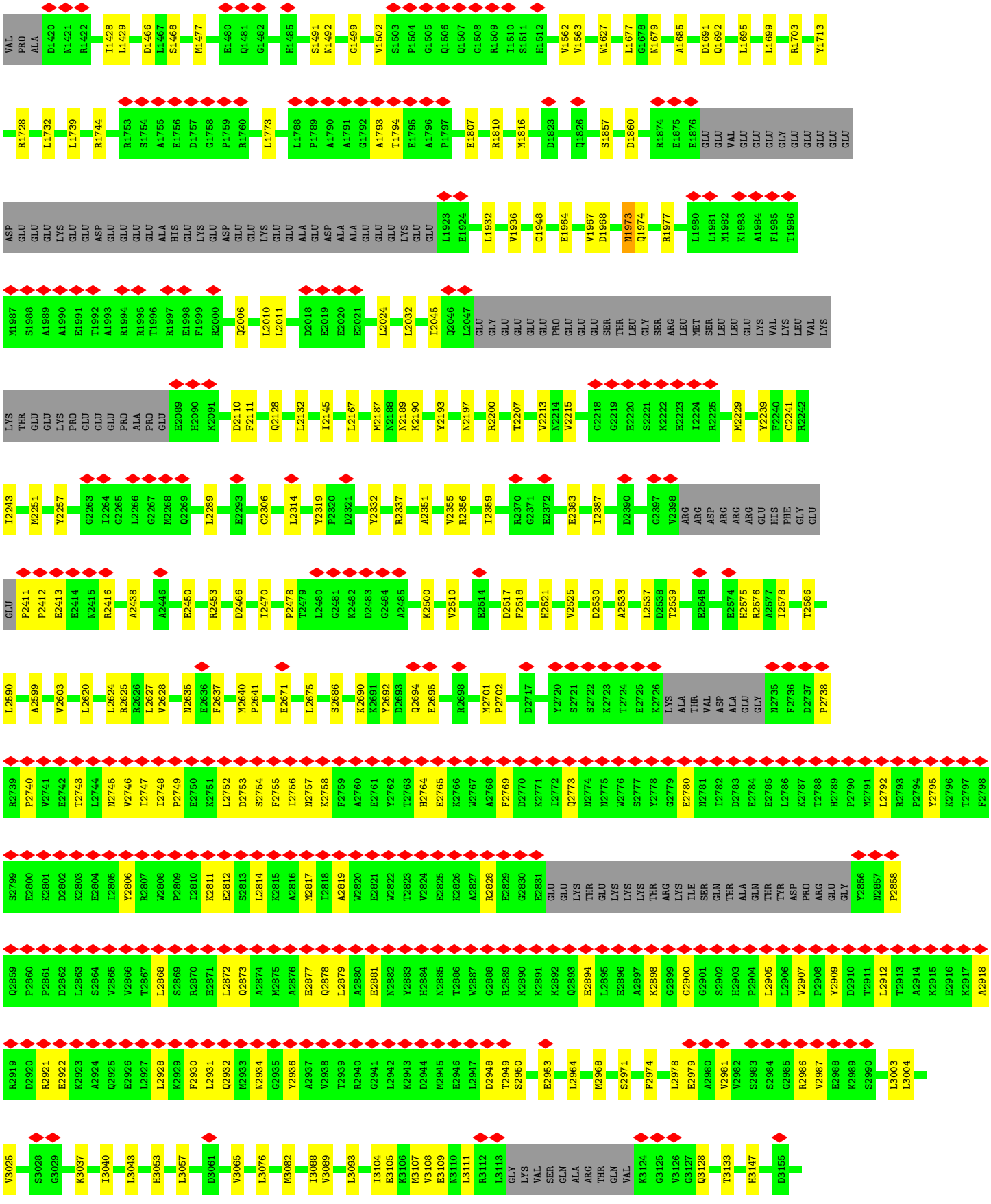


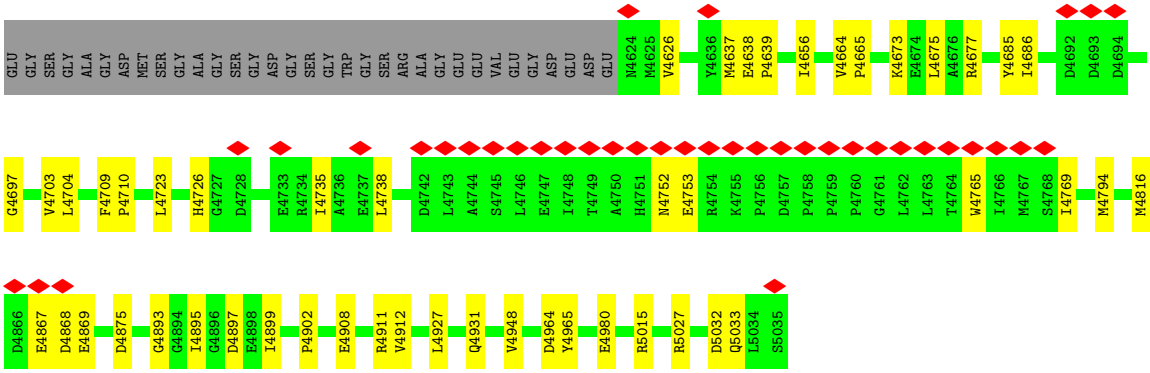






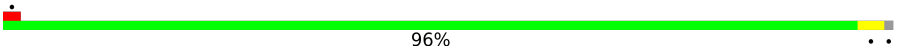


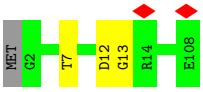

VAL PRO ALA D1420 N1421 R1422 I1428 L1429 D1466 L1467 S1468 M1477 E1480 Q1481 G1482 H1485 S1491 N1492 G1499 V1502 S1503 P1504 G1505 Q1506 Q1507 G1508 R1509 I1510 S1511 H1512 V1562 V1563 W1627 L1677 G1678 N1679 A1685 D1691 Q1692 L1695 L1699 R1703 Y1713
R1728 L1732 L1739 R1744 R1753 S1754 A1755 E1756 D1757 G1758 P1759 R1760 L1773 L1788 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 P1797 E1807 R1810 M1816 D1823 Q1826 S1857 D1860 R1874 E1875 E1876 GLU GLU VAL GLU GLU GLU GLY GLU GLU GLU GLU
ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU LYS GLU GLU L1923 E1924 L1932 V1936 C1948 E1964 V1967 D1968 N1973 Q1974 R1977 L1980 L1981 M1982 K1983 A1984 F1985 T1986
M1987 S1988 A1989 A1990 E1991 T1992 A1993 R1994 R1995 T1996 R1997 E1998 F1999 R2000 Q2006 L2010 L2011 D2018 E2019 E2020 E2021 L2024 L2032 I2045 Q2046 L2047 GLU GLY GLU GLU GLU PRO GLU GLU GLU SER THR LEU GLY SER ARG LEU MET SER LEU LEU GLU LYS VAL LYS LEU VAL LYS
LYS THR GLU GLU LYS PRO GLU GLU GLU PRO ALA PRO GLU E2089 H2090 K2091 D2110 F2111 Q2128 L2132 I2145 L2167 M2187 N2188 N2189 K2190 Y2193 N2197 R2200 T2207 V2213 N2214 V2215 G2218 G2219 E2220 S2221 K2222 E2223 I2224 R2225 M2229 Y2239 F2240 C2241 R2242
I2243 M2251 Y2257 G2263 I2264 G2265 L2266 G2267 M2268 Q2269 L2289 E2293 C2306 L2314 Y2319 P2320 D2321 Y2332 R2337 A2351 V2355 R2356 I2359 R2370 G2371 E2372 E2383 I2387 D2390 G2397 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU
GLU P2411 P2412 E2413 E2414 N2415 R2416 A2438 A2446 E2450 R2453 D2466 I2470 P2478 T2479 L2480 G2481 K2482 D2483 G2484 A2485 K2500 V2510 E2514 D2517 F2518 H2521 V2525 D2530 A2533 L2537 D2538 T2539 E2546 E2574 H2575 R2576 A2577 I2578 T2586
L2590 A2599 V2603 L2620 L2624 R2625 R2626 L2627 V2628 N2635 E2636 F2637 M2640 P2641 E2671 L2675 S2686 K2690 K2691 Y2692 D2693 Q2694 E2695 R2698 M2701 P2702 D2717 Y2720 S2721 S2722 K2723 T2724 E2725 K2726 LYS ALA THR VAL ASP ALA GLU GLY N2735 F2736 D2737 P2738
R2739 P2740 V2741 E2742 T2743 L2744 N2745 V2746 I2747 I2748 P2749 E2750 K2751 L2752 D2753 S2754 F2755 I2756 N2757 K2758 F2759 A2760 E2761 Y2762 T2763 H2764 E2765 K2766 W2767 A2768 F2769 D2770 K2771 I2772 Q2773 N2774 N2775 W2776 S2777 Y2778 G2779 E2780 N2781 I2782 D2783 E2784 E2785 L2786 K2787 T2788 H2789 P2790 M2791 L2792 R2793 P2794 Y2795 K2796 T2797 E2798
S2799 E2800 K2801 D2802 K2803 E2804 I2805 Y2806 R2807 W2808 P2809 I2810 K2811 E2812 S2813 L2814 K2815 A2816 M2817 I2818 A2819 W2820 E2821 W2822 T2823 V2824 E2825 K2826 A2827 R2828 E2829 G2830 E2831 GLU GLU LYS THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2856 N2857 P2858
Q2859 P2860 P2861 D2862 L2863 S2864 V2865 V2866 T2867 L2868 S2869 R2870 E2871 L2872 Q2873 A2874 M2875 A2876 E2877 Q2878 L2879 A2880 E2881 N2882 Y2883 H2884 N2885 T2886 W2887 G2888 R2889 K2890 K2891 K2892 Q2893 E2894 L2895 E2896 A2897 K2898 G2899 G2900 G2901 S2902 H2903 P2904 L2905 L2906 V2907 P2908 Y2909 D2910 T2911 L2912 T2913 A2914 K2915 E2916 K2917 A2918
R2919 D2920 R2921 E2922 K2923 A2924 Q2925 E2926 L2927 L2928 K2929 F2930 L2931 Q2932 M2933 N2934 G2935 Y2936 A2937 V2938 T2939 R2940 G2941 L2942 K2943 D2944 M2945 E2946 L2947 D2948 T2949 S2950 E2953 L2964 M2968 S2971 F2974 L2978 E2979 A2980 V2981 V2982 S2983 S2984 G2985 R2986 V2987 E2988 K2989 S2990 L3003 L3004
V3025 S3028 G3029 K3037 I3040 L3043 H3053 L3057 D3061 V3065 L3076 M3082 I3088 V3089 L3093 I3104 E3105 K3106 M3107 V3108 E3109 N3110 L3111 R3112 L3113 GLY LYS VAL SER GLN ALA ARG THR GLN VAL K3124 G3125 V3126 G3127 Q3128 T3133 H3147 D3155



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

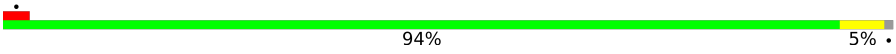
Chain E:

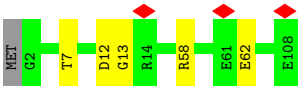




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

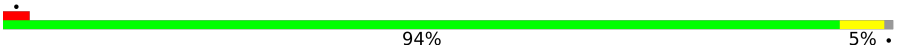
Chain H:

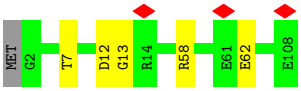




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

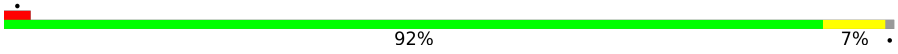
Chain F:

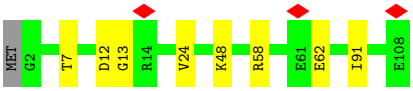




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

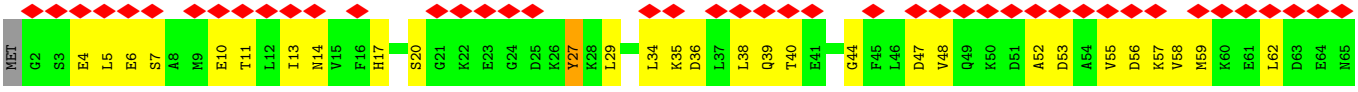
Chain G:

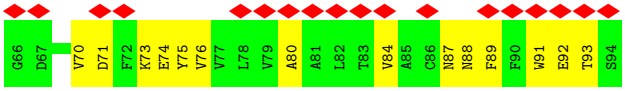




• Molecule 3: Protein S100A1

Chain J:



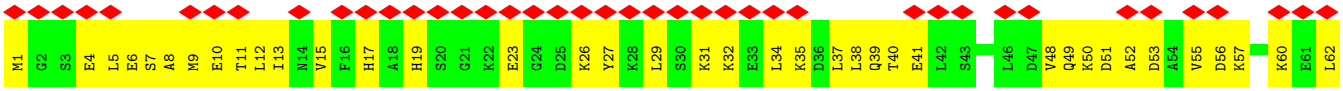


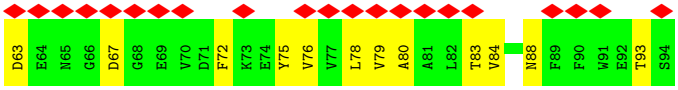
• Molecule 3: Protein S100A1

Chain I:

• Molecule 3: Protein S100A1

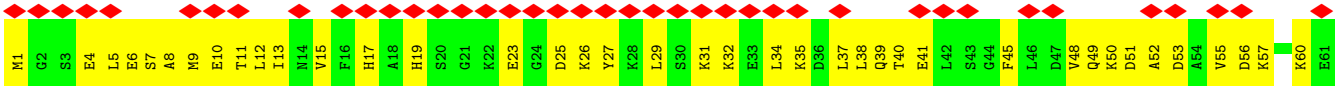
Chain K:





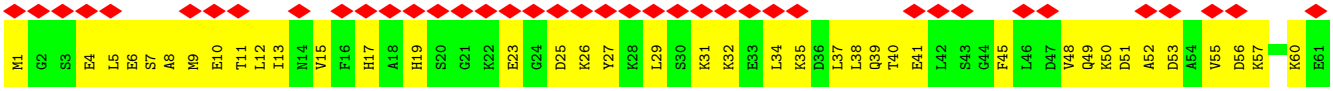
• Molecule 3: Protein S100A1

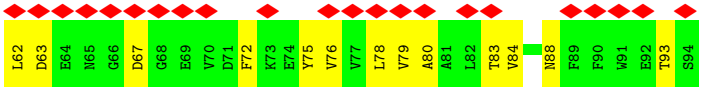
Chain M:



• Molecule 3: Protein S100A1

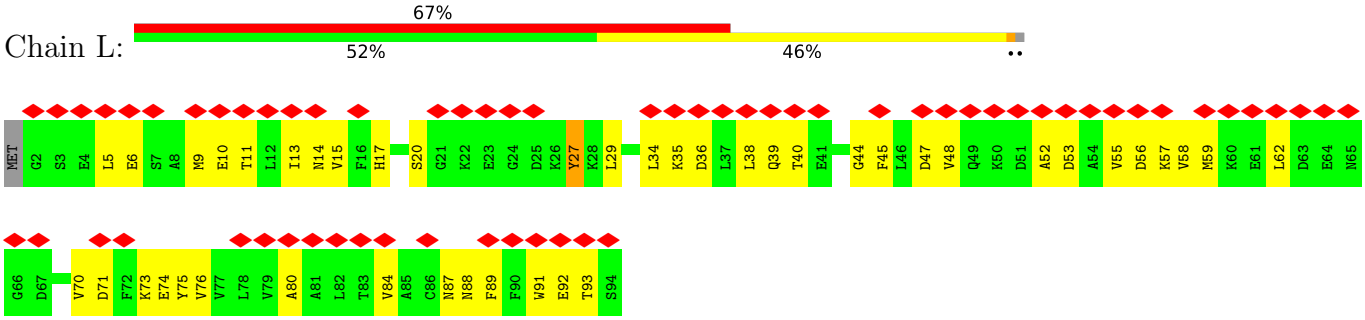
Chain O:





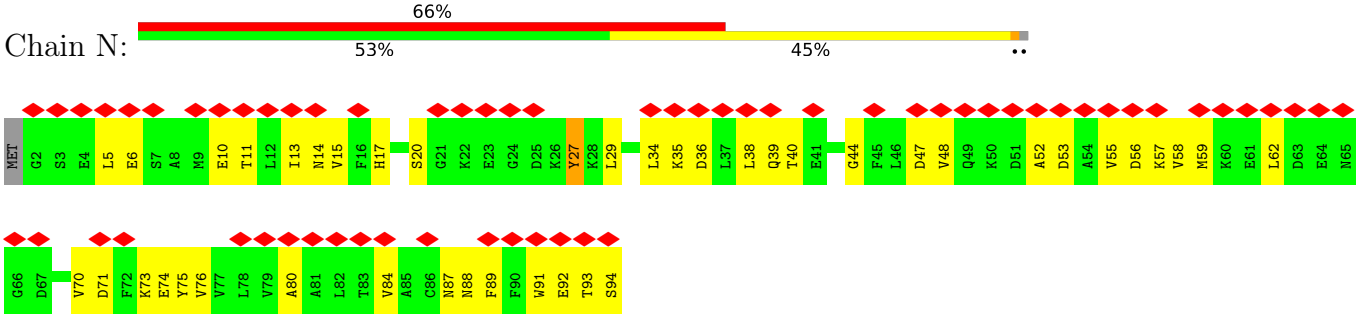
• Molecule 3: Protein S100A1

Chain L:



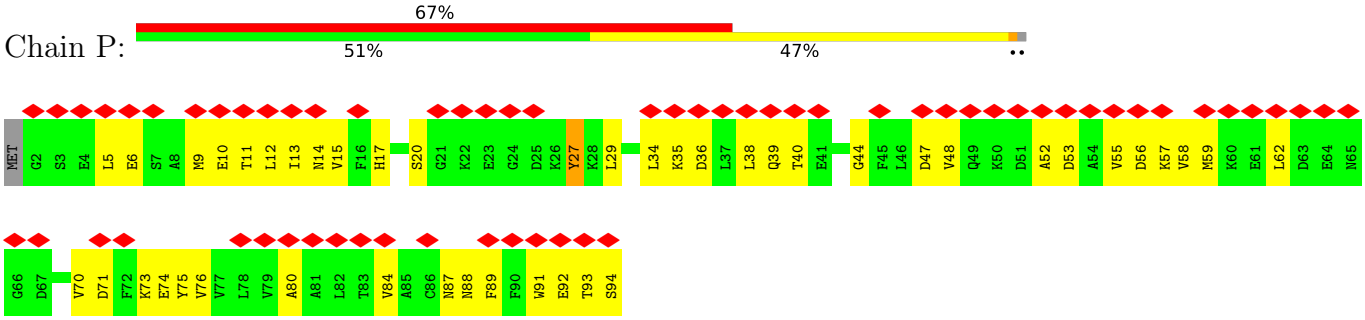
• Molecule 3: Protein S100A1

Chain N:



• Molecule 3: Protein S100A1

Chain P:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	36506	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)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.686	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/35601	0.48	0/48224
1	B	0.25	0/35601	0.48	0/48224
1	C	0.25	0/35601	0.48	0/48224
1	D	0.25	0/35601	0.48	0/48224
2	E	0.25	0/847	0.49	0/1142
2	F	0.25	0/847	0.50	0/1142
2	G	0.25	0/847	0.49	0/1142
2	H	0.25	0/847	0.49	0/1142
3	I	0.33	0/747	0.54	0/1002
3	J	0.29	0/739	0.50	0/992
3	K	0.33	0/747	0.54	0/1002
3	L	0.29	0/739	0.50	0/992
3	M	0.33	0/747	0.54	0/1002
3	N	0.29	0/739	0.50	0/992
3	O	0.33	0/747	0.54	0/1002
3	P	0.29	0/739	0.50	0/992
All	All	0.25	0/151736	0.49	0/205440

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3240	MET	Peptide
1	B	3240	MET	Peptide
1	C	3240	MET	Peptide
1	D	3240	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34809	0	34401	393	0
1	B	34809	0	34401	399	0
1	C	34809	0	34401	400	0
1	D	34809	0	34401	400	0
2	E	829	0	826	2	0
2	F	829	0	826	3	0
2	G	829	0	826	5	0
2	H	829	0	826	3	0
3	I	737	0	717	45	0
3	J	729	0	705	40	0
3	K	737	0	717	54	0
3	L	729	0	705	47	0
3	M	737	0	717	52	0
3	N	729	0	705	46	0
3	O	737	0	717	57	0
3	P	729	0	705	52	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	108	0	167	0	0
5	B	108	0	167	0	0
5	C	108	0	167	0	0
5	D	108	0	167	0	0
All	All	148852	0	147264	1911	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1911) 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:M:56:ASP:OD1	1:C:3638:ARG:NH2	1.59	1.34
1:A:3638:ARG:NH2	3:I:56:ASP:OD1	1.63	1.30
3:K:56:ASP:OD1	1:B:3638:ARG:NH2	1.63	1.30
3:O:56:ASP:OD1	1:D:3638:ARG:NH2	1.60	1.28
3:J:44:GLY:O	3:J:47:ASP:OD1	1.65	1.14
3:P:44:GLY:O	3:P:47:ASP:OD1	1.64	1.13
3:L:44:GLY:O	3:L:47:ASP:OD1	1.64	1.13
3:N:44:GLY:O	3:N:47:ASP:OD1	1.65	1.12
3:O:56:ASP:OD1	1:D:3638:ARG:CZ	2.01	1.08
3:M:56:ASP:OD1	1:C:3638:ARG:CZ	2.05	1.03
3:K:56:ASP:OD1	1:B:3638:ARG:CZ	2.05	1.03
1:D:2765:GLU:OE1	1:D:2795:TYR:OH	1.85	0.95
1:A:2765:GLU:OE1	1:A:2795:TYR:OH	1.85	0.94
1:C:2765:GLU:OE1	1:C:2795:TYR:OH	1.85	0.93
1:B:2765:GLU:OE1	1:B:2795:TYR:OH	1.85	0.93
3:J:5:LEU:HD13	3:I:15:VAL:HG11	1.52	0.92
1:C:979:THR:HG22	1:C:982:GLN:OE1	1.71	0.91
1:B:979:THR:HG22	1:B:982:GLN:OE1	1.71	0.91
1:A:3761:MET:SD	1:A:3765:ARG:NH1	2.44	0.91
1:D:979:THR:HG22	1:D:982:GLN:OE1	1.71	0.91
1:B:3761:MET:SD	1:B:3765:ARG:NH1	2.44	0.90
1:A:979:THR:HG22	1:A:982:GLN:OE1	1.71	0.90
1:C:3761:MET:SD	1:C:3765:ARG:NH1	2.44	0.90
1:D:3761:MET:SD	1:D:3765:ARG:NH1	2.44	0.89
1:C:2753:ASP:OD1	1:C:2811:LYS:NZ	2.06	0.89
3:L:47:ASP:OD2	1:B:2986:ARG:NH2	2.07	0.88
1:A:2753:ASP:OD1	1:A:2811:LYS:NZ	2.06	0.88
3:P:47:ASP:OD2	1:D:2986:ARG:NH2	2.07	0.88
1:B:2753:ASP:OD1	1:B:2811:LYS:NZ	2.06	0.87
1:D:2753:ASP:OD1	1:D:2811:LYS:NZ	2.06	0.87
1:A:3224:SER:OG	1:A:3227:GLU:OE1	1.94	0.86
1:B:3224:SER:OG	1:B:3227:GLU:OE1	1.94	0.85
1:C:3224:SER:OG	1:C:3227:GLU:OE1	1.94	0.85
3:M:5:LEU:HD23	3:M:9:MET:HE1	1.58	0.85
1:A:2986:ARG:NH2	3:J:47:ASP:OD2	2.08	0.85
1:D:3224:SER:OG	1:D:3227:GLU:OE1	1.94	0.85
3:K:93:THR:HG23	3:L:27:TYR:HB3	1.62	0.82

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3538:LYS:NZ	1:C:3608:ASP:OD2	2.13	0.82
3:N:47:ASP:OD2	1:C:2986:ARG:NH2	2.14	0.81
3:I:5:LEU:HD23	3:I:9:MET:HE1	1.62	0.81
1:A:1948:CYS:SG	1:A:2128:GLN:NE2	2.55	0.80
1:D:3538:LYS:NZ	1:D:3608:ASP:OD2	2.13	0.80
1:C:3761:MET:SD	1:C:3765:ARG:NH2	2.55	0.80
1:B:3761:MET:SD	1:B:3765:ARG:NH2	2.55	0.80
1:C:1948:CYS:SG	1:C:2128:GLN:NE2	2.55	0.80
1:A:3714:LYS:NZ	1:A:3718:ASP:OD2	2.16	0.79
1:D:1948:CYS:SG	1:D:2128:GLN:NE2	2.55	0.79
1:D:3761:MET:SD	1:D:3765:ARG:NH2	2.55	0.79
1:C:3714:LYS:NZ	1:C:3718:ASP:OD2	2.16	0.79
1:A:3761:MET:SD	1:A:3765:ARG:NH2	2.55	0.79
1:B:1948:CYS:SG	1:B:2128:GLN:NE2	2.55	0.79
3:L:92:GLU:O	3:L:93:THR:OG1	2.01	0.79
1:A:974:SER:O	1:A:977:ARG:NH1	2.16	0.78
3:J:92:GLU:O	3:J:93:THR:OG1	2.01	0.78
1:C:974:SER:O	1:C:977:ARG:NH1	2.16	0.78
1:D:3714:LYS:NZ	1:D:3718:ASP:OD2	2.16	0.78
1:A:3538:LYS:NZ	1:A:3608:ASP:OD2	2.13	0.78
1:D:974:SER:O	1:D:977:ARG:NH1	2.16	0.78
1:B:974:SER:O	1:B:977:ARG:NH1	2.16	0.78
1:B:3714:LYS:NZ	1:B:3718:ASP:OD2	2.16	0.78
1:A:70:LEU:HD13	1:A:102:LEU:HD11	1.65	0.77
1:A:3638:ARG:CZ	3:I:56:ASP:OD1	2.32	0.77
1:B:70:LEU:HD13	1:B:102:LEU:HD11	1.65	0.77
1:C:1691:ASP:OD1	1:C:1692:GLN:N	2.17	0.77
3:P:92:GLU:O	3:P:93:THR:OG1	2.01	0.77
1:B:1691:ASP:OD1	1:B:1692:GLN:N	2.17	0.77
3:N:92:GLU:O	3:N:93:THR:OG1	2.01	0.77
1:C:70:LEU:HD13	1:C:102:LEU:HD11	1.65	0.77
1:A:3082:MET:CE	1:A:3093:LEU:HD23	2.15	0.76
1:A:2877:GLU:OE2	1:A:2921:ARG:NH1	2.18	0.76
1:D:3082:MET:CE	1:D:3093:LEU:HD23	2.15	0.76
1:D:70:LEU:HD13	1:D:102:LEU:HD11	1.65	0.76
1:A:1691:ASP:OD1	1:A:1692:GLN:N	2.17	0.76
1:D:1691:ASP:OD1	1:D:1692:GLN:N	2.17	0.76
1:B:3538:LYS:NZ	1:B:3608:ASP:OD2	2.13	0.76
1:C:3082:MET:CE	1:C:3093:LEU:HD23	2.15	0.76
3:O:93:THR:HG23	3:P:27:TYR:HB3	1.66	0.76
1:D:2877:GLU:OE2	1:D:2921:ARG:NH1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3082:MET:CE	1:B:3093:LEU:HD23	2.15	0.76
1:B:1142:ARG:NH2	1:B:1168:GLU:OE2	2.19	0.76
1:C:2877:GLU:OE2	1:C:2921:ARG:NH1	2.18	0.76
3:O:26:LYS:HZ2	3:P:92:GLU:H	1.34	0.75
1:C:918:GLU:OE1	1:C:918:GLU:N	2.20	0.75
1:D:877:GLU:O	1:D:880:HIS:ND1	2.20	0.75
1:C:1142:ARG:NH2	1:C:1168:GLU:OE2	2.19	0.75
1:B:877:GLU:O	1:B:880:HIS:ND1	2.20	0.75
1:B:918:GLU:OE1	1:B:918:GLU:N	2.20	0.75
3:K:5:LEU:HD23	3:K:9:MET:HE1	1.69	0.75
1:A:1142:ARG:NH2	1:A:1168:GLU:OE2	2.19	0.75
1:A:877:GLU:O	1:A:880:HIS:ND1	2.20	0.75
1:C:877:GLU:O	1:C:880:HIS:ND1	2.20	0.75
1:B:2877:GLU:OE2	1:B:2921:ARG:NH1	2.18	0.75
3:M:15:VAL:HG11	3:N:5:LEU:HD13	1.68	0.74
3:O:5:LEU:HD23	3:O:9:MET:HE1	1.69	0.74
1:D:1142:ARG:NH2	1:D:1168:GLU:OE2	2.19	0.74
1:A:918:GLU:N	1:A:918:GLU:OE1	2.20	0.74
3:O:15:VAL:HG11	3:P:5:LEU:HD13	1.69	0.74
1:A:2625:ARG:NH1	1:A:2907:VAL:HG21	2.03	0.74
3:O:5:LEU:HD23	3:O:9:MET:CE	2.18	0.74
1:C:2625:ARG:NH1	1:C:2907:VAL:HG21	2.03	0.74
1:B:2625:ARG:NH1	1:B:2907:VAL:HG21	2.03	0.73
1:B:2949:THR:HG22	1:B:2950:SER:H	1.53	0.73
1:D:2625:ARG:NH1	1:D:2907:VAL:HG21	2.03	0.73
1:D:918:GLU:N	1:D:918:GLU:OE1	2.20	0.73
1:A:2757:ASN:OD1	1:A:2758:LYS:N	2.22	0.73
1:B:2757:ASN:OD1	1:B:2758:LYS:N	2.22	0.73
3:M:5:LEU:HD23	3:M:9:MET:CE	2.18	0.73
3:K:5:LEU:HD23	3:K:9:MET:CE	2.18	0.73
1:D:2757:ASN:OD1	1:D:2758:LYS:N	2.22	0.73
1:C:2757:ASN:OD1	1:C:2758:LYS:N	2.22	0.72
1:B:1466:ASP:OD2	1:B:1468:SER:OG	2.04	0.72
3:M:93:THR:HG23	3:N:27:TYR:HB3	1.72	0.72
1:C:2949:THR:HG22	1:C:2950:SER:H	1.53	0.72
3:J:87:ASN:OD1	3:I:27:TYR:OH	2.07	0.72
3:I:5:LEU:HD23	3:I:9:MET:CE	2.18	0.72
1:D:1466:ASP:OD2	1:D:1468:SER:OG	2.04	0.72
1:A:3547:ASP:OD2	1:A:3548:GLU:N	2.23	0.72
1:D:2949:THR:HG22	1:D:2950:SER:H	1.53	0.71
1:D:3547:ASP:OD2	1:D:3548:GLU:N	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1466:ASP:OD2	1:A:1468:SER:OG	2.04	0.71
1:A:2949:THR:HG22	1:A:2950:SER:H	1.53	0.71
1:D:4100:MET:HE3	1:D:4111:ILE:HG23	1.72	0.71
1:B:2907:VAL:HG23	1:B:2912:LEU:HD22	1.73	0.71
3:J:56:ASP:OD1	3:J:57:LYS:N	2.24	0.71
3:N:56:ASP:OD1	3:N:57:LYS:N	2.24	0.70
1:B:3547:ASP:OD2	1:B:3548:GLU:N	2.23	0.70
1:A:2907:VAL:HG23	1:A:2912:LEU:HD22	1.73	0.70
3:L:56:ASP:OD1	3:L:57:LYS:N	2.24	0.70
3:P:56:ASP:OD1	3:P:57:LYS:N	2.24	0.70
3:L:44:GLY:HA2	1:B:2986:ARG:NH2	2.06	0.70
3:K:15:VAL:HG11	3:L:5:LEU:HD13	1.73	0.70
1:C:3547:ASP:OD2	1:C:3548:GLU:N	2.23	0.69
1:C:1466:ASP:OD2	1:C:1468:SER:OG	2.04	0.69
1:C:2907:VAL:HG23	1:C:2912:LEU:HD22	1.73	0.69
1:C:4100:MET:HE3	1:C:4111:ILE:HG23	1.75	0.69
1:D:2907:VAL:HG23	1:D:2912:LEU:HD22	1.73	0.68
1:A:4138:PRO:O	1:A:4142:ILE:HD12	1.94	0.68
3:K:4:GLU:OE1	3:L:11:THR:HG23	1.93	0.68
3:M:53:ASP:OD2	3:M:57:LYS:NZ	2.27	0.68
1:B:4100:MET:HE3	1:B:4111:ILE:HG23	1.75	0.68
1:B:4138:PRO:O	1:B:4142:ILE:HD12	1.94	0.68
1:A:3589:ASP:OD1	1:A:3592:LYS:HB3	1.94	0.68
3:I:53:ASP:OD2	3:I:57:LYS:NZ	2.27	0.68
1:B:2635:ASN:OD1	1:B:2637:PHE:N	2.27	0.67
1:B:2748:ILE:HG21	1:B:2811:LYS:NZ	2.10	0.67
1:A:2635:ASN:OD1	1:A:2637:PHE:N	2.27	0.67
1:D:2635:ASN:OD1	1:D:2637:PHE:N	2.27	0.67
3:K:53:ASP:OD2	3:K:57:LYS:NZ	2.27	0.67
1:B:3869:ILE:O	1:B:3872:GLN:NE2	2.28	0.67
1:C:2635:ASN:OD1	1:C:2637:PHE:N	2.27	0.67
3:O:53:ASP:OD2	3:O:57:LYS:NZ	2.27	0.67
1:C:3869:ILE:O	1:C:3872:GLN:NE2	2.28	0.67
3:I:39:GLN:NE2	3:I:40:THR:OG1	2.28	0.67
3:M:39:GLN:NE2	3:M:40:THR:OG1	2.28	0.67
1:D:3589:ASP:OD1	1:D:3592:LYS:HB3	1.94	0.67
1:C:3589:ASP:OD1	1:C:3592:LYS:HB3	1.94	0.67
1:A:4100:MET:HE3	1:A:4111:ILE:HG23	1.77	0.67
1:B:3589:ASP:OD1	1:B:3592:LYS:HB3	1.94	0.67
1:C:4138:PRO:O	1:C:4142:ILE:HD12	1.94	0.67
1:A:3530:ASP:O	1:A:3534:ILE:HD12	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:39:GLN:NE2	3:K:40:THR:OG1	2.28	0.67
1:D:2748:ILE:HG21	1:D:2811:LYS:NZ	2.10	0.67
1:A:2748:ILE:HG21	1:A:2811:LYS:NZ	2.10	0.66
1:D:4138:PRO:O	1:D:4142:ILE:HD12	1.94	0.66
1:C:2748:ILE:HG21	1:C:2811:LYS:NZ	2.10	0.66
3:O:39:GLN:NE2	3:O:40:THR:OG1	2.28	0.66
1:D:3869:ILE:O	1:D:3872:GLN:NE2	2.28	0.66
1:A:3869:ILE:O	1:A:3872:GLN:NE2	2.28	0.66
1:D:3530:ASP:O	1:D:3534:ILE:HD12	1.95	0.66
1:C:1043:ALA:O	1:C:1046:THR:OG1	2.10	0.66
1:A:1043:ALA:O	1:A:1046:THR:OG1	2.10	0.66
1:D:2197:ASN:OD1	1:D:2200:ARG:NH2	2.29	0.66
1:B:1043:ALA:O	1:B:1046:THR:OG1	2.10	0.66
1:B:3249:ARG:O	1:B:3253:GLU:OE1	2.14	0.66
3:O:56:ASP:HA	1:D:3638:ARG:HH22	1.61	0.66
1:D:3249:ARG:O	1:D:3253:GLU:OE1	2.14	0.66
1:B:3530:ASP:O	1:B:3534:ILE:HD12	1.95	0.66
1:A:3589:ASP:O	1:A:3593:ILE:HD12	1.96	0.66
1:D:3532:ASP:OD1	1:D:3533:LEU:N	2.29	0.66
3:K:1:MET:O	3:K:7:SER:OG	2.14	0.66
3:M:1:MET:O	3:M:7:SER:OG	2.14	0.66
1:A:2197:ASN:OD1	1:A:2200:ARG:NH2	2.29	0.65
3:O:1:MET:O	3:O:7:SER:OG	2.14	0.65
1:B:3532:ASP:OD1	1:B:3533:LEU:N	2.29	0.65
1:A:3249:ARG:O	1:A:3253:GLU:OE1	2.14	0.65
1:A:3457:GLN:OE1	1:A:3504:TYR:N	2.30	0.65
3:O:4:GLU:OE1	3:P:11:THR:HG23	1.96	0.65
1:B:2197:ASN:OD1	1:B:2200:ARG:NH2	2.29	0.65
1:C:3082:MET:HE2	1:C:3093:LEU:HD23	1.77	0.65
1:C:3249:ARG:O	1:C:3253:GLU:OE1	2.14	0.65
1:C:3457:GLN:OE1	1:C:3504:TYR:N	2.30	0.65
3:I:1:MET:O	3:I:7:SER:OG	2.14	0.65
1:D:2599:ALA:O	1:D:2603:VAL:HG23	1.97	0.65
1:C:3532:ASP:OD1	1:C:3533:LEU:N	2.29	0.65
1:A:2599:ALA:O	1:A:2603:VAL:HG23	1.97	0.65
1:D:3589:ASP:O	1:D:3593:ILE:HD12	1.96	0.65
1:C:3589:ASP:O	1:C:3593:ILE:HD12	1.96	0.65
1:D:3457:GLN:OE1	1:D:3504:TYR:N	2.30	0.65
1:C:3530:ASP:O	1:C:3534:ILE:HD12	1.95	0.65
1:A:2045:ILE:HG13	1:A:2132:LEU:HD23	1.79	0.65
1:D:2045:ILE:HG13	1:D:2132:LEU:HD23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3589:ASP:O	1:B:3593:ILE:HD12	1.96	0.65
1:B:3457:GLN:OE1	1:B:3504:TYR:N	2.30	0.64
1:A:3532:ASP:OD1	1:A:3533:LEU:N	2.29	0.64
1:A:16:ARG:NH1	1:A:101:THR:OG1	2.31	0.64
1:B:2599:ALA:O	1:B:2603:VAL:HG23	1.97	0.64
1:C:3761:MET:SD	1:C:3765:ARG:CZ	2.86	0.64
1:B:1562:VAL:HG12	1:B:1563:VAL:HG13	1.80	0.64
1:C:16:ARG:NH1	1:C:101:THR:OG1	2.31	0.64
1:C:2599:ALA:O	1:C:2603:VAL:HG23	1.97	0.64
1:B:3761:MET:SD	1:B:3765:ARG:CZ	2.86	0.64
1:B:2045:ILE:HG13	1:B:2132:LEU:HD23	1.79	0.64
1:B:3170:LEU:HD12	1:B:3195:LEU:HD11	1.80	0.64
1:C:862:ILE:HG23	1:C:934:LEU:HD22	1.80	0.63
1:C:2045:ILE:HG13	1:C:2132:LEU:HD23	1.79	0.63
1:A:862:ILE:HG23	1:A:934:LEU:HD22	1.80	0.63
1:C:3564:VAL:HA	1:C:3570:LEU:HD22	1.80	0.63
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.80	0.63
1:D:1043:ALA:O	1:D:1046:THR:OG1	2.10	0.63
1:A:3170:LEU:HD12	1:A:3195:LEU:HD11	1.80	0.63
1:D:3761:MET:SD	1:D:3765:ARG:CZ	2.86	0.63
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.81	0.63
1:B:16:ARG:NH1	1:B:101:THR:OG1	2.31	0.63
1:B:862:ILE:HG23	1:B:934:LEU:HD22	1.80	0.63
1:B:3564:VAL:HA	1:B:3570:LEU:HD22	1.80	0.63
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.81	0.63
1:A:3761:MET:SD	1:A:3765:ARG:CZ	2.86	0.63
3:P:44:GLY:HA2	1:D:2986:ARG:NH2	2.14	0.63
1:B:2187:MET:O	1:B:2193:TYR:OH	2.14	0.63
1:C:2197:ASN:OD1	1:C:2200:ARG:NH2	2.29	0.63
1:A:2828:ARG:NH2	1:A:2932:GLN:OE1	2.32	0.62
2:E:12:ASP:OD1	2:E:13:GLY:N	2.33	0.62
2:F:12:ASP:OD1	2:F:13:GLY:N	2.33	0.62
1:D:16:ARG:NH1	1:D:101:THR:OG1	2.31	0.62
1:A:3564:VAL:HA	1:A:3570:LEU:HD22	1.80	0.62
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.81	0.62
2:G:12:ASP:OD1	2:G:13:GLY:N	2.33	0.62
1:B:216:THR:OG1	1:B:219:HIS:NE2	2.33	0.62
1:C:2828:ARG:NH2	1:C:2932:GLN:OE1	2.32	0.62
3:K:56:ASP:HA	1:B:3638:ARG:HH22	1.64	0.62
1:D:1562:VAL:HG12	1:D:1563:VAL:HG13	1.80	0.62
1:B:2828:ARG:NH2	1:B:2932:GLN:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1562:VAL:HG12	1:C:1563:VAL:HG13	1.80	0.62
1:A:909:VAL:HG22	1:A:913:SER:OG	2.00	0.62
2:H:12:ASP:OD1	2:H:13:GLY:N	2.33	0.62
1:D:3564:VAL:HA	1:D:3570:LEU:HD22	1.80	0.62
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.81	0.62
1:C:2746:VAL:HG21	1:C:2819:ALA:HB2	1.82	0.62
1:B:1857:SER:OG	1:B:1860:ASP:OD2	2.16	0.62
3:I:49:GLN:NE2	3:I:51:ASP:O	2.33	0.62
1:C:3170:LEU:HD12	1:C:3195:LEU:HD11	1.80	0.62
1:D:909:VAL:HG22	1:D:913:SER:OG	2.00	0.61
1:D:2828:ARG:NH2	1:D:2932:GLN:OE1	2.32	0.61
1:C:216:THR:OG1	1:C:219:HIS:NE2	2.33	0.61
1:C:885:LEU:O	1:C:888:ILE:HG22	2.00	0.61
1:D:3170:LEU:HD12	1:D:3195:LEU:HD11	1.80	0.61
1:B:865:PRO:HD2	1:B:868:LEU:HD12	1.82	0.61
1:B:909:VAL:HG22	1:B:913:SER:OG	2.00	0.61
1:C:1857:SER:OG	1:C:1860:ASP:OD2	2.16	0.61
3:M:4:GLU:OE1	3:N:11:THR:HG23	2.00	0.61
3:M:49:GLN:NE2	3:M:51:ASP:O	2.33	0.61
1:A:216:THR:OG1	1:A:219:HIS:NE2	2.33	0.61
1:D:862:ILE:HG23	1:D:934:LEU:HD22	1.80	0.61
1:A:2620:LEU:O	1:A:2624:LEU:HD23	2.01	0.61
3:O:49:GLN:NE2	3:O:51:ASP:O	2.33	0.61
1:A:2746:VAL:HG21	1:A:2819:ALA:HB2	1.82	0.61
1:D:216:THR:OG1	1:D:219:HIS:NE2	2.33	0.61
1:C:865:PRO:HD2	1:C:868:LEU:HD12	1.81	0.61
1:C:2620:LEU:O	1:C:2624:LEU:HD23	2.01	0.61
1:C:3771:SER:OG	1:C:3775:ASN:OD1	2.19	0.61
1:A:865:PRO:HD2	1:A:868:LEU:HD12	1.81	0.61
1:A:2624:LEU:O	1:A:2628:VAL:HG23	2.01	0.61
3:P:6:GLU:O	3:P:10:GLU:OE1	2.19	0.61
1:B:1967:VAL:HG21	1:B:3650:ALA:HB1	1.83	0.61
1:B:2624:LEU:O	1:B:2628:VAL:HG23	2.01	0.61
1:C:918:GLU:HA	1:C:921:TYR:CD1	2.36	0.61
1:C:2624:LEU:O	1:C:2628:VAL:HG23	2.01	0.61
1:A:1932:LEU:HD13	1:A:1936:VAL:HG11	1.83	0.61
3:N:6:GLU:O	3:N:10:GLU:OE1	2.19	0.61
1:D:865:PRO:HD2	1:D:868:LEU:HD12	1.81	0.61
1:D:2746:VAL:HG21	1:D:2819:ALA:HB2	1.82	0.61
1:D:1967:VAL:HG21	1:D:3650:ALA:HB1	1.83	0.61
1:D:2624:LEU:O	1:D:2628:VAL:HG23	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:LEU:O	1:B:888:ILE:HG22	2.00	0.61
1:B:2907:VAL:HG23	1:B:2912:LEU:CD2	2.31	0.61
1:C:1967:VAL:HG21	1:C:3650:ALA:HB1	1.83	0.61
3:K:12:LEU:HD13	3:L:5:LEU:HD11	1.83	0.60
3:K:49:GLN:NE2	3:K:51:ASP:O	2.33	0.60
3:L:35:LYS:O	3:L:39:GLN:OE1	2.20	0.60
3:L:6:GLU:O	3:L:10:GLU:OE1	2.19	0.60
1:D:918:GLU:HA	1:D:921:TYR:CD1	2.36	0.60
1:C:909:VAL:HG22	1:C:913:SER:OG	2.00	0.60
1:A:918:GLU:HA	1:A:921:TYR:CD1	2.36	0.60
1:A:2907:VAL:HG23	1:A:2912:LEU:CD2	2.31	0.60
3:J:6:GLU:O	3:J:10:GLU:OE1	2.19	0.60
3:N:35:LYS:O	3:N:39:GLN:OE1	2.19	0.60
1:D:885:LEU:O	1:D:888:ILE:HG22	2.00	0.60
1:B:2755:PHE:CD2	1:B:2814:LEU:HD11	2.37	0.60
1:C:2907:VAL:HG23	1:C:2912:LEU:CD2	2.31	0.60
1:D:2620:LEU:O	1:D:2624:LEU:HD23	2.01	0.60
1:B:1932:LEU:HD13	1:B:1936:VAL:HG11	1.83	0.60
1:B:2620:LEU:O	1:B:2624:LEU:HD23	2.01	0.60
1:C:1932:LEU:HD13	1:C:1936:VAL:HG11	1.83	0.60
3:J:35:LYS:O	3:J:39:GLN:OE1	2.20	0.60
3:P:35:LYS:O	3:P:39:GLN:OE1	2.20	0.60
1:A:885:LEU:O	1:A:888:ILE:HG22	2.00	0.60
1:D:1932:LEU:HD13	1:D:1936:VAL:HG11	1.83	0.60
1:C:2755:PHE:CD2	1:C:2814:LEU:HD11	2.36	0.60
1:C:1264:THR:OG1	1:C:1267:THR:OG1	2.18	0.60
1:D:4823:THR:O	1:D:4826:SER:OG	2.16	0.60
1:B:918:GLU:HA	1:B:921:TYR:CD1	2.36	0.60
1:B:2438:ALA:HB2	1:B:2510:VAL:HG22	1.84	0.60
1:A:2438:ALA:HB2	1:A:2510:VAL:HG22	1.84	0.60
1:A:2755:PHE:CD2	1:A:2814:LEU:HD11	2.36	0.60
3:I:6:GLU:O	3:I:10:GLU:OE1	2.20	0.60
1:D:722:LEU:HD12	1:D:1477:MET:CE	2.32	0.60
1:D:2438:ALA:HB2	1:D:2510:VAL:HG22	1.84	0.60
1:B:2746:VAL:HG21	1:B:2819:ALA:HB2	1.82	0.59
1:C:722:LEU:HD12	1:C:1477:MET:CE	2.32	0.59
1:A:1967:VAL:HG21	1:A:3650:ALA:HB1	1.83	0.59
3:O:6:GLU:O	3:O:10:GLU:OE1	2.20	0.59
1:B:722:LEU:HD12	1:B:1477:MET:CE	2.32	0.59
1:C:2006:GLN:NE2	1:C:3640:THR:O	2.36	0.59
1:C:2187:MET:O	1:C:2193:TYR:OH	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2438:ALA:HB2	1:C:2510:VAL:HG22	1.84	0.59
1:C:5032:ASP:OD1	1:C:5033:GLN:N	2.36	0.59
3:O:72:PHE:CZ	3:O:76:VAL:HG11	2.37	0.59
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.36	0.59
1:C:885:LEU:O	1:C:889:GLU:OE1	2.21	0.59
1:A:1857:SER:OG	1:A:1860:ASP:OD2	2.16	0.59
3:I:72:PHE:CZ	3:I:76:VAL:HG11	2.37	0.59
3:M:56:ASP:HA	1:C:3638:ARG:HH22	1.67	0.59
3:M:72:PHE:CZ	3:M:76:VAL:HG11	2.37	0.59
1:D:3771:SER:OG	1:D:3775:ASN:OD1	2.19	0.59
1:D:5032:ASP:OD1	1:D:5033:GLN:N	2.36	0.59
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.85	0.59
1:A:722:LEU:HD12	1:A:1477:MET:CE	2.32	0.59
1:D:885:LEU:O	1:D:889:GLU:OE1	2.21	0.59
1:D:2907:VAL:HG23	1:D:2912:LEU:CD2	2.31	0.59
1:A:5032:ASP:OD1	1:A:5033:GLN:N	2.36	0.59
3:M:27:TYR:CD2	3:N:93:THR:HA	2.38	0.59
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.85	0.59
1:B:885:LEU:O	1:B:889:GLU:OE1	2.21	0.58
3:J:47:ASP:OD1	3:J:48:VAL:N	2.37	0.58
3:L:47:ASP:OD1	3:L:48:VAL:N	2.37	0.58
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.85	0.58
3:K:6:GLU:O	3:K:10:GLU:OE1	2.20	0.58
3:N:34:LEU:HD11	3:N:75:TYR:CD1	2.39	0.58
1:B:71:GLU:OE2	1:B:111:ARG:NE	2.35	0.58
1:C:3865:ASP:OD1	1:C:3870:ASN:ND2	2.37	0.58
1:A:2006:GLN:NE2	1:A:3640:THR:O	2.36	0.58
1:A:2215:VAL:HG21	1:A:2229:MET:HE1	1.86	0.58
1:A:3865:ASP:OD1	1:A:3870:ASN:ND2	2.37	0.58
3:P:34:LEU:HD11	3:P:75:TYR:CD1	2.39	0.58
1:B:2006:GLN:NE2	1:B:3640:THR:O	2.36	0.58
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.85	0.58
3:P:47:ASP:OD1	3:P:48:VAL:N	2.37	0.58
1:B:5032:ASP:OD1	1:B:5033:GLN:N	2.35	0.58
1:A:3446:TRP:NE1	1:A:3456:GLU:OE2	2.37	0.58
3:J:34:LEU:HD11	3:J:75:TYR:CD1	2.39	0.58
3:K:72:PHE:CZ	3:K:76:VAL:HG11	2.37	0.58
1:D:2006:GLN:NE2	1:D:3640:THR:O	2.36	0.58
1:B:3865:ASP:OD1	1:B:3870:ASN:ND2	2.37	0.58
1:C:3366:LEU:HD23	1:C:3406:LEU:HD23	1.86	0.58
1:A:885:LEU:O	1:A:889:GLU:OE1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:6:GLU:O	3:M:10:GLU:OE1	2.20	0.58
3:N:47:ASP:OD1	3:N:48:VAL:N	2.37	0.58
1:D:3865:ASP:OD1	1:D:3870:ASN:ND2	2.37	0.58
1:A:2745:ASN:OD1	1:A:2746:VAL:N	2.37	0.58
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.34	0.58
1:C:1499:GLY:O	1:C:1502:VAL:HG12	2.04	0.58
1:A:3366:LEU:HD23	1:A:3406:LEU:HD23	1.86	0.57
1:D:980:PRO:O	1:D:983:THR:OG1	2.20	0.57
1:D:3587:ALA:HA	1:D:3593:ILE:HD11	1.86	0.57
1:D:2745:ASN:OD1	1:D:2746:VAL:N	2.37	0.57
1:D:3446:TRP:NE1	1:D:3456:GLU:OE2	2.37	0.57
1:B:1499:GLY:O	1:B:1502:VAL:HG12	2.04	0.57
3:L:88:ASN:OD1	3:L:89:PHE:N	2.38	0.57
3:N:88:ASN:OD1	3:N:89:PHE:N	2.37	0.57
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.34	0.57
1:C:2745:ASN:OD1	1:C:2746:VAL:N	2.37	0.57
1:A:1428:ILE:HG23	1:A:1429:LEU:HD22	1.87	0.57
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.34	0.57
3:J:88:ASN:OD1	3:J:89:PHE:N	2.38	0.57
3:O:27:TYR:CD2	3:P:93:THR:HA	2.38	0.57
1:B:3366:LEU:HD23	1:B:3406:LEU:HD23	1.86	0.57
1:C:1428:ILE:HG23	1:C:1429:LEU:HD22	1.87	0.57
3:P:88:ASN:OD1	3:P:89:PHE:N	2.37	0.57
1:B:2745:ASN:OD1	1:B:2746:VAL:N	2.37	0.57
3:N:44:GLY:HA2	1:C:2986:ARG:NH2	2.19	0.57
1:D:1499:GLY:O	1:D:1502:VAL:HG12	2.04	0.57
1:B:1428:ILE:HG23	1:B:1429:LEU:HD22	1.87	0.57
1:B:3174:TYR:O	1:B:3178:THR:HG23	2.05	0.57
1:B:3446:TRP:NE1	1:B:3456:GLU:OE2	2.37	0.57
1:C:71:GLU:OE2	1:C:111:ARG:NE	2.35	0.57
1:C:3174:TYR:O	1:C:3178:THR:HG23	2.05	0.57
3:L:34:LEU:HD11	3:L:75:TYR:CD1	2.39	0.57
1:D:1428:ILE:HG23	1:D:1429:LEU:HD22	1.87	0.57
1:B:3587:ALA:HA	1:B:3593:ILE:HD11	1.86	0.57
1:C:3446:TRP:NE1	1:C:3456:GLU:OE2	2.37	0.57
1:D:875:LEU:O	1:D:879:ILE:HG12	2.05	0.57
1:B:1080:LYS:HA	1:B:1190:LEU:HD11	1.86	0.57
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.34	0.57
1:A:1080:LYS:HA	1:A:1190:LEU:HD11	1.86	0.57
1:A:3174:TYR:O	1:A:3178:THR:HG23	2.05	0.57
1:D:3174:TYR:O	1:D:3178:THR:HG23	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:875:LEU:O	1:C:879:ILE:HG12	2.05	0.57
1:C:982:GLN:HG2	1:C:1054:ILE:HD11	1.86	0.57
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.87	0.57
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.87	0.56
1:A:875:LEU:O	1:A:879:ILE:HG12	2.05	0.56
1:A:1264:THR:OG1	1:A:1267:THR:OG1	2.18	0.56
3:O:12:LEU:HD13	3:P:5:LEU:HD11	1.87	0.56
1:B:875:LEU:O	1:B:879:ILE:HG12	2.05	0.56
1:A:310:THR:O	1:A:314:SER:OG	2.14	0.56
1:D:1080:LYS:HA	1:D:1190:LEU:HD11	1.86	0.56
1:D:1132:ARG:NH1	1:D:1179:ALA:O	2.38	0.56
1:D:2215:VAL:HG21	1:D:2229:MET:HE1	1.87	0.56
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.87	0.56
1:D:3366:LEU:HD23	1:D:3406:LEU:HD23	1.86	0.56
1:B:982:GLN:HG2	1:B:1054:ILE:HD11	1.86	0.56
1:C:1080:LYS:HA	1:C:1190:LEU:HD11	1.86	0.56
1:C:3595:ARG:O	1:C:3599:GLU:OE1	2.24	0.56
1:A:3053:HIS:O	1:A:3128:GLN:NE2	2.38	0.56
1:D:2692:TYR:OH	1:D:2694:GLN:HG2	2.06	0.56
1:D:2743:THR:OG1	1:D:2812:GLU:O	2.20	0.56
1:B:1132:ARG:NH1	1:B:1179:ALA:O	2.39	0.56
1:B:4823:THR:O	1:B:4826:SER:OG	2.16	0.56
3:O:25:ASP:HB3	3:P:94:SER:CB	2.36	0.56
1:D:1042:GLN:O	1:D:1046:THR:HG23	2.06	0.56
1:D:4868:ASP:OD1	1:D:4869:GLU:N	2.39	0.56
1:B:878:ASN:ND2	1:B:1046:THR:HG22	2.21	0.56
1:A:878:ASN:ND2	1:A:1046:THR:HG22	2.21	0.56
1:A:1499:GLY:O	1:A:1502:VAL:HG12	2.04	0.56
1:A:4823:THR:O	1:A:4826:SER:OG	2.16	0.56
1:D:982:GLN:HG2	1:D:1054:ILE:HD11	1.86	0.56
1:B:3771:SER:OG	1:B:3775:ASN:OD1	2.19	0.56
1:A:1132:ARG:NH1	1:A:1179:ALA:O	2.38	0.56
1:A:3771:SER:OG	1:A:3775:ASN:OD1	2.19	0.56
1:B:2743:THR:OG1	1:B:2812:GLU:O	2.20	0.56
1:B:4868:ASP:OD1	1:B:4869:GLU:N	2.39	0.56
1:C:3587:ALA:HA	1:C:3593:ILE:HD11	1.86	0.56
1:A:3587:ALA:HA	1:A:3593:ILE:HD11	1.86	0.56
1:B:4235:GLU:OE2	1:B:5015:ARG:NH2	2.39	0.56
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.87	0.56
1:C:34:LEU:HD23	1:C:36:LEU:HD11	1.88	0.56
1:C:1132:ARG:NH1	1:C:1179:ALA:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:GLN:O	1:A:1046:THR:HG23	2.06	0.56
1:B:1042:GLN:O	1:B:1046:THR:HG23	2.06	0.56
1:C:2692:TYR:OH	1:C:2694:GLN:HG2	2.06	0.56
1:A:287:THR:HG21	1:A:482:GLU:OE1	2.06	0.55
3:M:12:LEU:HD13	3:N:5:LEU:HD11	1.88	0.55
1:D:878:ASN:ND2	1:D:1046:THR:HG22	2.21	0.55
1:B:2213:VAL:HG21	1:B:2257:TYR:OH	2.06	0.55
1:C:2213:VAL:HG21	1:C:2257:TYR:OH	2.06	0.55
1:C:4235:GLU:OE2	1:C:5015:ARG:NH2	2.39	0.55
1:A:982:GLN:HG2	1:A:1054:ILE:HD11	1.86	0.55
1:A:2971:SER:HA	1:A:2974:PHE:CE1	2.41	0.55
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.87	0.55
1:B:3595:ARG:O	1:B:3599:GLU:OE1	2.24	0.55
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.87	0.55
1:D:4235:GLU:OE2	1:D:5015:ARG:NH2	2.39	0.55
1:A:3595:ARG:O	1:A:3599:GLU:OE1	2.24	0.55
1:A:4868:ASP:OD1	1:A:4869:GLU:N	2.39	0.55
3:K:84:VAL:HG23	3:L:27:TYR:CZ	2.41	0.55
1:D:287:THR:HG21	1:D:482:GLU:OE1	2.06	0.55
1:C:287:THR:HG21	1:C:482:GLU:OE1	2.06	0.55
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.87	0.55
1:B:287:THR:HG21	1:B:482:GLU:OE1	2.06	0.55
1:B:2971:SER:HA	1:B:2974:PHE:CE1	2.42	0.55
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.87	0.55
1:A:1236:THR:OG1	1:A:1703:ARG:NH1	2.40	0.55
1:D:3351:ARG:HG2	1:D:3353:GLU:OE1	2.06	0.55
1:B:34:LEU:HD23	1:B:36:LEU:HD11	1.88	0.55
1:B:3351:ARG:HG2	1:B:3353:GLU:OE1	2.06	0.55
1:B:3053:HIS:O	1:B:3128:GLN:NE2	2.38	0.55
1:C:878:ASN:ND2	1:C:1046:THR:HG22	2.21	0.55
1:C:4823:THR:O	1:C:4826:SER:OG	2.16	0.55
1:A:4235:GLU:OE2	1:A:5015:ARG:NH2	2.39	0.55
3:M:27:TYR:OH	3:N:87:ASN:OD1	2.25	0.55
1:D:34:LEU:HD23	1:D:36:LEU:HD11	1.88	0.55
1:B:2828:ARG:NH2	1:B:2936:TYR:O	2.40	0.55
1:C:4868:ASP:OD1	1:C:4869:GLU:N	2.39	0.55
3:K:27:TYR:CD2	3:L:93:THR:HA	2.42	0.55
1:D:2478:PRO:HD2	1:D:2537:LEU:HD21	1.89	0.55
1:D:3595:ARG:O	1:D:3599:GLU:OE1	2.24	0.55
1:C:1236:THR:OG1	1:C:1703:ARG:NH1	2.40	0.55
1:C:3053:HIS:O	1:C:3128:GLN:NE2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:OE2	1:A:111:ARG:NE	2.35	0.55
1:A:2045:ILE:CG1	1:A:2132:LEU:HD23	2.37	0.55
1:A:2748:ILE:HG21	1:A:2811:LYS:HZ1	1.70	0.55
1:D:3292:ALA:O	1:D:3294:PRO:HD3	2.07	0.55
1:B:1236:THR:OG1	1:B:1703:ARG:NH1	2.40	0.55
1:B:2692:TYR:OH	1:B:2694:GLN:HG2	2.06	0.55
1:C:1042:GLN:O	1:C:1046:THR:HG23	2.06	0.55
1:C:2478:PRO:HD2	1:C:2537:LEU:HD21	1.89	0.55
1:C:3351:ARG:HG2	1:C:3353:GLU:OE1	2.06	0.55
1:B:3082:MET:HE1	1:B:3093:LEU:HD23	1.87	0.54
1:C:3460:VAL:HG23	1:C:3465:ILE:HG13	1.89	0.54
1:A:2213:VAL:HG21	1:A:2257:TYR:OH	2.06	0.54
1:A:2743:THR:OG1	1:A:2812:GLU:O	2.20	0.54
1:A:2756:ILE:CG1	1:A:2814:LEU:HD12	2.38	0.54
1:A:2828:ARG:NH2	1:A:2936:TYR:O	2.40	0.54
1:A:3351:ARG:HG2	1:A:3353:GLU:OE1	2.06	0.54
1:D:2213:VAL:HG21	1:D:2257:TYR:OH	2.06	0.54
1:A:4964:ASP:OD1	1:A:4965:TYR:N	2.41	0.54
1:D:3053:HIS:O	1:D:3128:GLN:NE2	2.38	0.54
1:B:3460:VAL:HG23	1:B:3465:ILE:HG13	1.90	0.54
1:C:297:ASP:OD1	1:C:298:GLN:N	2.41	0.54
1:C:3292:ALA:O	1:C:3294:PRO:HD3	2.08	0.54
1:A:2692:TYR:OH	1:A:2694:GLN:HG2	2.06	0.54
1:D:1236:THR:OG1	1:D:1703:ARG:NH1	2.40	0.54
1:D:1793:ALA:O	1:D:1794:THR:OG1	2.20	0.54
1:D:2828:ARG:NH2	1:D:2936:TYR:O	2.40	0.54
1:D:2971:SER:HA	1:D:2974:PHE:CE1	2.41	0.54
1:C:980:PRO:O	1:C:983:THR:OG1	2.20	0.54
1:C:4964:ASP:OD1	1:C:4965:TYR:N	2.41	0.54
1:A:34:LEU:HD23	1:A:36:LEU:HD11	1.88	0.54
1:A:3460:VAL:HG23	1:A:3465:ILE:HG13	1.89	0.54
1:A:3570:LEU:HD23	1:A:3570:LEU:O	2.07	0.54
3:O:27:TYR:OH	3:P:87:ASN:OD1	2.24	0.54
1:D:4964:ASP:OD1	1:D:4965:TYR:N	2.41	0.54
1:C:2045:ILE:CG1	1:C:2132:LEU:HD23	2.37	0.54
1:C:3570:LEU:O	1:C:3570:LEU:HD23	2.07	0.54
1:A:980:PRO:O	1:A:983:THR:OG1	2.20	0.54
1:D:2045:ILE:CG1	1:D:2132:LEU:HD23	2.37	0.54
1:B:3025:VAL:HG23	1:B:3025:VAL:O	2.08	0.54
1:B:3292:ALA:O	1:B:3294:PRO:HD3	2.07	0.54
1:B:3570:LEU:HD23	1:B:3570:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2971:SER:HA	1:C:2974:PHE:CE1	2.42	0.54
1:A:2478:PRO:HD2	1:A:2537:LEU:HD21	1.89	0.54
1:B:2215:VAL:HG21	1:B:2229:MET:HE1	1.90	0.54
1:C:2215:VAL:HG21	1:C:2229:MET:HE1	1.90	0.54
1:A:297:ASP:OD1	1:A:298:GLN:N	2.41	0.54
3:O:5:LEU:HD12	3:P:15:VAL:HG11	1.89	0.54
1:D:71:GLU:OE2	1:D:111:ARG:NE	2.35	0.54
1:D:2756:ILE:CG1	1:D:2814:LEU:HD12	2.38	0.54
1:D:3570:LEU:HD23	1:D:3570:LEU:O	2.07	0.54
1:B:980:PRO:O	1:B:983:THR:OG1	2.20	0.54
1:B:2756:ILE:CG1	1:B:2814:LEU:HD12	2.38	0.54
1:A:914:LEU:O	1:A:919:ARG:NH2	2.41	0.54
1:A:3292:ALA:O	1:A:3294:PRO:HD3	2.08	0.54
3:O:48:VAL:O	3:O:50:LYS:NZ	2.38	0.54
1:B:2045:ILE:CG1	1:B:2132:LEU:HD23	2.38	0.54
1:C:2828:ARG:NH2	1:C:2936:TYR:O	2.40	0.54
1:A:3188:ARG:HG2	1:A:3273:ILE:HD11	1.90	0.54
1:A:4107:THR:O	1:A:4111:ILE:HD12	2.08	0.54
1:D:1857:SER:OG	1:D:1860:ASP:OD2	2.16	0.54
1:B:4107:THR:O	1:B:4111:ILE:HD12	2.08	0.54
1:B:4964:ASP:OD1	1:B:4965:TYR:N	2.41	0.54
1:C:3188:ARG:HG2	1:C:3273:ILE:HD11	1.90	0.54
1:C:914:LEU:O	1:C:919:ARG:NH2	2.41	0.53
1:A:964:ASN:OD1	1:A:965:GLY:N	2.42	0.53
1:A:4816:MET:O	1:A:4822:ARG:NH1	2.42	0.53
1:D:914:LEU:O	1:D:919:ARG:NH2	2.41	0.53
1:A:3025:VAL:HG23	1:A:3025:VAL:O	2.08	0.53
1:D:3025:VAL:HG23	1:D:3025:VAL:O	2.08	0.53
1:D:4107:THR:O	1:D:4111:ILE:HD12	2.08	0.53
1:B:2478:PRO:HD2	1:B:2537:LEU:HD21	1.89	0.53
1:B:3868:VAL:HG22	1:B:3869:ILE:H	1.74	0.53
1:B:4816:MET:O	1:B:4822:ARG:NH1	2.42	0.53
1:C:4816:MET:O	1:C:4822:ARG:NH1	2.42	0.53
1:A:2872:LEU:HB3	1:A:2928:LEU:HD21	1.91	0.53
1:A:3082:MET:HE1	1:A:3093:LEU:HD23	1.89	0.53
1:A:3450:HIS:O	1:A:3454:ARG:NE	2.42	0.53
1:C:2756:ILE:CG1	1:C:2814:LEU:HD12	2.38	0.53
1:D:297:ASP:OD1	1:D:298:GLN:N	2.41	0.53
1:D:2872:LEU:HB3	1:D:2928:LEU:HD21	1.91	0.53
1:B:297:ASP:OD1	1:B:298:GLN:N	2.41	0.53
1:B:3188:ARG:HG2	1:B:3273:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2872:LEU:HB3	1:C:2928:LEU:HD21	1.91	0.53
1:A:3868:VAL:HG22	1:A:3869:ILE:H	1.74	0.53
3:K:4:GLU:OE1	3:L:11:THR:CG2	2.56	0.53
3:O:84:VAL:HG23	3:P:27:TYR:CZ	2.43	0.53
1:D:2533:ALA:O	1:D:2537:LEU:HD13	2.09	0.53
1:D:3460:VAL:HG23	1:D:3465:ILE:HG13	1.90	0.53
1:D:4083:TYR:O	1:D:4085:THR:HG23	2.09	0.53
1:B:914:LEU:O	1:B:919:ARG:NH2	2.41	0.53
1:B:2872:LEU:HB3	1:B:2928:LEU:HD21	1.91	0.53
1:A:2533:ALA:O	1:A:2537:LEU:HD13	2.09	0.53
3:L:59:MET:HA	3:L:62:LEU:HD23	1.91	0.53
3:N:59:MET:HA	3:N:62:LEU:HD23	1.91	0.53
1:D:4816:MET:O	1:D:4822:ARG:NH1	2.42	0.53
1:B:2918:ALA:HA	1:B:2921:ARG:HG2	1.91	0.53
1:B:3450:HIS:O	1:B:3454:ARG:NE	2.42	0.53
1:C:3025:VAL:HG23	1:C:3025:VAL:O	2.08	0.53
1:C:3868:VAL:HG22	1:C:3869:ILE:H	1.74	0.53
3:L:44:GLY:O	3:L:48:VAL:HG22	2.09	0.53
1:D:3188:ARG:HG2	1:D:3273:ILE:HD11	1.90	0.53
1:B:964:ASN:OD1	1:B:965:GLY:N	2.42	0.53
1:C:4083:TYR:O	1:C:4085:THR:HG23	2.09	0.53
3:J:44:GLY:O	3:J:48:VAL:HG22	2.09	0.53
1:D:3082:MET:HE1	1:D:3093:LEU:HD23	1.89	0.53
1:B:2533:ALA:O	1:B:2537:LEU:HD13	2.09	0.53
1:C:2949:THR:HG22	1:C:2950:SER:N	2.23	0.53
1:D:3105:GLU:O	1:D:3109:GLU:OE1	2.27	0.53
1:D:3450:HIS:O	1:D:3454:ARG:NE	2.42	0.53
1:C:862:ILE:O	1:C:931:LYS:NZ	2.42	0.53
1:C:2533:ALA:O	1:C:2537:LEU:HD13	2.08	0.53
1:C:2918:ALA:HA	1:C:2921:ARG:HG2	1.91	0.53
3:N:10:GLU:HA	3:N:13:ILE:HG22	1.91	0.52
1:D:2949:THR:HG22	1:D:2950:SER:N	2.23	0.52
1:D:3107:MET:SD	1:D:3133:THR:HG21	2.49	0.52
1:B:862:ILE:O	1:B:931:LYS:NZ	2.42	0.52
1:C:722:LEU:HD12	1:C:1477:MET:HE2	1.89	0.52
1:C:4107:THR:O	1:C:4111:ILE:HD12	2.08	0.52
1:A:3107:MET:SD	1:A:3133:THR:HG21	2.49	0.52
1:A:4083:TYR:O	1:A:4085:THR:HG23	2.09	0.52
3:J:59:MET:HA	3:J:62:LEU:HD23	1.91	0.52
3:L:47:ASP:OD1	3:L:48:VAL:HG13	2.09	0.52
3:N:44:GLY:O	3:N:48:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:862:ILE:O	1:D:931:LYS:NZ	2.43	0.52
1:D:964:ASN:OD1	1:D:965:GLY:N	2.42	0.52
1:C:918:GLU:HA	1:C:921:TYR:CE1	2.45	0.52
1:A:4016:LEU:HD23	1:A:4135:PHE:HE1	1.75	0.52
3:K:5:LEU:HD12	3:L:15:VAL:HG21	1.91	0.52
3:P:44:GLY:O	3:P:48:VAL:HG22	2.09	0.52
3:P:59:MET:HA	3:P:62:LEU:HD23	1.91	0.52
1:D:918:GLU:HA	1:D:921:TYR:CE1	2.45	0.52
1:D:3868:VAL:HG22	1:D:3869:ILE:H	1.74	0.52
1:D:4249:GLN:O	1:D:4253:GLN:HG3	2.10	0.52
1:C:4249:GLN:O	1:C:4253:GLN:HG3	2.10	0.52
1:A:3173:ILE:HG21	1:A:3195:LEU:HD13	1.90	0.52
3:O:5:LEU:CD1	3:P:15:VAL:HG21	2.39	0.52
1:C:964:ASN:OD1	1:C:965:GLY:N	2.42	0.52
1:A:878:ASN:HD22	1:A:1046:THR:HG22	1.75	0.52
1:A:2918:ALA:HA	1:A:2921:ARG:HG2	1.91	0.52
1:A:4580:VAL:HG12	1:B:4875:ASP:O	2.10	0.52
3:P:10:GLU:HA	3:P:13:ILE:HG22	1.91	0.52
1:D:3173:ILE:HG21	1:D:3195:LEU:HD13	1.90	0.52
1:B:2167:LEU:HD11	1:B:2207:THR:HG23	1.92	0.52
1:B:4016:LEU:HD23	1:B:4135:PHE:HE1	1.75	0.52
1:A:918:GLU:HA	1:A:921:TYR:CE1	2.45	0.52
1:A:3105:GLU:O	1:A:3109:GLU:OE1	2.27	0.52
1:D:878:ASN:HD22	1:D:1046:THR:HG22	1.75	0.52
1:C:3173:ILE:HG21	1:C:3195:LEU:HD13	1.90	0.52
3:P:34:LEU:HD11	3:P:75:TYR:CE1	2.45	0.52
1:C:878:ASN:HD22	1:C:1046:THR:HG22	1.75	0.52
1:C:3547:ASP:O	1:C:3598:GLN:NE2	2.43	0.52
3:L:10:GLU:HA	3:L:13:ILE:HG22	1.91	0.52
1:D:2539:THR:HG21	1:D:2900:GLY:HA2	1.91	0.52
1:B:722:LEU:HD12	1:B:1477:MET:HE2	1.92	0.52
1:B:878:ASN:HD22	1:B:1046:THR:HG22	1.75	0.52
1:B:3105:GLU:O	1:B:3109:GLU:OE1	2.28	0.52
1:B:3173:ILE:HG21	1:B:3195:LEU:HD13	1.91	0.52
1:B:4083:TYR:O	1:B:4085:THR:HG23	2.09	0.52
1:C:2625:ARG:HH11	1:C:2907:VAL:HG21	1.75	0.52
1:C:3930:GLN:HB3	1:C:3995:PHE:CE1	2.45	0.52
3:I:8:ALA:O	3:I:11:THR:OG1	2.24	0.52
1:D:569:LEU:HD12	1:D:603:VAL:HG13	1.92	0.52
1:B:2539:THR:HG21	1:B:2900:GLY:HA2	1.92	0.52
1:B:3547:ASP:O	1:B:3598:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2167:LEU:HD11	1:C:2207:THR:HG23	1.92	0.52
1:C:2987:VAL:O	1:C:2987:VAL:HG13	2.10	0.52
1:A:2167:LEU:HD11	1:A:2207:THR:HG23	1.92	0.52
3:O:37:LEU:O	3:O:41:GLU:OE1	2.28	0.52
1:A:2539:THR:HG21	1:A:2900:GLY:HA2	1.91	0.51
3:J:34:LEU:HD11	3:J:75:TYR:CE1	2.45	0.51
3:O:5:LEU:HD12	3:P:15:VAL:HG21	1.91	0.51
3:N:47:ASP:OD1	3:N:48:VAL:HG13	2.09	0.51
1:B:569:LEU:HD12	1:B:603:VAL:HG13	1.92	0.51
1:B:3107:MET:SD	1:B:3133:THR:HG21	2.50	0.51
1:C:554:ARG:NH2	1:C:556:GLU:OE2	2.40	0.51
1:C:3450:HIS:O	1:C:3454:ARG:NE	2.42	0.51
3:J:47:ASP:OD1	3:J:48:VAL:HG13	2.09	0.51
3:I:37:LEU:O	3:I:41:GLU:OE1	2.28	0.51
3:O:31:LYS:NZ	3:O:62:LEU:O	2.38	0.51
3:L:34:LEU:HD11	3:L:75:TYR:CE1	2.45	0.51
1:D:2500:LYS:NZ	1:D:2530:ASP:OD2	2.36	0.51
1:D:2918:ALA:HA	1:D:2921:ARG:HG2	1.91	0.51
1:D:3930:GLN:HB3	1:D:3995:PHE:CE1	2.45	0.51
1:B:2949:THR:HG22	1:B:2950:SER:N	2.23	0.51
1:B:4249:GLN:O	1:B:4253:GLN:HG3	2.10	0.51
1:C:2517:ASP:OD2	1:C:2518:PHE:N	2.43	0.51
1:C:3107:MET:SD	1:C:3133:THR:HG21	2.50	0.51
1:A:2517:ASP:OD2	1:A:2518:PHE:N	2.43	0.51
1:A:3547:ASP:O	1:A:3598:GLN:NE2	2.43	0.51
3:K:37:LEU:O	3:K:41:GLU:OE1	2.28	0.51
3:M:37:LEU:O	3:M:41:GLU:OE1	2.28	0.51
1:D:932:THR:O	1:D:936:LEU:HD23	2.10	0.51
1:B:918:GLU:HA	1:B:921:TYR:CE1	2.45	0.51
1:B:2987:VAL:O	1:B:2987:VAL:HG13	2.10	0.51
1:C:1932:LEU:HD13	1:C:1936:VAL:CG1	2.41	0.51
1:A:2383:GLU:O	1:A:2387:ILE:HG12	2.11	0.51
1:A:4249:GLN:O	1:A:4253:GLN:HG3	2.10	0.51
3:M:84:VAL:HG23	3:N:27:TYR:CZ	2.45	0.51
1:D:3547:ASP:O	1:D:3598:GLN:NE2	2.43	0.51
1:B:4752:ASN:OD1	1:B:4753:GLU:N	2.42	0.51
1:C:569:LEU:HD12	1:C:603:VAL:HG13	1.92	0.51
1:C:3105:GLU:O	1:C:3109:GLU:OE1	2.27	0.51
1:A:877:GLU:O	1:A:880:HIS:CE1	2.63	0.51
1:A:2949:THR:HG22	1:A:2950:SER:N	2.23	0.51
1:A:2987:VAL:HG13	1:A:2987:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2517:ASP:OD2	1:D:2518:PHE:N	2.43	0.51
1:B:2383:GLU:O	1:B:2387:ILE:HG12	2.11	0.51
1:C:4016:LEU:HD23	1:C:4135:PHE:HE1	1.75	0.51
1:A:569:LEU:HD12	1:A:603:VAL:HG13	1.92	0.51
1:B:877:GLU:O	1:B:880:HIS:CE1	2.63	0.51
1:B:1932:LEU:HD13	1:B:1936:VAL:CG1	2.41	0.51
1:B:2625:ARG:HH11	1:B:2907:VAL:HG21	1.75	0.51
1:B:3930:GLN:HB3	1:B:3995:PHE:CE1	2.45	0.51
3:N:34:LEU:HD11	3:N:75:TYR:CE1	2.45	0.51
3:P:47:ASP:OD1	3:P:48:VAL:HG13	2.09	0.51
1:D:722:LEU:HD12	1:D:1477:MET:HE2	1.92	0.51
1:D:877:GLU:O	1:D:880:HIS:CE1	2.63	0.51
1:A:862:ILE:O	1:A:931:LYS:NZ	2.42	0.51
3:O:38:LEU:HD12	3:O:39:GLN:N	2.26	0.51
1:D:2167:LEU:HD11	1:D:2207:THR:HG23	1.92	0.51
1:B:3250:LEU:HD23	1:B:3253:GLU:OE2	2.11	0.51
1:C:877:GLU:O	1:C:880:HIS:CE1	2.63	0.51
1:C:932:THR:O	1:C:936:LEU:HD23	2.10	0.51
1:A:932:THR:O	1:A:936:LEU:HD23	2.10	0.51
3:J:10:GLU:HA	3:J:13:ILE:HG22	1.91	0.51
1:D:1932:LEU:HD13	1:D:1936:VAL:CG1	2.41	0.51
1:A:3250:LEU:HD23	1:A:3253:GLU:OE2	2.11	0.51
1:A:3930:GLN:HB3	1:A:3995:PHE:CE1	2.45	0.51
3:I:31:LYS:NZ	3:I:62:LEU:O	2.38	0.51
1:D:3250:LEU:HD23	1:D:3253:GLU:OE2	2.11	0.51
1:D:2987:VAL:HG13	1:D:2987:VAL:O	2.10	0.50
1:C:1264:THR:HG1	1:C:1267:THR:HG1	1.54	0.50
1:C:2539:THR:HG21	1:C:2900:GLY:HA2	1.91	0.50
1:A:722:LEU:HD12	1:A:1477:MET:HE1	1.93	0.50
1:A:1932:LEU:HD13	1:A:1936:VAL:CG1	2.41	0.50
1:A:4685:TYR:CD1	1:A:4704:LEU:HD11	2.47	0.50
3:M:38:LEU:HD12	3:M:39:GLN:N	2.26	0.50
1:D:4685:TYR:CD1	1:D:4704:LEU:HD11	2.47	0.50
1:B:3433:GLU:OE1	1:B:3525:MET:CG	2.59	0.50
1:C:330:ARG:NH2	1:C:331:ASP:OD1	2.45	0.50
1:C:3467:ASN:ND2	1:C:3508:THR:O	2.44	0.50
1:A:664:TYR:OH	1:A:666:GLU:OE2	2.30	0.50
1:D:3169:THR:O	1:D:3173:ILE:HG12	2.11	0.50
1:C:3433:GLU:OE1	1:C:3525:MET:CG	2.59	0.50
1:D:2625:ARG:HH11	1:D:2907:VAL:HG21	1.75	0.50
1:C:664:TYR:OH	1:C:666:GLU:OE2	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2383:GLU:O	1:C:2387:ILE:HG12	2.11	0.50
1:A:3169:THR:O	1:A:3173:ILE:HG12	2.11	0.50
3:N:29:LEU:HD23	3:N:34:LEU:HD13	1.93	0.50
1:D:4016:LEU:HD23	1:D:4135:PHE:HE1	1.75	0.50
1:B:2517:ASP:OD2	1:B:2518:PHE:N	2.43	0.50
1:A:2755:PHE:CE2	1:A:2814:LEU:HD11	2.47	0.50
3:L:29:LEU:HD23	3:L:34:LEU:HD13	1.93	0.50
1:D:3467:ASN:ND2	1:D:3508:THR:O	2.44	0.50
1:C:3250:LEU:HD23	1:C:3253:GLU:OE2	2.11	0.50
1:B:664:TYR:OH	1:B:666:GLU:OE2	2.30	0.50
1:B:932:THR:O	1:B:936:LEU:HD23	2.10	0.50
1:C:3771:SER:HA	1:C:3774:HIS:CE1	2.47	0.50
1:A:2625:ARG:HH11	1:A:2907:VAL:HG21	1.75	0.50
3:J:29:LEU:HD23	3:J:34:LEU:HD13	1.93	0.50
3:I:38:LEU:HD12	3:I:39:GLN:N	2.26	0.50
1:D:4574:ILE:HG23	1:D:4637:MET:HG2	1.93	0.50
1:B:1739:LEU:HD12	1:B:1964:GLU:CD	2.32	0.50
1:B:4685:TYR:CD1	1:B:4704:LEU:HD11	2.47	0.50
3:M:48:VAL:O	3:M:50:LYS:NZ	2.38	0.50
1:D:330:ARG:NH2	1:D:331:ASP:OD1	2.45	0.50
1:B:3467:ASN:ND2	1:B:3508:THR:O	2.44	0.50
1:C:4685:TYR:CD1	1:C:4704:LEU:HD11	2.47	0.50
3:K:5:LEU:CD1	3:L:15:VAL:HG21	2.42	0.49
3:N:34:LEU:HD23	3:N:70:VAL:HG21	1.95	0.49
1:D:3433:GLU:OE1	1:D:3525:MET:CG	2.59	0.49
1:D:3554:LEU:HB2	1:D:3594:VAL:HG13	1.93	0.49
1:B:330:ARG:NH2	1:B:331:ASP:OD1	2.45	0.49
1:B:3554:LEU:HB2	1:B:3594:VAL:HG13	1.93	0.49
1:C:3316:LEU:HD23	1:C:3346:ILE:HD13	1.94	0.49
1:A:3467:ASN:ND2	1:A:3508:THR:O	2.44	0.49
1:B:2755:PHE:CE2	1:B:2814:LEU:HD11	2.47	0.49
1:C:2755:PHE:CE2	1:C:2814:LEU:HD11	2.47	0.49
1:A:2110:ASP:OD1	1:A:2111:PHE:N	2.45	0.49
1:A:3771:SER:HA	1:A:3774:HIS:CE1	2.47	0.49
3:M:5:LEU:HD12	3:N:15:VAL:HG21	1.94	0.49
3:P:29:LEU:HD23	3:P:34:LEU:HD13	1.93	0.49
1:B:2110:ASP:OD1	1:B:2111:PHE:N	2.45	0.49
1:B:2979:GLU:OE2	1:B:3057:LEU:HD22	2.13	0.49
1:C:2110:ASP:OD1	1:C:2111:PHE:N	2.45	0.49
3:K:6:GLU:HG2	3:L:45:PHE:HE2	1.77	0.49
3:L:52:ALA:HA	3:L:55:VAL:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1264:THR:OG1	1:D:1267:THR:OG1	2.18	0.49
1:D:1739:LEU:HD12	1:D:1964:GLU:CD	2.32	0.49
1:D:2383:GLU:O	1:D:2387:ILE:HG12	2.11	0.49
1:D:2755:PHE:CE2	1:D:2814:LEU:HD11	2.47	0.49
1:C:1739:LEU:HD12	1:C:1964:GLU:CD	2.32	0.49
1:C:2979:GLU:OE2	1:C:3057:LEU:HD22	2.13	0.49
1:C:4574:ILE:HG23	1:C:4637:MET:HG2	1.93	0.49
1:D:2110:ASP:OD1	1:D:2111:PHE:N	2.45	0.49
1:B:234:ILE:O	1:B:258:ARG:NH1	2.46	0.49
1:B:3316:LEU:HD23	1:B:3346:ILE:HD13	1.94	0.49
1:C:2743:THR:OG1	1:C:2812:GLU:O	2.20	0.49
1:A:4574:ILE:HG23	1:A:4637:MET:HG2	1.93	0.49
3:K:60:LYS:O	3:K:63:ASP:OD1	2.31	0.49
1:D:4709:PHE:HB3	1:D:4710:PRO:HD3	1.94	0.49
1:B:41:GLU:OE2	1:B:407:SER:OG	2.29	0.49
1:B:3169:THR:O	1:B:3173:ILE:HG12	2.11	0.49
1:C:3927:LEU:O	1:C:3930:GLN:HG3	2.13	0.49
1:A:234:ILE:O	1:A:258:ARG:NH1	2.46	0.49
3:K:38:LEU:HD12	3:K:39:GLN:N	2.26	0.49
1:D:41:GLU:OE2	1:D:407:SER:OG	2.29	0.49
1:D:664:TYR:OH	1:D:666:GLU:OE2	2.30	0.49
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.13	0.49
1:B:3927:LEU:O	1:B:3930:GLN:HG3	2.13	0.49
1:B:4574:ILE:HG23	1:B:4637:MET:HG2	1.93	0.49
1:C:3271:ILE:H	1:C:3271:ILE:HD12	1.78	0.49
1:A:1739:LEU:HD12	1:A:1964:GLU:CD	2.32	0.49
1:A:3433:GLU:OE1	1:A:3525:MET:CG	2.59	0.49
3:J:27:TYR:HB3	3:I:93:THR:HG23	1.95	0.49
3:J:34:LEU:HD23	3:J:70:VAL:HG21	1.95	0.49
3:P:34:LEU:HD23	3:P:70:VAL:HG21	1.95	0.49
1:B:902:LYS:HZ2	1:B:904:LEU:HB2	1.78	0.49
1:B:1164:THR:HG22	1:B:1169:VAL:HA	1.94	0.49
1:B:3771:SER:HA	1:B:3774:HIS:CE1	2.47	0.49
1:C:234:ILE:O	1:C:258:ARG:NH1	2.46	0.49
3:P:53:ASP:O	3:P:57:LYS:HG2	2.13	0.49
1:D:3927:LEU:O	1:D:3930:GLN:HG3	2.13	0.49
1:C:41:GLU:OE2	1:C:407:SER:OG	2.29	0.49
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.13	0.49
1:A:330:ARG:NH2	1:A:331:ASP:OD1	2.45	0.49
1:A:3554:LEU:HB2	1:A:3594:VAL:HG13	1.93	0.49
3:J:53:ASP:O	3:J:57:LYS:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:60:LYS:O	3:M:63:ASP:OD1	2.31	0.49
1:D:2979:GLU:OE2	1:D:3057:LEU:HD22	2.13	0.49
1:C:2500:LYS:NZ	1:C:2530:ASP:OD2	2.36	0.49
1:C:3169:THR:O	1:C:3173:ILE:HG12	2.11	0.49
1:C:3554:LEU:HB2	1:C:3594:VAL:HG13	1.93	0.49
1:A:3181:ASN:O	1:A:3185:GLU:OE1	2.31	0.48
1:A:3316:LEU:HD23	1:A:3346:ILE:HD13	1.94	0.48
1:A:3927:LEU:O	1:A:3930:GLN:HG3	2.13	0.48
3:I:60:LYS:O	3:I:63:ASP:OD1	2.31	0.48
3:O:60:LYS:O	3:O:63:ASP:OD1	2.31	0.48
1:D:1164:THR:HG22	1:D:1169:VAL:HA	1.94	0.48
1:D:3181:ASN:O	1:D:3185:GLU:OE1	2.31	0.48
1:D:3771:SER:HA	1:D:3774:HIS:CE1	2.47	0.48
1:B:4927:LEU:O	1:B:4931:GLN:OE1	2.32	0.48
1:C:883:TRP:O	1:C:887:ARG:HD3	2.13	0.48
1:C:1164:THR:HG22	1:C:1169:VAL:HA	1.94	0.48
1:A:1164:THR:HG22	1:A:1169:VAL:HA	1.94	0.48
1:A:1973:ASN:ND2	1:A:1973:ASN:O	2.47	0.48
1:A:4875:ASP:O	1:D:4580:VAL:HG12	2.13	0.48
1:A:4927:LEU:O	1:A:4931:GLN:OE1	2.32	0.48
3:K:8:ALA:O	3:K:11:THR:OG1	2.24	0.48
3:O:19:HIS:CE1	3:O:37:LEU:HD13	2.49	0.48
1:D:883:TRP:O	1:D:887:ARG:HD3	2.13	0.48
1:B:554:ARG:NH2	1:B:556:GLU:OE2	2.40	0.48
1:B:883:TRP:O	1:B:887:ARG:HD3	2.13	0.48
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.13	0.48
1:B:4709:PHE:HB3	1:B:4710:PRO:HD3	1.94	0.48
3:N:53:ASP:O	3:N:57:LYS:HG2	2.13	0.48
3:P:52:ALA:HA	3:P:55:VAL:HG12	1.94	0.48
1:D:2011:LEU:HD11	1:D:2032:LEU:HD21	1.95	0.48
1:D:3271:ILE:H	1:D:3271:ILE:HD12	1.78	0.48
1:D:3316:LEU:HD23	1:D:3346:ILE:HD13	1.94	0.48
3:J:80:ALA:O	3:J:84:VAL:HG12	2.14	0.48
1:B:4580:VAL:HG12	1:C:4875:ASP:O	2.13	0.48
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.13	0.48
1:A:4908:GLU:O	1:A:4912:VAL:HG13	2.13	0.48
3:J:52:ALA:HA	3:J:55:VAL:HG12	1.95	0.48
3:K:48:VAL:O	3:K:50:LYS:NZ	2.38	0.48
1:D:902:LYS:HZ2	1:D:904:LEU:HB2	1.78	0.48
1:D:3236:SER:OG	1:D:3238:GLU:OE1	2.32	0.48
1:D:3467:ASN:O	1:D:3471:LEU:HD13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2011:LEU:HD11	1:B:2032:LEU:HD21	1.95	0.48
1:B:3164:VAL:HG22	1:B:3233:LEU:HD21	1.96	0.48
1:A:2450:GLU:OE1	1:A:2453:ARG:NH1	2.47	0.48
1:A:2979:GLU:OE2	1:A:3057:LEU:HD22	2.13	0.48
3:I:19:HIS:CE1	3:I:37:LEU:HD13	2.49	0.48
3:N:52:ALA:HA	3:N:55:VAL:HG12	1.95	0.48
1:D:2450:GLU:OE1	1:D:2453:ARG:NH1	2.47	0.48
1:B:1973:ASN:O	1:B:1973:ASN:ND2	2.47	0.48
1:A:41:GLU:OE2	1:A:407:SER:OG	2.29	0.48
1:A:2918:ALA:O	1:A:2922:GLU:OE1	2.32	0.48
1:A:4709:PHE:HB3	1:A:4710:PRO:HD3	1.94	0.48
3:K:93:THR:HG23	3:L:27:TYR:CB	2.38	0.48
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.79	0.48
1:D:4908:GLU:O	1:D:4912:VAL:HG13	2.13	0.48
1:B:2686:SER:O	1:B:2690:LYS:HG2	2.14	0.48
1:B:2817:MET:SD	1:B:2879:LEU:HD12	2.54	0.48
1:A:883:TRP:O	1:A:887:ARG:HD3	2.13	0.48
1:A:2817:MET:SD	1:A:2879:LEU:HD12	2.54	0.48
1:A:3236:SER:OG	1:A:3238:GLU:OE1	2.32	0.48
1:A:4632:GLU:OE1	1:A:4634:THR:OG1	2.27	0.48
1:B:2764:HIS:N	1:B:2806:TYR:OH	2.47	0.48
1:B:3271:ILE:H	1:B:3271:ILE:HD12	1.78	0.48
1:C:2764:HIS:N	1:C:2806:TYR:OH	2.47	0.48
1:C:3868:VAL:HG22	1:C:3869:ILE:N	2.29	0.48
3:M:31:LYS:NZ	3:M:62:LEU:O	2.38	0.48
3:L:80:ALA:O	3:L:84:VAL:HG12	2.14	0.48
1:D:2764:HIS:N	1:D:2806:TYR:OH	2.47	0.48
1:D:4685:TYR:OH	1:D:4697:GLY:O	2.30	0.48
1:B:2450:GLU:OE1	1:B:2453:ARG:NH1	2.47	0.48
1:B:3316:LEU:O	1:B:3320:ILE:HG12	2.14	0.48
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.72	0.48
1:C:2011:LEU:HD11	1:C:2032:LEU:HD21	1.96	0.48
1:C:3467:ASN:O	1:C:3471:LEU:HD13	2.14	0.48
1:C:4927:LEU:O	1:C:4931:GLN:OE1	2.32	0.48
1:A:2500:LYS:NZ	1:A:2530:ASP:OD2	2.36	0.47
3:I:7:SER:O	3:I:11:THR:HG23	2.14	0.47
3:L:34:LEU:HD23	3:L:70:VAL:HG21	1.95	0.47
1:B:3324:ILE:HG21	1:B:3409:LEU:HD21	1.96	0.47
1:B:4686:ILE:HD11	1:B:4738:LEU:HD23	1.96	0.47
1:C:2817:MET:SD	1:C:2879:LEU:HD12	2.54	0.47
1:C:3164:VAL:HG22	1:C:3233:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3181:ASN:O	1:C:3185:GLU:OE1	2.32	0.47
1:C:3236:SER:OG	1:C:3238:GLU:OE1	2.32	0.47
1:C:4709:PHE:HB3	1:C:4710:PRO:HD3	1.94	0.47
1:A:880:HIS:CE1	1:A:911:PHE:HB2	2.49	0.47
1:A:2686:SER:O	1:A:2690:LYS:HG2	2.14	0.47
1:A:3082:MET:HE2	1:A:3093:LEU:HD23	1.94	0.47
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.72	0.47
1:D:234:ILE:O	1:D:258:ARG:NH1	2.46	0.47
1:D:3324:ILE:HG21	1:D:3409:LEU:HD21	1.97	0.47
1:D:4875:ASP:O	1:C:4580:VAL:HG12	2.13	0.47
1:C:2671:GLU:O	1:C:2675:LEU:HD13	2.15	0.47
1:C:4752:ASN:OD1	1:C:4753:GLU:N	2.42	0.47
1:A:2011:LEU:HD11	1:A:2032:LEU:HD21	1.95	0.47
1:A:3271:ILE:H	1:A:3271:ILE:HD12	1.78	0.47
3:K:7:SER:O	3:K:11:THR:HG23	2.14	0.47
3:O:7:SER:O	3:O:11:THR:HG23	2.14	0.47
3:L:53:ASP:O	3:L:57:LYS:HG2	2.13	0.47
1:D:3770:GLN:O	1:D:3774:HIS:ND1	2.47	0.47
1:D:3868:VAL:HG22	1:D:3869:ILE:N	2.29	0.47
1:D:4927:LEU:O	1:D:4931:GLN:OE1	2.32	0.47
1:B:3181:ASN:O	1:B:3185:GLU:OE1	2.31	0.47
1:B:4908:GLU:O	1:B:4912:VAL:HG13	2.13	0.47
1:C:3770:GLN:O	1:C:3774:HIS:ND1	2.47	0.47
1:C:4686:ILE:HD11	1:C:4738:LEU:HD23	1.96	0.47
1:A:1793:ALA:O	1:A:1794:THR:OG1	2.20	0.47
1:A:3467:ASN:O	1:A:3471:LEU:HD13	2.14	0.47
3:I:48:VAL:O	3:I:50:LYS:NZ	2.38	0.47
1:D:4876:ASP:OD2	1:D:4879:THR:OG1	2.28	0.47
1:B:3467:ASN:O	1:B:3471:LEU:HD13	2.14	0.47
1:C:2450:GLU:OE1	1:C:2453:ARG:NH1	2.47	0.47
1:C:4908:GLU:O	1:C:4912:VAL:HG13	2.13	0.47
1:A:2671:GLU:O	1:A:2675:LEU:HD13	2.15	0.47
1:A:3316:LEU:O	1:A:3320:ILE:HG12	2.14	0.47
3:M:19:HIS:CE1	3:M:37:LEU:HD13	2.49	0.47
3:M:26:LYS:HZ2	3:N:92:GLU:H	1.62	0.47
1:D:880:HIS:CE1	1:D:911:PHE:HB2	2.49	0.47
1:D:980:PRO:HA	1:D:983:THR:OG1	2.15	0.47
1:D:2686:SER:O	1:D:2690:LYS:HG2	2.14	0.47
1:D:4055:SER:HG	1:D:4166:PHE:HE1	1.60	0.47
1:D:4686:ILE:HD11	1:D:4738:LEU:HD23	1.96	0.47
1:B:2918:ALA:O	1:B:2922:GLU:OE1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2747:ILE:HG22	1:C:2748:ILE:N	2.30	0.47
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.79	0.47
1:A:3770:GLN:O	1:A:3774:HIS:ND1	2.47	0.47
1:A:3868:VAL:HG22	1:A:3869:ILE:N	2.29	0.47
3:N:80:ALA:O	3:N:84:VAL:HG12	2.14	0.47
3:P:80:ALA:O	3:P:84:VAL:HG12	2.14	0.47
1:D:2918:ALA:O	1:D:2922:GLU:OE1	2.32	0.47
1:D:3954:PHE:O	1:D:3958:MET:HG3	2.14	0.47
1:B:2500:LYS:NZ	1:B:2530:ASP:OD2	2.36	0.47
1:B:4703:VAL:HG13	1:B:4709:PHE:HE1	1.80	0.47
1:C:926:SER:O	1:C:929:THR:OG1	2.27	0.47
1:C:2930:PHE:O	1:C:2934:ASN:ND2	2.48	0.47
1:A:2747:ILE:HG22	1:A:2748:ILE:N	2.30	0.47
1:A:2764:HIS:N	1:A:2806:TYR:OH	2.47	0.47
1:A:3164:VAL:HG22	1:A:3233:LEU:HD21	1.96	0.47
3:O:8:ALA:O	3:O:11:THR:OG1	2.24	0.47
1:D:2289:LEU:HD21	1:D:3855:LYS:HD2	1.97	0.47
1:D:2671:GLU:O	1:D:2675:LEU:HD13	2.15	0.47
1:D:2747:ILE:HG22	1:D:2748:ILE:H	1.80	0.47
1:D:2747:ILE:HG22	1:D:2748:ILE:N	2.30	0.47
1:B:2930:PHE:O	1:B:2934:ASN:ND2	2.48	0.47
1:B:3868:VAL:HG22	1:B:3869:ILE:N	2.29	0.47
1:C:980:PRO:HA	1:C:983:THR:OG1	2.15	0.47
1:C:1967:VAL:CG2	1:C:3650:ALA:HB1	2.45	0.47
1:C:2918:ALA:O	1:C:2922:GLU:OE1	2.32	0.47
1:C:3316:LEU:O	1:C:3320:ILE:HG12	2.14	0.47
1:C:3324:ILE:HG21	1:C:3409:LEU:HD21	1.97	0.47
1:A:2930:PHE:O	1:A:2934:ASN:ND2	2.48	0.47
1:A:3954:PHE:O	1:A:3958:MET:HG3	2.14	0.47
3:M:5:LEU:CD1	3:N:15:VAL:HG21	2.45	0.47
3:O:4:GLU:OE1	3:P:11:THR:CG2	2.63	0.47
1:D:694:SER:O	1:D:694:SER:OG	2.31	0.47
1:D:2817:MET:SD	1:D:2879:LEU:HD12	2.54	0.47
1:D:3004:LEU:HD21	1:D:3065:VAL:HG22	1.97	0.47
1:D:3316:LEU:O	1:D:3320:ILE:HG12	2.14	0.47
1:D:3600:VAL:O	1:D:3604:LEU:HD13	2.15	0.47
1:B:1264:THR:OG1	1:B:1267:THR:OG1	2.18	0.47
1:C:4893:GLY:N	1:C:4897:ASP:OD2	2.47	0.47
1:A:614:ALA:HB2	1:A:1677:LEU:HD12	1.97	0.47
1:A:980:PRO:HA	1:A:983:THR:OG1	2.15	0.47
1:A:3600:VAL:O	1:A:3604:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4686:ILE:HD11	1:A:4738:LEU:HD23	1.96	0.47
1:A:4703:VAL:HG13	1:A:4709:PHE:HE1	1.80	0.47
3:M:7:SER:O	3:M:11:THR:HG23	2.14	0.47
1:D:978:LEU:HD12	1:D:982:GLN:CB	2.45	0.47
1:D:2930:PHE:O	1:D:2934:ASN:ND2	2.48	0.47
1:D:3163:GLN:NE2	1:D:3204:VAL:HG11	2.30	0.47
1:B:3600:VAL:O	1:B:3604:LEU:HD13	2.15	0.47
1:C:2289:LEU:HD21	1:C:3855:LYS:HD2	1.97	0.47
1:C:3600:VAL:O	1:C:3604:LEU:HD13	2.15	0.47
1:A:3163:GLN:NE2	1:A:3204:VAL:HG11	2.30	0.47
1:A:3540:ARG:NH2	1:A:3545:ASP:OD2	2.49	0.47
3:K:19:HIS:CE1	3:K:37:LEU:HD13	2.49	0.47
3:K:31:LYS:NZ	3:K:62:LEU:O	2.38	0.47
3:K:32:LYS:HA	3:K:35:LYS:HE3	1.97	0.47
3:O:32:LYS:HA	3:O:35:LYS:HE3	1.97	0.47
3:N:13:ILE:HD11	3:N:17:HIS:HE1	1.80	0.47
1:B:880:HIS:CE1	1:B:911:PHE:HB2	2.49	0.47
1:B:978:LEU:HD12	1:B:982:GLN:CB	2.45	0.47
1:C:978:LEU:HD12	1:C:982:GLN:CB	2.45	0.47
1:A:554:ARG:NH2	1:A:556:GLU:OE2	2.40	0.46
1:A:3324:ILE:HG21	1:A:3409:LEU:HD21	1.96	0.46
3:J:93:THR:HA	3:I:27:TYR:CD2	2.50	0.46
3:P:13:ILE:HD11	3:P:17:HIS:HE1	1.80	0.46
1:D:1713:TYR:OH	1:D:1816:MET:SD	2.73	0.46
1:D:1967:VAL:CG2	1:D:3650:ALA:HB1	2.45	0.46
1:D:1973:ASN:O	1:D:1973:ASN:ND2	2.47	0.46
1:D:2187:MET:O	1:D:2193:TYR:OH	2.14	0.46
1:B:3163:GLN:NE2	1:B:3204:VAL:HG11	2.30	0.46
1:B:3954:PHE:O	1:B:3958:MET:HG3	2.14	0.46
1:B:4107:THR:O	1:B:4110:GLU:N	2.48	0.46
1:C:2627:LEU:HD22	1:C:2641:PRO:HB3	1.97	0.46
1:C:2747:ILE:HG22	1:C:2748:ILE:H	1.80	0.46
1:C:2748:ILE:HG21	1:C:2811:LYS:CE	2.46	0.46
1:C:3954:PHE:O	1:C:3958:MET:HG3	2.14	0.46
1:C:4107:THR:O	1:C:4110:GLU:N	2.48	0.46
1:A:722:LEU:HD12	1:A:1477:MET:HE2	1.97	0.46
3:O:93:THR:HG23	3:P:27:TYR:CB	2.41	0.46
1:D:3164:VAL:HG22	1:D:3233:LEU:HD21	1.96	0.46
1:D:3540:ARG:NH2	1:D:3545:ASP:OD2	2.49	0.46
1:D:4013:ILE:O	1:D:4017:LYS:HG2	2.16	0.46
1:B:2671:GLU:O	1:B:2675:LEU:HD13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3236:SER:OG	1:B:3238:GLU:OE1	2.32	0.46
1:C:24:GLN:OE1	1:C:204:ASN:ND2	2.49	0.46
1:C:880:HIS:CE1	1:C:911:PHE:HB2	2.49	0.46
1:C:3372:LYS:O	1:C:3376:GLU:OE1	2.33	0.46
1:A:929:THR:O	1:A:932:THR:OG1	2.28	0.46
1:A:1807:GLU:HA	1:A:1810:ARG:NH1	2.31	0.46
1:A:2747:ILE:HG22	1:A:2748:ILE:H	1.80	0.46
1:A:3559:ASN:O	1:A:3560:LEU:HB2	2.15	0.46
1:A:4107:THR:O	1:A:4110:GLU:N	2.48	0.46
3:K:26:LYS:HZ2	3:L:92:GLU:H	1.62	0.46
1:D:3372:LYS:O	1:D:3376:GLU:OE1	2.33	0.46
1:B:722:LEU:HD12	1:B:1477:MET:HE1	1.98	0.46
1:B:3372:LYS:O	1:B:3376:GLU:OE1	2.33	0.46
1:C:3163:GLN:NE2	1:C:3204:VAL:HG11	2.30	0.46
1:C:4703:VAL:HG13	1:C:4709:PHE:HE1	1.80	0.46
1:A:3004:LEU:HD21	1:A:3065:VAL:HG22	1.97	0.46
3:I:32:LYS:HA	3:I:35:LYS:HE3	1.97	0.46
3:O:25:ASP:HB3	3:P:94:SER:HB3	1.96	0.46
1:D:926:SER:O	1:D:929:THR:OG1	2.27	0.46
1:D:1807:GLU:HA	1:D:1810:ARG:NH1	2.31	0.46
1:B:614:ALA:HB2	1:B:1677:LEU:HD12	1.97	0.46
1:B:2747:ILE:HG22	1:B:2748:ILE:N	2.29	0.46
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.79	0.46
1:B:3540:ARG:NH2	1:B:3545:ASP:OD2	2.48	0.46
1:C:1807:GLU:HA	1:C:1810:ARG:NH1	2.31	0.46
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.97	0.46
1:A:868:LEU:CD2	1:A:871:ILE:HD12	2.46	0.46
1:A:902:LYS:HZ2	1:A:904:LEU:HB2	1.80	0.46
1:A:4013:ILE:O	1:A:4017:LYS:HG2	2.16	0.46
1:A:4100:MET:CE	1:A:4111:ILE:HG23	2.45	0.46
1:D:982:GLN:CG	1:D:1054:ILE:HD11	2.46	0.46
1:D:3559:ASN:O	1:D:3560:LEU:HB2	2.15	0.46
1:B:24:GLN:OE1	1:B:204:ASN:ND2	2.49	0.46
1:B:2627:LEU:HD22	1:B:2641:PRO:HB3	1.97	0.46
1:C:982:GLN:CG	1:C:1054:ILE:HD11	2.46	0.46
1:C:4013:ILE:O	1:C:4017:LYS:HG2	2.16	0.46
1:A:3372:LYS:O	1:A:3376:GLU:OE1	2.33	0.46
1:A:3458:ASN:O	1:A:3459:PHE:C	2.54	0.46
1:A:3567:SER:O	1:A:3571:ARG:NH1	2.49	0.46
1:D:929:THR:O	1:D:932:THR:OG1	2.29	0.46
1:B:2747:ILE:HG22	1:B:2748:ILE:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3770:GLN:O	1:B:3774:HIS:ND1	2.47	0.46
1:C:1713:TYR:OH	1:C:1816:MET:SD	2.73	0.46
1:C:1973:ASN:O	1:C:1973:ASN:ND2	2.47	0.46
1:C:2686:SER:O	1:C:2690:LYS:HG2	2.14	0.46
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.31	0.46
1:C:3540:ARG:NH2	1:C:3545:ASP:OD2	2.49	0.46
1:A:24:GLN:OE1	1:A:204:ASN:ND2	2.49	0.46
1:A:877:GLU:HA	1:A:880:HIS:ND1	2.31	0.46
1:A:978:LEU:HD12	1:A:982:GLN:CB	2.45	0.46
3:K:67:ASP:N	3:K:67:ASP:OD1	2.49	0.46
3:M:32:LYS:HA	3:M:35:LYS:HE3	1.97	0.46
1:B:3373:VAL:HG12	1:B:3399:PHE:CE2	2.51	0.46
1:C:47:LEU:HD13	1:C:126:ARG:HH12	1.81	0.46
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.97	0.46
1:C:921:TYR:O	1:C:925:MET:HG2	2.16	0.46
1:A:921:TYR:O	1:A:925:MET:HG2	2.16	0.46
1:A:2193:TYR:HE1	1:A:2239:TYR:HH	1.63	0.46
1:A:2627:LEU:HD22	1:A:2641:PRO:HB3	1.97	0.46
1:A:2765:GLU:OE2	1:A:2858:PRO:HA	2.16	0.46
3:J:5:LEU:HD11	3:I:12:LEU:HD13	1.98	0.46
3:J:13:ILE:HD11	3:J:17:HIS:HE1	1.80	0.46
3:M:67:ASP:OD1	3:M:67:ASP:N	2.49	0.46
1:D:3337:LYS:HD2	1:D:3465:ILE:CG2	2.46	0.46
1:D:4703:VAL:HG13	1:D:4709:PHE:HE1	1.80	0.46
1:B:1807:GLU:HA	1:B:1810:ARG:NH1	2.31	0.46
1:B:3082:MET:HE2	1:B:3093:LEU:HD23	1.96	0.46
1:B:3559:ASN:O	1:B:3560:LEU:HB2	2.15	0.46
1:C:3559:ASN:O	1:C:3560:LEU:HB2	2.15	0.46
1:A:47:LEU:HD13	1:A:126:ARG:HH12	1.81	0.46
1:A:3820:LEU:HD21	1:A:3901:ASP:HB3	1.98	0.46
1:D:614:ALA:HB2	1:D:1677:LEU:HD12	1.97	0.46
1:D:868:LEU:CD2	1:D:871:ILE:HD12	2.46	0.46
1:D:2765:GLU:OE2	1:D:2858:PRO:HA	2.16	0.46
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.72	0.46
1:D:4656:ILE:HD11	1:D:4794:MET:HB2	1.98	0.46
1:D:4765:TRP:O	1:D:4769:ILE:HG12	2.15	0.46
1:C:877:GLU:HA	1:C:880:HIS:ND1	2.31	0.46
1:A:1713:TYR:OH	1:A:1816:MET:SD	2.73	0.46
1:A:3337:LYS:HD2	1:A:3465:ILE:CG2	2.46	0.46
1:A:3526:CYS:SG	1:A:3600:VAL:HG11	2.56	0.46
3:K:5:LEU:HD12	3:L:15:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:34:LEU:HD23	3:K:38:LEU:HD23	1.98	0.46
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.31	0.46
1:D:3567:SER:O	1:D:3571:ARG:NH1	2.49	0.46
1:B:980:PRO:HA	1:B:983:THR:OG1	2.15	0.46
1:B:1713:TYR:OH	1:B:1816:MET:SD	2.73	0.46
1:B:1967:VAL:CG2	1:B:3650:ALA:HB1	2.45	0.46
1:C:868:LEU:CD2	1:C:871:ILE:HD12	2.46	0.46
1:C:1172:SER:OG	1:C:1176:SER:N	2.47	0.46
1:C:3076:LEU:O	1:C:3147:HIS:NE2	2.48	0.46
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.72	0.46
1:A:2289:LEU:HD21	1:A:3855:LYS:HD2	1.97	0.45
1:A:4765:TRP:O	1:A:4769:ILE:HG12	2.15	0.45
2:E:7:THR:HG23	2:E:7:THR:O	2.16	0.45
1:D:47:LEU:HD13	1:D:126:ARG:HH12	1.81	0.45
1:B:47:LEU:HD13	1:B:126:ARG:HH12	1.81	0.45
1:B:2748:ILE:HG21	1:B:2811:LYS:CE	2.45	0.45
1:B:3004:LEU:HD21	1:B:3065:VAL:HG22	1.97	0.45
1:C:421:SER:O	1:C:425:LYS:NZ	2.44	0.45
1:C:3567:SER:O	1:C:3571:ARG:NH1	2.49	0.45
1:A:1967:VAL:CG2	1:A:3650:ALA:HB1	2.45	0.45
3:I:34:LEU:HD23	3:I:38:LEU:HD23	1.98	0.45
3:I:80:ALA:HA	3:I:83:THR:HG22	1.98	0.45
1:D:2748:ILE:HG21	1:D:2811:LYS:CE	2.45	0.45
1:D:2881:GLU:OE1	1:D:2909:TYR:HB3	2.17	0.45
1:D:3373:VAL:HG12	1:D:3399:PHE:CE2	2.51	0.45
1:B:868:LEU:CD2	1:B:871:ILE:HD12	2.46	0.45
1:B:982:GLN:CG	1:B:1054:ILE:HD11	2.46	0.45
1:B:3567:SER:O	1:B:3571:ARG:NH1	2.49	0.45
1:B:4685:TYR:OH	1:B:4697:GLY:O	2.30	0.45
1:A:982:GLN:CG	1:A:1054:ILE:HD11	2.46	0.45
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.97	0.45
1:D:921:TYR:O	1:D:925:MET:HG2	2.16	0.45
1:D:3526:CYS:SG	1:D:3600:VAL:HG11	2.56	0.45
1:D:4107:THR:O	1:D:4110:GLU:N	2.48	0.45
1:B:877:GLU:HA	1:B:880:HIS:ND1	2.31	0.45
1:B:2289:LEU:HD21	1:B:3855:LYS:HD2	1.97	0.45
1:B:3458:ASN:O	1:B:3459:PHE:C	2.54	0.45
1:C:3004:LEU:HD21	1:C:3065:VAL:HG22	1.97	0.45
1:C:3337:LYS:HD2	1:C:3465:ILE:CG2	2.46	0.45
1:C:3820:LEU:HD21	1:C:3901:ASP:HB3	1.98	0.45
1:C:4765:TRP:O	1:C:4769:ILE:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3177:GLY:HA3	1:A:3273:ILE:HD13	1.98	0.45
3:I:67:ASP:N	3:I:67:ASP:OD1	2.49	0.45
1:D:2814:LEU:HA	1:D:2817:MET:HE2	1.98	0.45
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.97	0.45
1:B:4013:ILE:O	1:B:4017:LYS:HG2	2.16	0.45
1:C:614:ALA:HB2	1:C:1677:LEU:HD12	1.97	0.45
1:C:3373:VAL:HG12	1:C:3399:PHE:CE2	2.51	0.45
1:C:3434:GLU:O	1:C:3438:MET:HG3	2.17	0.45
1:A:2780:GLU:OE1	1:A:2780:GLU:N	2.49	0.45
1:A:2894:GLU:OE1	1:A:2898:LYS:NZ	2.50	0.45
3:I:12:LEU:O	3:I:15:VAL:HG12	2.17	0.45
3:M:5:LEU:HD12	3:N:15:VAL:HG11	1.98	0.45
3:O:67:ASP:OD1	3:O:67:ASP:N	2.49	0.45
3:L:13:ILE:HD11	3:L:17:HIS:HE1	1.80	0.45
1:D:24:GLN:OE1	1:D:204:ASN:ND2	2.49	0.45
1:D:1773:LEU:HD11	1:D:2145:ILE:HD11	1.99	0.45
1:D:2780:GLU:OE1	1:D:2780:GLU:N	2.49	0.45
1:B:3337:LYS:HD2	1:B:3465:ILE:CG2	2.46	0.45
1:A:1773:LEU:HD11	1:A:2145:ILE:HD11	1.99	0.45
1:A:2881:GLU:OE1	1:A:2909:TYR:HB3	2.17	0.45
1:A:3373:VAL:HG12	1:A:3399:PHE:CE2	2.51	0.45
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.31	0.45
3:M:80:ALA:HA	3:M:83:THR:HG22	1.98	0.45
1:D:2627:LEU:HD22	1:D:2641:PRO:HB3	1.97	0.45
1:D:3434:GLU:O	1:D:3438:MET:HG3	2.17	0.45
1:D:4893:GLY:N	1:D:4897:ASP:OD2	2.47	0.45
1:B:1773:LEU:HD11	1:B:2145:ILE:HD11	1.99	0.45
1:B:4765:TRP:O	1:B:4769:ILE:HG12	2.15	0.45
1:C:1773:LEU:HD11	1:C:2145:ILE:HD11	1.99	0.45
1:A:473:ARG:NH2	1:A:476:GLN:OE1	2.44	0.45
1:A:760:ILE:HG23	1:A:760:ILE:O	2.17	0.45
3:O:34:LEU:HD23	3:O:38:LEU:HD23	1.98	0.45
3:P:87:ASN:OD1	3:P:91:TRP:CE3	2.70	0.45
1:D:3082:MET:HE2	1:D:3093:LEU:HD23	1.94	0.45
1:B:921:TYR:O	1:B:925:MET:HG2	2.16	0.45
1:B:2193:TYR:HE1	1:B:2239:TYR:HH	1.62	0.45
1:B:3820:LEU:HD21	1:B:3901:ASP:HB3	1.98	0.45
1:B:4876:ASP:OD2	1:B:4879:THR:OG1	2.28	0.45
1:C:2765:GLU:OE2	1:C:2858:PRO:HA	2.16	0.45
1:C:2964:LEU:CD2	1:C:3003:LEU:HD22	2.47	0.45
1:A:2351:ALA:O	1:A:2355:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:92:GLU:C	3:N:93:THR:HG1	2.11	0.45
1:D:421:SER:O	1:D:425:LYS:NZ	2.44	0.45
1:D:877:GLU:HA	1:D:880:HIS:ND1	2.31	0.45
1:D:2894:GLU:OE1	1:D:2898:LYS:NZ	2.50	0.45
1:D:3282:LEU:CD1	1:D:3316:LEU:HD22	2.46	0.45
1:D:3820:LEU:HD21	1:D:3901:ASP:HB3	1.98	0.45
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	1.98	0.45
1:B:3107:MET:O	1:B:3111:LEU:HD23	2.17	0.45
1:B:3526:CYS:SG	1:B:3600:VAL:HG11	2.56	0.45
1:C:902:LYS:HZ2	1:C:904:LEU:HB2	1.82	0.45
1:C:3460:VAL:HG23	1:C:3465:ILE:CG1	2.47	0.45
1:C:3526:CYS:SG	1:C:3600:VAL:HG11	2.56	0.45
3:J:20:SER:HA	3:J:29:LEU:HD13	1.99	0.45
3:J:87:ASN:OD1	3:J:91:TRP:CE3	2.70	0.45
3:M:34:LEU:HD23	3:M:38:LEU:HD23	1.98	0.45
3:L:87:ASN:OD1	3:L:91:TRP:CE3	2.70	0.45
1:D:554:ARG:NH2	1:D:556:GLU:OE2	2.40	0.45
1:D:2964:LEU:CD2	1:D:3003:LEU:HD22	2.47	0.45
1:D:3177:GLY:HA3	1:D:3273:ILE:HD13	1.98	0.45
1:B:3460:VAL:HG23	1:B:3465:ILE:CG1	2.47	0.45
1:A:2748:ILE:HG21	1:A:2811:LYS:CE	2.46	0.45
2:H:7:THR:HG23	2:H:7:THR:O	2.17	0.45
3:K:12:LEU:O	3:K:15:VAL:HG12	2.17	0.45
3:O:17:HIS:CE1	3:P:87:ASN:HD21	2.35	0.45
1:B:2521:HIS:O	1:B:2525:VAL:HG23	2.17	0.45
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.31	0.45
1:C:929:THR:O	1:C:932:THR:OG1	2.28	0.45
1:C:2894:GLU:OE1	1:C:2898:LYS:NZ	2.50	0.45
1:C:4656:ILE:HD11	1:C:4794:MET:HB2	1.98	0.45
1:A:3107:MET:O	1:A:3111:LEU:HD23	2.17	0.44
3:K:12:LEU:HD21	3:L:9:MET:CE	2.47	0.44
3:K:34:LEU:HD21	3:K:78:LEU:HD21	2.00	0.44
3:M:8:ALA:O	3:M:11:THR:OG1	2.24	0.44
1:D:3460:VAL:HG23	1:D:3465:ILE:CG1	2.47	0.44
1:B:4656:ILE:HD11	1:B:4794:MET:HB2	1.98	0.44
1:A:3434:GLU:O	1:A:3438:MET:HG3	2.17	0.44
1:A:3460:VAL:HG23	1:A:3465:ILE:CG1	2.47	0.44
1:A:3564:VAL:HG13	1:A:3565:GLU:N	2.33	0.44
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	1.98	0.44
3:K:75:TYR:O	3:K:79:VAL:HG22	2.18	0.44
3:M:34:LEU:HD21	3:M:78:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:75:TYR:O	3:O:79:VAL:HG22	2.18	0.44
3:L:36:ASP:O	3:L:40:THR:HG23	2.17	0.44
1:D:2351:ALA:O	1:D:2355:VAL:HG23	2.17	0.44
1:B:760:ILE:HG23	1:B:760:ILE:O	2.17	0.44
1:B:1695:LEU:O	1:B:1699:LEU:HD13	2.17	0.44
1:B:3076:LEU:O	1:B:3147:HIS:NE2	2.48	0.44
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.33	0.44
1:C:3107:MET:O	1:C:3111:LEU:HD23	2.17	0.44
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	1.98	0.44
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.32	0.44
3:P:36:ASP:O	3:P:40:THR:HG23	2.18	0.44
1:D:4703:VAL:HG13	1:D:4709:PHE:CE1	2.53	0.44
1:B:370:LEU:HB3	1:B:372:VAL:HG22	1.99	0.44
1:B:623:THR:HG23	1:B:627:LEU:HD12	1.99	0.44
1:B:2351:ALA:O	1:B:2355:VAL:HG23	2.17	0.44
1:B:2894:GLU:OE1	1:B:2898:LYS:NZ	2.50	0.44
1:B:3434:GLU:O	1:B:3438:MET:HG3	2.17	0.44
1:B:3564:VAL:HG13	1:B:3565:GLU:N	2.33	0.44
1:C:2351:ALA:O	1:C:2355:VAL:HG23	2.17	0.44
1:C:2881:GLU:OE1	1:C:2909:TYR:HB3	2.17	0.44
1:C:3564:VAL:HG13	1:C:3565:GLU:N	2.33	0.44
1:C:4100:MET:CE	1:C:4111:ILE:HG23	2.45	0.44
1:A:3275:LEU:HB3	1:A:3276:PRO:HD3	2.00	0.44
1:A:4656:ILE:HD11	1:A:4794:MET:HB2	1.98	0.44
1:A:4723:LEU:HA	1:A:4735:ILE:HG21	2.00	0.44
3:K:8:ALA:O	3:K:12:LEU:HD23	2.18	0.44
3:O:34:LEU:HD21	3:O:78:LEU:HD21	1.99	0.44
3:N:87:ASN:OD1	3:N:91:TRP:CE3	2.70	0.44
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.32	0.44
1:B:3282:LEU:CD1	1:B:3316:LEU:HD22	2.46	0.44
1:C:4107:THR:HG22	1:C:4109:PRO:HD2	2.00	0.44
1:A:1695:LEU:O	1:A:1699:LEU:HD13	2.18	0.44
1:A:2964:LEU:CD2	1:A:3003:LEU:HD22	2.47	0.44
3:I:8:ALA:O	3:I:12:LEU:HD23	2.18	0.44
3:M:8:ALA:O	3:M:12:LEU:HD23	2.18	0.44
3:O:12:LEU:O	3:O:15:VAL:HG12	2.17	0.44
3:N:36:ASP:O	3:N:40:THR:HG23	2.18	0.44
1:D:869:GLU:HA	1:D:872:ARG:HG2	2.00	0.44
1:D:3458:ASN:O	1:D:3459:PHE:C	2.54	0.44
1:D:3564:VAL:HG13	1:D:3565:GLU:N	2.33	0.44
1:B:979:THR:HG22	1:B:982:GLN:CD	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2964:LEU:CD2	1:B:3003:LEU:HD22	2.47	0.44
1:B:3275:LEU:HB3	1:B:3276:PRO:HD3	2.00	0.44
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.98	0.44
1:B:4893:GLY:N	1:B:4897:ASP:OD2	2.47	0.44
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.79	0.44
1:A:70:LEU:HD23	1:A:110:LEU:HD23	2.00	0.44
3:O:45:PHE:CE2	3:P:6:GLU:HG2	2.52	0.44
3:O:80:ALA:HA	3:O:83:THR:HG22	1.98	0.44
3:N:55:VAL:O	3:N:58:VAL:HG12	2.18	0.44
1:B:1172:SER:OG	1:B:1176:SER:N	2.47	0.44
1:B:3360:ILE:HB	1:B:3361:PRO:HD3	2.00	0.44
1:B:4107:THR:HG22	1:B:4109:PRO:HD2	2.00	0.44
1:B:4723:LEU:HA	1:B:4735:ILE:HG21	2.00	0.44
1:C:1695:LEU:O	1:C:1699:LEU:HD13	2.17	0.44
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.20	0.44
1:C:2521:HIS:O	1:C:2525:VAL:HG23	2.17	0.44
1:A:2215:VAL:CG2	1:A:2229:MET:HE1	2.48	0.44
1:A:4703:VAL:HG13	1:A:4709:PHE:CE1	2.53	0.44
3:J:36:ASP:O	3:J:40:THR:HG23	2.17	0.44
3:M:12:LEU:O	3:M:15:VAL:HG12	2.17	0.44
1:A:623:THR:HG23	1:A:627:LEU:HD12	1.99	0.44
1:A:3282:LEU:CD1	1:A:3316:LEU:HD22	2.46	0.44
3:L:20:SER:HA	3:L:29:LEU:HD13	1.99	0.44
1:D:3107:MET:O	1:D:3111:LEU:HD23	2.17	0.44
1:D:4107:THR:HG22	1:D:4109:PRO:HD2	2.00	0.44
1:B:473:ARG:NH2	1:B:476:GLN:OE1	2.44	0.44
1:B:869:GLU:HA	1:B:872:ARG:HG2	2.00	0.44
1:B:2765:GLU:OE2	1:B:2858:PRO:HA	2.16	0.44
1:C:3177:GLY:HA3	1:C:3273:ILE:HD13	1.98	0.44
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.32	0.44
1:C:4723:LEU:HA	1:C:4735:ILE:HG21	2.00	0.44
1:A:3380:LEU:HD12	1:A:3395:VAL:HG21	2.00	0.44
3:I:75:TYR:O	3:I:79:VAL:HG22	2.18	0.44
3:K:80:ALA:HA	3:K:83:THR:HG22	1.98	0.44
3:O:8:ALA:O	3:O:12:LEU:HD23	2.18	0.44
3:P:20:SER:HA	3:P:29:LEU:HD13	1.99	0.44
1:D:70:LEU:HD23	1:D:110:LEU:HD23	2.00	0.44
1:D:722:LEU:HD12	1:D:1477:MET:HE1	1.98	0.44
1:D:1744:ARG:NE	1:D:1964:GLU:OE2	2.50	0.44
1:D:2738:PRO:O	1:D:2740:PRO:HD3	2.18	0.44
1:D:3275:LEU:HB3	1:D:3276:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3443:PHE:CD2	1:B:3515:LEU:HD13	2.53	0.44
1:C:232:LEU:HD11	1:C:246:VAL:CG1	2.48	0.44
1:C:760:ILE:HG23	1:C:760:ILE:O	2.17	0.44
1:C:2749:PRO:HD2	1:C:2752:LEU:HD12	2.00	0.44
1:C:3360:ILE:HB	1:C:3361:PRO:HD3	2.00	0.44
1:C:3443:PHE:CD2	1:C:3515:LEU:HD13	2.53	0.44
1:C:4703:VAL:HG13	1:C:4709:PHE:CE1	2.53	0.44
1:A:216:THR:OG1	1:A:219:HIS:CD2	2.71	0.43
1:A:370:LEU:HB3	1:A:372:VAL:HG22	2.00	0.43
1:A:1172:SER:OG	1:A:1176:SER:N	2.47	0.43
1:A:1744:ARG:NE	1:A:1964:GLU:OE2	2.50	0.43
1:A:2738:PRO:O	1:A:2740:PRO:HD3	2.18	0.43
1:A:2749:PRO:HD2	1:A:2752:LEU:HD12	2.00	0.43
1:A:3443:PHE:CD2	1:A:3515:LEU:HD13	2.53	0.43
1:D:216:THR:OG1	1:D:219:HIS:CD2	2.71	0.43
1:D:760:ILE:O	1:D:760:ILE:HG23	2.17	0.43
1:D:2749:PRO:HD2	1:D:2752:LEU:HD12	2.00	0.43
1:D:3380:LEU:HD12	1:D:3395:VAL:HG21	2.00	0.43
1:D:4723:LEU:HA	1:D:4735:ILE:HG21	2.00	0.43
1:B:2749:PRO:HD2	1:B:2752:LEU:HD12	2.00	0.43
1:C:1144:TRP:HB2	1:C:1148:ASP:HB2	2.00	0.43
1:C:3267:MET:HG3	1:C:3267:MET:O	2.18	0.43
1:C:3380:LEU:HD12	1:C:3395:VAL:HG21	2.00	0.43
1:C:3458:ASN:O	1:C:3459:PHE:C	2.54	0.43
1:A:869:GLU:HA	1:A:872:ARG:HG2	2.00	0.43
1:A:2521:HIS:O	1:A:2525:VAL:HG23	2.17	0.43
3:J:84:VAL:HG11	3:I:73:LYS:HD2	2.01	0.43
3:I:34:LEU:HD21	3:I:78:LEU:HD21	1.99	0.43
3:M:48:VAL:O	3:M:48:VAL:HG12	2.18	0.43
3:O:48:VAL:O	3:O:48:VAL:HG12	2.18	0.43
3:L:55:VAL:O	3:L:58:VAL:HG12	2.18	0.43
1:D:1695:LEU:O	1:D:1699:LEU:HD13	2.18	0.43
1:B:2881:GLU:OE1	1:B:2909:TYR:HB3	2.17	0.43
1:B:3177:GLY:HA3	1:B:3273:ILE:HD13	1.98	0.43
1:B:4664:VAL:N	1:B:4665:PRO:CD	2.81	0.43
1:C:3275:LEU:HB3	1:C:3276:PRO:HD3	2.00	0.43
1:A:2411:PRO:N	1:A:2412:PRO:CD	2.81	0.43
1:A:2578:ILE:H	1:A:2578:ILE:HD12	1.84	0.43
1:A:3360:ILE:HB	1:A:3361:PRO:HD3	2.00	0.43
1:A:4107:THR:HG22	1:A:4109:PRO:HD2	2.00	0.43
3:N:20:SER:HA	3:N:29:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2521:HIS:O	1:D:2525:VAL:HG23	2.17	0.43
1:D:3360:ILE:HB	1:D:3361:PRO:HD3	2.00	0.43
1:B:978:LEU:HD12	1:B:982:GLN:HB2	2.01	0.43
1:B:2738:PRO:O	1:B:2740:PRO:HD3	2.18	0.43
1:A:979:THR:OG1	1:A:980:PRO:HD2	2.18	0.43
1:A:3267:MET:HG3	1:A:3267:MET:O	2.19	0.43
1:A:3515:LEU:HD11	1:A:3603:VAL:HG13	2.01	0.43
3:I:48:VAL:O	3:I:48:VAL:HG12	2.18	0.43
2:F:7:THR:HG23	2:F:7:THR:O	2.18	0.43
3:K:48:VAL:O	3:K:48:VAL:HG12	2.18	0.43
1:D:979:THR:OG1	1:D:980:PRO:HD2	2.18	0.43
1:D:4752:ASN:OD1	1:D:4753:GLU:N	2.42	0.43
1:B:216:THR:OG1	1:B:219:HIS:CD2	2.71	0.43
1:C:1968:ASP:C	1:C:1968:ASP:OD2	2.57	0.43
1:A:2748:ILE:HG21	1:A:2811:LYS:HE3	2.01	0.43
3:J:87:ASN:HD21	3:I:17:HIS:CE1	2.36	0.43
3:P:56:ASP:OD1	3:P:56:ASP:C	2.57	0.43
1:D:978:LEU:HD12	1:D:982:GLN:HB2	2.01	0.43
1:D:2215:VAL:CG2	1:D:2229:MET:HE1	2.49	0.43
1:D:2748:ILE:HG21	1:D:2811:LYS:HE3	2.01	0.43
1:D:3443:PHE:CD2	1:D:3515:LEU:HD13	2.53	0.43
1:B:791:ARG:HA	1:B:1627:TRP:O	2.19	0.43
1:B:979:THR:OG1	1:B:980:PRO:HD2	2.18	0.43
1:B:1968:ASP:C	1:B:1968:ASP:OD2	2.57	0.43
1:B:2411:PRO:N	1:B:2412:PRO:CD	2.81	0.43
1:B:2792:LEU:HD12	1:B:2792:LEU:O	2.19	0.43
1:B:3380:LEU:HD12	1:B:3395:VAL:HG21	2.00	0.43
1:B:4703:VAL:HG13	1:B:4709:PHE:CE1	2.53	0.43
1:C:370:LEU:HB3	1:C:372:VAL:HG22	2.00	0.43
1:C:619:GLN:OE1	1:C:1679:ASN:ND2	2.50	0.43
1:C:868:LEU:HD21	1:C:940:VAL:HG21	2.01	0.43
1:A:978:LEU:HD12	1:A:982:GLN:HB2	2.01	0.43
1:A:3859:LEU:HB3	1:A:3871:ARG:NH2	2.34	0.43
3:L:56:ASP:OD1	3:L:56:ASP:C	2.57	0.43
1:D:3461:VAL:HG23	1:D:3462:GLN:OE1	2.19	0.43
1:D:3515:LEU:HD11	1:D:3603:VAL:HG13	2.01	0.43
1:B:576:LEU:HA	1:B:579:ILE:HG12	2.01	0.43
1:C:4664:VAL:N	1:C:4665:PRO:CD	2.82	0.43
1:A:1144:TRP:HB2	1:A:1148:ASP:HB2	2.00	0.43
1:A:1968:ASP:OD2	1:A:1968:ASP:C	2.57	0.43
3:J:56:ASP:OD1	3:J:56:ASP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:55:VAL:O	3:P:58:VAL:HG12	2.18	0.43
1:D:2356:ARG:O	1:D:2359:ILE:HG12	2.19	0.43
1:D:4664:VAL:N	1:D:4665:PRO:CD	2.81	0.43
1:B:1282:ASN:OD1	1:B:1282:ASN:C	2.57	0.43
1:B:3267:MET:O	1:B:3267:MET:HG3	2.19	0.43
1:B:3859:LEU:HB3	1:B:3871:ARG:NH2	2.34	0.43
1:C:70:LEU:HD23	1:C:110:LEU:HD23	2.00	0.43
1:C:216:THR:OG1	1:C:219:HIS:CD2	2.71	0.43
1:C:623:THR:HG23	1:C:627:LEU:HD12	1.99	0.43
1:C:869:GLU:HA	1:C:872:ARG:HG2	2.00	0.43
1:C:1744:ARG:NE	1:C:1964:GLU:OE2	2.50	0.43
1:C:2748:ILE:HG21	1:C:2811:LYS:HE3	2.01	0.43
1:C:2769:PHE:O	1:C:2773:GLN:HG2	2.19	0.43
1:A:576:LEU:HA	1:A:579:ILE:HG12	2.01	0.43
1:A:2769:PHE:O	1:A:2773:GLN:HG2	2.19	0.43
1:A:4664:VAL:N	1:A:4665:PRO:CD	2.82	0.43
3:K:6:GLU:HG2	3:L:45:PHE:CE2	2.53	0.43
3:M:75:TYR:O	3:M:79:VAL:HG22	2.18	0.43
1:D:791:ARG:HA	1:D:1627:TRP:O	2.18	0.43
1:D:1127:GLY:HA3	1:D:1144:TRP:CZ3	2.54	0.43
1:D:2411:PRO:N	1:D:2412:PRO:CD	2.81	0.43
1:D:2578:ILE:HD12	1:D:2578:ILE:H	1.84	0.43
1:D:2792:LEU:O	1:D:2792:LEU:HD12	2.19	0.43
1:D:3267:MET:HG3	1:D:3267:MET:O	2.19	0.43
1:B:70:LEU:HD23	1:B:110:LEU:HD23	2.00	0.43
1:B:2748:ILE:HG21	1:B:2811:LYS:HE3	2.01	0.43
1:B:2780:GLU:OE1	1:B:2780:GLU:N	2.49	0.43
1:C:224:PHE:HD2	1:C:392:THR:HG1	1.66	0.43
1:C:576:LEU:HA	1:C:579:ILE:HG12	2.01	0.43
1:C:791:ARG:HA	1:C:1627:TRP:O	2.18	0.43
1:C:868:LEU:HA	1:C:871:ILE:HD12	2.00	0.43
1:C:2356:ARG:O	1:C:2359:ILE:HG12	2.19	0.43
1:C:2411:PRO:N	1:C:2412:PRO:CD	2.81	0.43
1:C:2792:LEU:HD12	1:C:2792:LEU:O	2.19	0.43
1:A:791:ARG:HA	1:A:1627:TRP:O	2.18	0.43
1:A:4685:TYR:OH	1:A:4697:GLY:O	2.30	0.43
3:J:11:THR:HG21	3:I:8:ALA:HB2	2.01	0.43
1:D:619:GLN:OE1	1:D:1679:ASN:ND2	2.50	0.43
1:D:979:THR:HG22	1:D:982:GLN:CD	2.37	0.43
1:D:1491:SER:OG	1:D:1492:ASN:N	2.52	0.43
1:B:232:LEU:HD11	1:B:246:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2769:PHE:O	1:B:2773:GLN:HG2	2.19	0.43
1:C:978:LEU:HD12	1:C:982:GLN:HB2	2.01	0.43
1:C:2978:LEU:HA	1:C:2981:VAL:HG22	2.01	0.43
2:G:7:THR:O	2:G:7:THR:HG23	2.18	0.43
3:N:56:ASP:OD1	3:N:56:ASP:C	2.57	0.43
1:D:232:LEU:HD11	1:D:246:VAL:CG1	2.49	0.43
1:D:308:ALA:HB1	1:D:313:THR:HG21	2.01	0.43
1:B:3461:VAL:HG23	1:B:3462:GLN:OE1	2.19	0.43
1:C:2780:GLU:OE1	1:C:2780:GLU:N	2.49	0.43
1:A:1282:ASN:C	1:A:1282:ASN:OD1	2.57	0.42
1:A:2694:GLN:NE2	3:J:4:GLU:OE2	2.52	0.42
1:A:2792:LEU:O	1:A:2792:LEU:HD12	2.19	0.42
1:A:4752:ASN:OD1	1:A:4753:GLU:N	2.42	0.42
3:J:55:VAL:O	3:J:58:VAL:HG12	2.18	0.42
1:D:623:THR:HG23	1:D:627:LEU:HD12	1.99	0.42
1:D:868:LEU:HD21	1:D:940:VAL:HG21	2.01	0.42
1:D:1282:ASN:OD1	1:D:1282:ASN:C	2.57	0.42
1:D:3765:ARG:NH2	1:D:4753:GLU:HB2	2.34	0.42
1:B:302:VAL:HG23	1:B:302:VAL:O	2.19	0.42
1:B:3568:PRO:HA	1:B:3571:ARG:CZ	2.49	0.42
1:C:1282:ASN:C	1:C:1282:ASN:OD1	2.57	0.42
1:C:2738:PRO:O	1:C:2740:PRO:HD3	2.18	0.42
1:A:4893:GLY:N	1:A:4897:ASP:OD2	2.47	0.42
2:G:91:ILE:HD11	1:C:1685:ALA:HA	2.00	0.42
1:D:868:LEU:HA	1:D:871:ILE:HD12	2.00	0.42
1:D:4980:GLU:OE2	1:D:5027:ARG:NH2	2.53	0.42
1:B:929:THR:O	1:B:932:THR:OG1	2.28	0.42
1:B:2748:ILE:HG21	1:B:2811:LYS:HZ1	1.85	0.42
1:B:3515:LEU:HD11	1:B:3603:VAL:HG13	2.01	0.42
1:C:216:THR:HG22	1:C:274:HIS:HA	2.01	0.42
1:C:869:GLU:O	1:C:872:ARG:HG2	2.19	0.42
1:C:979:THR:HG22	1:C:982:GLN:CD	2.37	0.42
1:C:979:THR:OG1	1:C:980:PRO:HD2	2.18	0.42
1:C:2578:ILE:H	1:C:2578:ILE:HD12	1.84	0.42
1:A:619:GLN:OE1	1:A:1679:ASN:ND2	2.50	0.42
1:A:910:ASN:O	1:A:914:LEU:N	2.52	0.42
1:A:2356:ARG:O	1:A:2359:ILE:HG12	2.19	0.42
1:A:2413:GLU:CG	1:A:2416:ARG:NH2	2.83	0.42
1:A:3104:ILE:O	1:A:3108:VAL:HG23	2.20	0.42
1:A:4895:ILE:O	1:A:4899:ILE:HG12	2.19	0.42
3:J:27:TYR:CZ	3:I:84:VAL:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:72:PHE:O	3:M:76:VAL:HG22	2.20	0.42
3:N:10:GLU:O	3:N:14:ASN:OD1	2.38	0.42
3:P:10:GLU:O	3:P:14:ASN:OD1	2.38	0.42
1:D:1144:TRP:HB2	1:D:1148:ASP:HB2	2.00	0.42
1:D:2953:GLU:OE1	1:D:2953:GLU:N	2.49	0.42
1:D:4895:ILE:O	1:D:4899:ILE:HG12	2.19	0.42
1:B:1144:TRP:HB2	1:B:1148:ASP:HB2	2.00	0.42
1:B:2413:GLU:CG	1:B:2416:ARG:NH2	2.83	0.42
1:B:4100:MET:CE	1:B:4111:ILE:HG23	2.45	0.42
1:B:4686:ILE:HD12	1:B:4735:ILE:CD1	2.50	0.42
1:C:722:LEU:HD12	1:C:1477:MET:HE1	2.01	0.42
1:C:1127:GLY:HA3	1:C:1144:TRP:CZ3	2.54	0.42
1:C:3461:VAL:HG23	1:C:3462:GLN:OE1	2.19	0.42
1:A:302:VAL:HG23	1:A:302:VAL:O	2.19	0.42
1:A:1491:SER:OG	1:A:1492:ASN:N	2.52	0.42
1:A:3076:LEU:O	1:A:3147:HIS:NE2	2.48	0.42
3:K:72:PHE:O	3:K:76:VAL:HG22	2.20	0.42
3:O:52:ALA:HA	3:O:55:VAL:HG12	2.01	0.42
3:N:73:LYS:O	3:N:76:VAL:HG22	2.20	0.42
1:D:370:LEU:HB3	1:D:372:VAL:HG22	2.00	0.42
1:D:869:GLU:O	1:D:872:ARG:HG2	2.19	0.42
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.20	0.42
1:D:3568:PRO:HA	1:D:3571:ARG:CZ	2.49	0.42
1:B:1491:SER:OG	1:B:1492:ASN:N	2.52	0.42
1:C:910:ASN:O	1:C:914:LEU:N	2.52	0.42
1:C:2413:GLU:CG	1:C:2416:ARG:NH2	2.83	0.42
1:C:2968:MET:HG3	1:C:3043:LEU:HD12	2.02	0.42
1:C:3104:ILE:O	1:C:3108:VAL:HG23	2.20	0.42
1:C:3282:LEU:CD1	1:C:3316:LEU:HD22	2.46	0.42
1:C:3351:ARG:HG2	1:C:3352:PRO:HD2	2.02	0.42
1:C:3515:LEU:HD11	1:C:3603:VAL:HG13	2.01	0.42
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.20	0.42
3:K:12:LEU:HD11	3:L:9:MET:HE3	2.02	0.42
3:K:23:GLU:OE2	3:K:29:LEU:HA	2.20	0.42
3:M:4:GLU:OE1	3:N:11:THR:CG2	2.65	0.42
1:D:216:THR:HG22	1:D:274:HIS:HA	2.01	0.42
1:D:1023:VAL:HG13	1:D:1024:PRO:HD2	2.02	0.42
1:D:1124:VAL:HG23	1:D:1133:TRP:HB2	2.01	0.42
1:D:2878:GLN:O	1:D:2881:GLU:HB3	2.20	0.42
1:D:3173:ILE:CG2	1:D:3195:LEU:HD13	2.50	0.42
1:B:216:THR:HG22	1:B:274:HIS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:GLN:OE1	1:B:1679:ASN:ND2	2.50	0.42
1:B:868:LEU:HA	1:B:871:ILE:HD12	2.00	0.42
1:B:1124:VAL:HG23	1:B:1133:TRP:HB2	2.01	0.42
1:B:1793:ALA:O	1:B:1794:THR:OG1	2.20	0.42
1:B:2575:HIS:ND1	1:B:2576:ARG:HG2	2.35	0.42
1:B:2978:LEU:HA	1:B:2981:VAL:HG22	2.01	0.42
1:B:3351:ARG:HG2	1:B:3352:PRO:HD2	2.01	0.42
1:C:3037:LYS:O	1:C:3040:ILE:HG22	2.20	0.42
1:C:3458:ASN:O	1:C:3462:GLN:OE1	2.37	0.42
1:C:3568:PRO:HA	1:C:3571:ARG:CZ	2.49	0.42
1:C:3600:VAL:HG12	1:C:3604:LEU:HD13	2.02	0.42
1:C:4980:GLU:OE2	1:C:5027:ARG:NH2	2.53	0.42
1:A:34:LEU:HD12	1:A:54:SER:HB2	2.01	0.42
1:A:232:LEU:HD11	1:A:246:VAL:CG1	2.48	0.42
1:A:2575:HIS:ND1	1:A:2576:ARG:HG2	2.35	0.42
1:A:2814:LEU:HA	1:A:2817:MET:HE2	2.02	0.42
1:A:3088:ILE:HG13	1:A:3089:VAL:N	2.35	0.42
3:M:52:ALA:HA	3:M:55:VAL:HG12	2.01	0.42
3:O:45:PHE:HE2	3:P:6:GLU:HG2	1.85	0.42
1:D:576:LEU:HA	1:D:579:ILE:HG12	2.01	0.42
1:D:1172:SER:OG	1:D:1176:SER:N	2.47	0.42
1:D:2314:LEU:HD12	1:D:2319:TYR:CD1	2.55	0.42
1:D:2586:THR:O	1:D:2590:LEU:HD13	2.20	0.42
1:D:3104:ILE:O	1:D:3108:VAL:HG23	2.20	0.42
1:D:3458:ASN:O	1:D:3462:GLN:OE1	2.37	0.42
1:D:4100:MET:CE	1:D:4111:ILE:HG23	2.45	0.42
1:B:868:LEU:HD21	1:B:940:VAL:HG21	2.01	0.42
1:B:2578:ILE:H	1:B:2578:ILE:HD12	1.84	0.42
1:B:2878:GLN:O	1:B:2881:GLU:HB3	2.20	0.42
1:B:3104:ILE:O	1:B:3108:VAL:HG23	2.20	0.42
1:B:3181:ASN:O	1:B:3184:VAL:N	2.53	0.42
1:C:302:VAL:HG23	1:C:302:VAL:O	2.19	0.42
1:C:1124:VAL:HG23	1:C:1133:TRP:HB2	2.01	0.42
1:C:3859:LEU:HB3	1:C:3871:ARG:NH2	2.34	0.42
1:C:4686:ILE:HD12	1:C:4735:ILE:CD1	2.50	0.42
1:A:1124:VAL:HG23	1:A:1133:TRP:HB2	2.01	0.42
1:A:3181:ASN:O	1:A:3184:VAL:N	2.53	0.42
1:A:3182:PRO:HA	1:A:3185:GLU:OE1	2.20	0.42
1:A:3461:VAL:HG23	1:A:3462:GLN:OE1	2.19	0.42
1:A:4867:GLU:N	1:A:4867:GLU:OE2	2.53	0.42
1:A:4980:GLU:OE2	1:A:5027:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:73:LYS:O	3:J:76:VAL:HG22	2.20	0.42
3:I:52:ALA:HA	3:I:55:VAL:HG12	2.01	0.42
3:L:71:ASP:HB2	3:L:74:GLU:OE1	2.20	0.42
3:P:73:LYS:O	3:P:76:VAL:HG22	2.19	0.42
1:D:34:LEU:HD12	1:D:54:SER:HB2	2.01	0.42
1:D:2868:LEU:HD23	1:D:2873:GLN:HG2	2.02	0.42
1:D:2978:LEU:HA	1:D:2981:VAL:HG22	2.01	0.42
1:D:3088:ILE:HG13	1:D:3089:VAL:N	2.35	0.42
1:D:3600:VAL:HG12	1:D:3604:LEU:HD13	2.02	0.42
1:D:3643:TYR:CD1	1:D:3644:ASN:OD1	2.73	0.42
1:B:869:GLU:O	1:B:872:ARG:HG2	2.19	0.42
1:B:1023:VAL:HG13	1:B:1024:PRO:HD2	2.02	0.42
1:B:1744:ARG:NE	1:B:1964:GLU:OE2	2.50	0.42
1:B:3088:ILE:HG13	1:B:3089:VAL:N	2.35	0.42
1:B:3354:LEU:HD12	1:B:3358:HIS:ND1	2.35	0.42
1:B:4895:ILE:O	1:B:4899:ILE:HG12	2.19	0.42
1:C:2878:GLN:O	1:C:2881:GLU:HB3	2.20	0.42
1:C:3088:ILE:HG13	1:C:3089:VAL:N	2.35	0.42
1:C:4016:LEU:HD23	1:C:4135:PHE:CE1	2.54	0.42
1:C:4685:TYR:OH	1:C:4697:GLY:O	2.30	0.42
1:A:2878:GLN:O	1:A:2881:GLU:HB3	2.20	0.42
3:M:13:ILE:O	3:M:17:HIS:ND1	2.33	0.42
1:D:2575:HIS:ND1	1:D:2576:ARG:HG2	2.35	0.42
1:D:3076:LEU:O	1:D:3147:HIS:NE2	2.48	0.42
1:D:3717:LEU:HD21	1:D:3785:MET:HE3	2.02	0.42
1:C:1491:SER:OG	1:C:1492:ASN:N	2.52	0.42
1:A:185:THR:HG22	1:A:190:LEU:HD22	2.02	0.42
1:A:868:LEU:HA	1:A:871:ILE:HD12	2.00	0.42
1:A:1127:GLY:HA3	1:A:1144:TRP:CZ3	2.54	0.42
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	2.02	0.42
1:A:2314:LEU:HD12	1:A:2319:TYR:CD1	2.55	0.42
1:A:3173:ILE:CG2	1:A:3195:LEU:HD13	2.50	0.42
1:A:3458:ASN:O	1:A:3462:GLN:OE1	2.37	0.42
1:A:3643:TYR:CD1	1:A:3644:ASN:OD1	2.73	0.42
1:A:3765:ARG:NH2	1:A:4753:GLU:HB2	2.34	0.42
1:A:4686:ILE:HD12	1:A:4735:ILE:CD1	2.50	0.42
3:K:52:ALA:HA	3:K:55:VAL:HG12	2.01	0.42
3:O:23:GLU:OE2	3:O:29:LEU:HA	2.20	0.42
3:L:73:LYS:O	3:L:76:VAL:HG22	2.19	0.42
3:P:38:LEU:HD12	3:P:39:GLN:N	2.35	0.42
1:D:185:THR:HG22	1:D:190:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	2.01	0.42
1:D:2769:PHE:O	1:D:2773:GLN:HG2	2.19	0.42
1:D:3907:ARG:HG2	1:D:3908:THR:HG23	2.02	0.42
1:B:1014:ILE:HB	1:B:1015:PRO:HD3	2.02	0.42
1:B:3765:ARG:NH2	1:B:4753:GLU:HB2	2.34	0.42
1:B:4632:GLU:OE1	1:B:4634:THR:OG1	2.27	0.42
1:C:245:LEU:HD22	1:C:376:LYS:HE2	2.02	0.42
1:C:2314:LEU:HD12	1:C:2319:TYR:CD1	2.55	0.42
1:C:2586:THR:O	1:C:2590:LEU:HD13	2.19	0.42
1:C:3643:TYR:CD1	1:C:3644:ASN:OD1	2.73	0.42
1:A:868:LEU:HD21	1:A:940:VAL:HG21	2.01	0.42
3:I:23:GLU:OE2	3:I:29:LEU:HA	2.20	0.42
3:M:45:PHE:CE2	3:N:6:GLU:HG2	2.55	0.42
3:N:71:ASP:HB2	3:N:74:GLU:OE1	2.20	0.42
1:D:671:GLU:HG2	1:D:789:LYS:HB3	2.01	0.42
1:D:2413:GLU:CG	1:D:2416:ARG:NH2	2.83	0.42
1:D:3351:ARG:HG2	1:D:3352:PRO:HD2	2.01	0.42
1:D:4538:PHE:N	1:D:4541:GLU:OE1	2.53	0.42
1:B:308:ALA:HB1	1:B:313:THR:HG21	2.01	0.42
1:B:2241:CYS:SG	1:B:2251:MET:HG3	2.60	0.42
1:B:2356:ARG:O	1:B:2359:ILE:HG12	2.19	0.42
1:B:4980:GLU:OE2	1:B:5027:ARG:NH2	2.53	0.42
1:C:308:ALA:HB1	1:C:313:THR:HG21	2.01	0.42
1:C:1023:VAL:HG13	1:C:1024:PRO:HD2	2.02	0.42
1:C:2241:CYS:SG	1:C:2251:MET:HG3	2.60	0.42
1:C:3457:GLN:O	1:C:3460:VAL:HG12	2.20	0.42
1:C:4538:PHE:N	1:C:4541:GLU:OE1	2.53	0.42
1:A:3907:ARG:HG2	1:A:3908:THR:HG23	2.02	0.41
3:O:56:ASP:HA	1:D:3638:ARG:NH2	2.33	0.41
3:P:71:ASP:HB2	3:P:74:GLU:OE1	2.20	0.41
1:D:302:VAL:O	1:D:302:VAL:HG23	2.19	0.41
1:D:3859:LEU:HB3	1:D:3871:ARG:NH2	2.34	0.41
1:B:3173:ILE:CG2	1:B:3195:LEU:HD13	2.50	0.41
1:C:34:LEU:HD12	1:C:54:SER:HB2	2.01	0.41
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	2.02	0.41
1:C:2575:HIS:ND1	1:C:2576:ARG:HG2	2.35	0.41
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.03	0.41
1:C:3765:ARG:NH2	1:C:4753:GLU:HB2	2.34	0.41
1:C:3907:ARG:HG2	1:C:3908:THR:HG23	2.02	0.41
1:C:4895:ILE:O	1:C:4899:ILE:HG12	2.20	0.41
1:A:216:THR:HG22	1:A:274:HIS:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:GLU:O	1:A:872:ARG:HG2	2.19	0.41
1:A:3351:ARG:HG2	1:A:3352:PRO:HD2	2.02	0.41
1:A:3855:LYS:O	1:A:3859:LEU:HD13	2.20	0.41
3:M:23:GLU:OE2	3:M:29:LEU:HA	2.20	0.41
3:N:38:LEU:HD12	3:N:39:GLN:N	2.35	0.41
1:D:3590:PRO:O	1:D:3594:VAL:HG23	2.21	0.41
1:D:3919:ILE:HG22	1:D:3983:LEU:HD21	2.02	0.41
1:D:4686:ILE:HD12	1:D:4735:ILE:CD1	2.50	0.41
1:B:910:ASN:O	1:B:914:LEU:N	2.52	0.41
1:B:1127:GLY:HA3	1:B:1144:TRP:CZ3	2.54	0.41
1:B:2755:PHE:CZ	1:B:2931:LEU:HG	2.55	0.41
1:B:4675:LEU:HD23	1:B:4709:PHE:CE1	2.55	0.41
1:C:4673:LYS:O	1:C:4677:ARG:HD3	2.20	0.41
1:A:2241:CYS:SG	1:A:2251:MET:HG3	2.60	0.41
1:A:2978:LEU:HA	1:A:2981:VAL:HG22	2.01	0.41
1:A:3108:VAL:HA	1:A:3176:LEU:HD12	2.02	0.41
3:J:10:GLU:O	3:J:14:ASN:OD1	2.38	0.41
3:I:72:PHE:O	3:I:76:VAL:HG22	2.20	0.41
2:G:24:VAL:HG22	2:G:48:LYS:HG2	2.02	0.41
1:D:245:LEU:HD22	1:D:376:LYS:HE2	2.02	0.41
1:D:910:ASN:O	1:D:914:LEU:N	2.52	0.41
1:D:3181:ASN:O	1:D:3184:VAL:N	2.53	0.41
1:D:3182:PRO:HA	1:D:3185:GLU:OE1	2.20	0.41
1:D:3354:LEU:HD12	1:D:3358:HIS:ND1	2.35	0.41
1:D:4016:LEU:HD23	1:D:4135:PHE:CE1	2.54	0.41
1:B:671:GLU:HG2	1:B:789:LYS:HB3	2.02	0.41
1:B:1974:GLN:OE1	1:B:1977:ARG:NH1	2.54	0.41
1:B:3458:ASN:O	1:B:3462:GLN:OE1	2.37	0.41
1:C:23:LEU:HD23	1:C:203:MET:HG2	2.02	0.41
1:C:3410:TYR:HB2	1:C:3510:LEU:HD21	2.03	0.41
1:C:3919:ILE:HG22	1:C:3983:LEU:HD21	2.02	0.41
1:A:979:THR:HG23	1:A:981:ALA:HB3	2.02	0.41
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.03	0.41
1:A:3354:LEU:HD12	1:A:3358:HIS:ND1	2.35	0.41
3:M:51:ASP:OD2	3:M:88:ASN:HB3	2.21	0.41
3:M:72:PHE:CE2	3:M:76:VAL:HG11	2.55	0.41
3:O:72:PHE:CE2	3:O:76:VAL:HG11	2.55	0.41
1:D:1968:ASP:OD2	1:D:1968:ASP:C	2.57	0.41
1:D:2968:MET:HG3	1:D:3043:LEU:HD12	2.02	0.41
1:D:3367:ARG:NH1	1:D:3441:GLU:OE2	2.53	0.41
1:B:400:GLN:O	1:B:404:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:SER:O	1:B:694:SER:OG	2.31	0.41
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	2.01	0.41
1:B:2586:THR:O	1:B:2590:LEU:HD13	2.20	0.41
1:C:1974:GLN:OE1	1:C:1977:ARG:NH1	2.54	0.41
1:C:3181:ASN:O	1:C:3184:VAL:N	2.53	0.41
1:C:4675:LEU:HD23	1:C:4709:PHE:CE1	2.56	0.41
1:C:4867:GLU:N	1:C:4867:GLU:OE2	2.53	0.41
1:A:245:LEU:HD22	1:A:376:LYS:HE2	2.02	0.41
1:A:1974:GLN:OE1	1:A:1977:ARG:NH1	2.54	0.41
1:A:3568:PRO:HA	1:A:3571:ARG:CZ	2.50	0.41
1:A:4675:LEU:HD23	1:A:4709:PHE:CE1	2.55	0.41
3:J:38:LEU:HD12	3:J:39:GLN:N	2.35	0.41
3:J:71:ASP:HB2	3:J:74:GLU:OE1	2.20	0.41
1:D:3440:GLY:O	1:D:3444:ILE:HG13	2.21	0.41
1:D:4673:LYS:O	1:D:4677:ARG:HD3	2.21	0.41
1:B:1728:ARG:O	1:B:1732:LEU:HG	2.21	0.41
1:B:2570:PHE:O	1:B:2573:THR:HG23	2.21	0.41
1:B:2968:MET:HG3	1:B:3043:LEU:HD12	2.02	0.41
1:B:3182:PRO:HA	1:B:3185:GLU:OE1	2.20	0.41
1:B:3367:ARG:NH1	1:B:3441:GLU:OE2	2.53	0.41
1:B:3907:ARG:HG2	1:B:3908:THR:HG23	2.02	0.41
1:B:4538:PHE:N	1:B:4541:GLU:OE1	2.53	0.41
1:C:1014:ILE:HB	1:C:1015:PRO:HD3	2.02	0.41
1:C:2306:CYS:HG	1:C:2332:TYR:HE2	1.67	0.41
1:C:3182:PRO:HA	1:C:3185:GLU:OE1	2.20	0.41
1:A:2755:PHE:CZ	1:A:2931:LEU:HG	2.55	0.41
1:A:2968:MET:HG3	1:A:3043:LEU:HD12	2.02	0.41
3:J:4:GLU:O	3:J:7:SER:OG	2.30	0.41
3:K:51:ASP:OD2	3:K:88:ASN:HB3	2.21	0.41
3:L:10:GLU:O	3:L:14:ASN:OD1	2.38	0.41
1:D:1728:ARG:O	1:D:1732:LEU:HG	2.21	0.41
1:D:1974:GLN:OE1	1:D:1977:ARG:NH1	2.54	0.41
1:D:2281:VAL:O	1:D:2281:VAL:HG22	2.21	0.41
1:D:3410:TYR:HB2	1:D:3510:LEU:HD21	2.03	0.41
1:D:3457:GLN:O	1:D:3460:VAL:HG12	2.20	0.41
1:D:3855:LYS:O	1:D:3859:LEU:HD13	2.20	0.41
1:D:4675:LEU:HD23	1:D:4709:PHE:CE1	2.55	0.41
1:B:3108:VAL:HA	1:B:3176:LEU:HD12	2.02	0.41
1:C:185:THR:HG22	1:C:190:LEU:HD22	2.02	0.41
1:C:2215:VAL:CG2	1:C:2229:MET:HE1	2.50	0.41
1:C:2868:LEU:HD23	1:C:2873:GLN:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3590:PRO:O	1:C:3594:VAL:HG23	2.21	0.41
1:C:4703:VAL:O	1:C:4703:VAL:HG22	2.21	0.41
1:A:308:ALA:HB1	1:A:313:THR:HG21	2.01	0.41
1:A:1014:ILE:HB	1:A:1015:PRO:HD3	2.02	0.41
1:A:2189:ASN:OD1	1:A:2190:LYS:N	2.54	0.41
1:A:2757:ASN:OD1	1:A:2757:ASN:C	2.59	0.41
1:A:3590:PRO:O	1:A:3594:VAL:HG23	2.21	0.41
1:D:400:GLN:O	1:D:404:MET:HG3	2.21	0.41
1:B:34:LEU:HD12	1:B:54:SER:HB2	2.01	0.41
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.03	0.41
1:B:3919:ILE:HG22	1:B:3983:LEU:HD21	2.02	0.41
1:C:485:LEU:HD11	1:C:527:LEU:HD12	2.03	0.41
1:C:3173:ILE:CG2	1:C:3195:LEU:HD13	2.50	0.41
1:A:868:LEU:HB3	1:A:930:LEU:HD23	2.03	0.41
1:A:2239:TYR:O	1:A:2243:ILE:HG13	2.21	0.41
1:A:4186:ILE:CD1	1:A:4196:ILE:HD11	2.51	0.41
1:D:2466:ASP:O	1:D:2470:ILE:HG13	2.21	0.41
1:D:3108:VAL:HA	1:D:3176:LEU:HD12	2.02	0.41
1:B:23:LEU:HD23	1:B:203:MET:HG2	2.02	0.41
1:B:2189:ASN:OD1	1:B:2190:LYS:N	2.54	0.41
1:B:2314:LEU:HD12	1:B:2319:TYR:CD1	2.55	0.41
1:B:2625:ARG:HH12	1:B:2907:VAL:HG21	1.84	0.41
1:B:2868:LEU:HD23	1:B:2873:GLN:HG2	2.02	0.41
1:B:3600:VAL:HG12	1:B:3604:LEU:HD13	2.02	0.41
1:B:3643:TYR:CD1	1:B:3644:ASN:OD1	2.73	0.41
1:C:35:LYS:C	1:C:36:LEU:HD12	2.41	0.41
1:C:3440:GLY:O	1:C:3444:ILE:HG13	2.21	0.41
1:A:35:LYS:C	1:A:36:LEU:HD12	2.41	0.41
1:A:1023:VAL:HG13	1:A:1024:PRO:HD2	2.02	0.41
1:A:1102:ARG:HG2	1:A:1126:ASN:HB2	2.03	0.41
1:A:2281:VAL:HG22	1:A:2281:VAL:O	2.21	0.41
1:A:2413:GLU:HG3	1:A:2416:ARG:NH2	2.36	0.41
1:A:2466:ASP:O	1:A:2470:ILE:HG13	2.21	0.41
1:A:2570:PHE:O	1:A:2573:THR:HG23	2.21	0.41
1:A:2586:THR:O	1:A:2590:LEU:HD13	2.20	0.41
1:A:2868:LEU:HD23	1:A:2873:GLN:HG2	2.02	0.41
1:A:3457:GLN:O	1:A:3460:VAL:HG12	2.20	0.41
1:A:3717:LEU:HD21	1:A:3785:MET:HE3	2.03	0.41
1:A:3756:PHE:CD1	1:A:3756:PHE:C	2.94	0.41
1:A:3758:GLU:OE1	1:A:3761:MET:CE	2.69	0.41
1:A:3919:ILE:HG22	1:A:3983:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4673:LYS:O	1:A:4677:ARG:HD3	2.20	0.41
3:I:13:ILE:O	3:I:17:HIS:ND1	2.33	0.41
3:K:72:PHE:CE2	3:K:76:VAL:HG11	2.55	0.41
3:M:25:ASP:HB3	3:N:94:SER:CB	2.51	0.41
3:O:13:ILE:HG23	3:O:17:HIS:CE1	2.56	0.41
3:O:51:ASP:OD2	3:O:88:ASN:HB3	2.21	0.41
3:O:72:PHE:O	3:O:76:VAL:HG22	2.20	0.41
1:D:1795:GLU:N	1:D:1795:GLU:OE2	2.54	0.41
1:D:2701:MET:HB3	1:D:2702:PRO:HD3	2.03	0.41
1:D:3758:GLU:OE1	1:D:3761:MET:CE	2.69	0.41
1:D:4638:GLU:HB3	1:D:4639:PRO:HD3	2.03	0.41
1:D:4703:VAL:O	1:D:4703:VAL:HG22	2.21	0.41
1:D:4867:GLU:N	1:D:4867:GLU:OE2	2.53	0.41
1:B:35:LYS:C	1:B:36:LEU:HD12	2.41	0.41
1:B:979:THR:HG23	1:B:981:ALA:HB3	2.02	0.41
1:B:1102:ARG:HG2	1:B:1126:ASN:HB2	2.03	0.41
1:B:2754:SER:O	1:B:2757:ASN:OD1	2.39	0.41
1:B:3440:GLY:O	1:B:3444:ILE:HG13	2.21	0.41
1:B:3758:GLU:OE1	1:B:3761:MET:CE	2.69	0.41
1:B:3855:LYS:O	1:B:3859:LEU:HD13	2.20	0.41
1:B:4638:GLU:HB3	1:B:4639:PRO:HD3	2.03	0.41
1:B:4867:GLU:OE2	1:B:4867:GLU:N	2.53	0.41
1:C:400:GLN:O	1:C:404:MET:HG3	2.21	0.41
1:C:868:LEU:HB3	1:C:930:LEU:HD23	2.03	0.41
1:C:2189:ASN:OD1	1:C:2190:LYS:N	2.54	0.41
1:C:2754:SER:O	1:C:2757:ASN:OD1	2.39	0.41
1:C:2757:ASN:OD1	1:C:2757:ASN:C	2.59	0.41
1:C:3108:VAL:HA	1:C:3176:LEU:HD12	2.02	0.41
1:C:3354:LEU:HD12	1:C:3358:HIS:ND1	2.35	0.41
1:C:3855:LYS:O	1:C:3859:LEU:HD13	2.20	0.41
1:C:3972:ILE:CG2	1:C:3983:LEU:HD12	2.51	0.41
1:A:671:GLU:HG2	1:A:789:LYS:HB3	2.02	0.41
1:A:868:LEU:HD22	1:A:871:ILE:HD12	2.03	0.41
1:A:4538:PHE:N	1:A:4541:GLU:OE1	2.53	0.41
1:A:4670:LYS:O	1:A:4673:LYS:HG2	2.21	0.41
3:L:38:LEU:HD12	3:L:39:GLN:N	2.35	0.41
1:D:485:LEU:HD11	1:D:527:LEU:HD12	2.03	0.41
1:D:2189:ASN:OD1	1:D:2190:LYS:N	2.54	0.41
1:D:2570:PHE:O	1:D:2573:THR:HG23	2.21	0.41
1:D:2695:GLU:OE1	1:D:2695:GLU:HA	2.21	0.41
1:D:4632:GLU:OE1	1:D:4634:THR:OG1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:LEU:HD22	1:B:871:ILE:HD12	2.03	0.41
1:B:2757:ASN:OD1	1:B:2757:ASN:C	2.59	0.41
1:B:3457:GLN:O	1:B:3460:VAL:HG12	2.20	0.41
1:B:3590:PRO:O	1:B:3594:VAL:HG23	2.21	0.41
1:B:4186:ILE:CD1	1:B:4196:ILE:HD11	2.51	0.41
1:C:575:VAL:O	1:C:579:ILE:HG12	2.21	0.41
1:C:671:GLU:HG2	1:C:789:LYS:HB3	2.02	0.41
1:A:400:GLN:O	1:A:404:MET:HG3	2.21	0.40
1:A:575:VAL:O	1:A:579:ILE:HG12	2.21	0.40
1:A:3367:ARG:NH1	1:A:3441:GLU:OE2	2.53	0.40
1:A:3440:GLY:O	1:A:3444:ILE:HG13	2.21	0.40
3:I:37:LEU:HD23	3:I:75:TYR:CE1	2.56	0.40
2:F:58:ARG:O	2:F:62:GLU:HG3	2.21	0.40
3:K:13:ILE:HG23	3:K:17:HIS:CE1	2.56	0.40
3:M:13:ILE:HG23	3:M:17:HIS:CE1	2.56	0.40
3:O:5:LEU:HD12	3:P:15:VAL:CB	2.52	0.40
3:O:12:LEU:HD11	3:P:9:MET:HE3	2.03	0.40
3:O:62:LEU:HD12	3:O:63:ASP:N	2.36	0.40
1:D:2124:LEU:O	1:D:2128:GLN:HG2	2.22	0.40
1:D:2241:CYS:SG	1:D:2251:MET:HG3	2.60	0.40
1:D:2757:ASN:OD1	1:D:2757:ASN:C	2.59	0.40
1:B:245:LEU:HD22	1:B:376:LYS:HE2	2.02	0.40
1:B:1795:GLU:N	1:B:1795:GLU:OE2	2.54	0.40
1:B:3362:THR:O	1:B:3366:LEU:HD13	2.21	0.40
1:B:3593:ILE:HD12	1:B:3593:ILE:H	1.86	0.40
1:B:4703:VAL:HG22	1:B:4703:VAL:O	2.21	0.40
1:C:2695:GLU:OE1	1:C:2695:GLU:HA	2.21	0.40
1:C:3286:TRP:HA	1:C:3308:VAL:HG13	2.04	0.40
1:C:3758:GLU:OE1	1:C:3761:MET:CE	2.69	0.40
1:C:3989:TRP:HE3	1:C:4050:MET:SD	2.44	0.40
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	2.03	0.40
1:A:3362:THR:O	1:A:3366:LEU:HD13	2.21	0.40
1:A:3593:ILE:HD12	1:A:3593:ILE:H	1.86	0.40
3:I:51:ASP:OD2	3:I:88:ASN:HB3	2.21	0.40
3:I:72:PHE:CE2	3:I:76:VAL:HG11	2.55	0.40
2:G:58:ARG:O	2:G:62:GLU:HG3	2.21	0.40
3:M:17:HIS:CE1	3:N:87:ASN:HD21	2.39	0.40
3:O:12:LEU:HD11	3:P:9:MET:CE	2.51	0.40
1:D:919:ARG:O	1:D:923:LEU:HG	2.22	0.40
1:D:3362:THR:O	1:D:3366:LEU:HD13	2.21	0.40
1:D:4186:ILE:CD1	1:D:4196:ILE:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:HG22	1:B:190:LEU:HD22	2.02	0.40
1:B:2215:VAL:CG2	1:B:2229:MET:HE1	2.50	0.40
1:B:3037:LYS:O	1:B:3040:ILE:HG22	2.20	0.40
1:B:3410:TYR:HB2	1:B:3510:LEU:HD21	2.03	0.40
1:B:3989:TRP:HE3	1:B:4050:MET:SD	2.44	0.40
1:B:4670:LYS:O	1:B:4673:LYS:HG2	2.21	0.40
1:B:4673:LYS:O	1:B:4677:ARG:HD3	2.20	0.40
1:A:3406:LEU:HD22	1:A:3410:TYR:CZ	2.56	0.40
1:A:3600:VAL:HG12	1:A:3604:LEU:HD13	2.02	0.40
1:A:4876:ASP:OD2	1:A:4879:THR:OG1	2.28	0.40
3:I:31:LYS:HA	3:I:34:LEU:HB3	2.03	0.40
3:I:62:LEU:HD12	3:I:63:ASP:N	2.36	0.40
3:K:37:LEU:HD23	3:K:75:TYR:CE1	2.56	0.40
3:M:31:LYS:HA	3:M:34:LEU:HB3	2.03	0.40
1:D:23:LEU:HD23	1:D:203:MET:HG2	2.02	0.40
1:D:2306:CYS:HG	1:D:2332:TYR:HE2	1.68	0.40
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	2.03	0.40
1:B:4016:LEU:HD23	1:B:4135:PHE:CE1	2.54	0.40
1:C:979:THR:HG23	1:C:981:ALA:HB3	2.02	0.40
1:C:2010:LEU:O	1:C:2024:LEU:HD12	2.22	0.40
1:C:3362:THR:O	1:C:3366:LEU:HD13	2.21	0.40
1:C:4686:ILE:HG21	1:C:4726:HIS:HB3	2.03	0.40
1:A:3989:TRP:HE3	1:A:4050:MET:SD	2.44	0.40
3:K:12:LEU:HD11	3:L:9:MET:CE	2.51	0.40
3:K:31:LYS:HA	3:K:34:LEU:HB3	2.03	0.40
3:M:37:LEU:HD23	3:M:75:TYR:CE1	2.56	0.40
1:D:2239:TYR:O	1:D:2243:ILE:HG13	2.21	0.40
1:D:2413:GLU:HG3	1:D:2416:ARG:NH2	2.36	0.40
1:D:2755:PHE:CZ	1:D:2931:LEU:HG	2.55	0.40
1:D:3534:ILE:HD12	1:D:3534:ILE:H	1.87	0.40
1:D:4696:LYS:HA	1:D:4696:LYS:HE2	2.04	0.40
1:B:633:LEU:HD13	1:B:1667:THR:HG23	2.04	0.40
1:B:868:LEU:HB3	1:B:930:LEU:HD23	2.03	0.40
1:B:1425:PRO:O	1:B:1429:LEU:HD23	2.22	0.40
1:B:2413:GLU:HG3	1:B:2416:ARG:NH2	2.36	0.40
1:B:3286:TRP:HA	1:B:3308:VAL:HG13	2.04	0.40
1:C:473:ARG:NH2	1:C:476:GLN:OE1	2.44	0.40
1:C:1102:ARG:HG2	1:C:1126:ASN:HB2	2.03	0.40
1:C:2466:ASP:O	1:C:2470:ILE:HG13	2.21	0.40
1:C:2755:PHE:CZ	1:C:2931:LEU:HG	2.55	0.40
1:C:3367:ARG:NH1	1:C:3441:GLU:OE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4186:ILE:CD1	1:C:4196:ILE:HD11	2.51	0.40
1:C:4638:GLU:HB3	1:C:4639:PRO:HD3	2.03	0.40
1:A:23:LEU:HD23	1:A:203:MET:HG2	2.02	0.40
1:A:3410:TYR:HB2	1:A:3510:LEU:HD21	2.03	0.40
1:A:4638:GLU:HB3	1:A:4639:PRO:HD3	2.03	0.40
1:A:4703:VAL:HG22	1:A:4703:VAL:O	2.21	0.40
2:H:58:ARG:O	2:H:62:GLU:HG3	2.21	0.40
3:K:62:LEU:HD12	3:K:63:ASP:N	2.36	0.40
3:P:12:LEU:O	3:P:15:VAL:HG22	2.22	0.40
1:D:868:LEU:HB3	1:D:930:LEU:HD23	2.03	0.40
1:D:979:THR:HG23	1:D:981:ALA:HB3	2.02	0.40
1:D:1014:ILE:HB	1:D:1015:PRO:HD3	2.02	0.40
1:D:2010:LEU:O	1:D:2024:LEU:HD12	2.21	0.40
1:B:864:LEU:HD21	1:B:872:ARG:HD2	2.04	0.40
1:B:2210:GLU:HA	1:B:2213:VAL:HG22	2.04	0.40
1:B:2387:ILE:HD13	1:B:2393:ARG:NE	2.37	0.40
1:B:2905:LEU:HD12	1:B:2912:LEU:HD11	2.04	0.40
1:C:902:LYS:HZ2	1:C:904:LEU:HD12	1.86	0.40
1:C:1728:ARG:O	1:C:1732:LEU:HG	2.21	0.40
1:C:2239:TYR:O	1:C:2243:ILE:HG13	2.21	0.40
1:C:2640:MET:HB3	1:C:2641:PRO:HD3	2.04	0.40
1:C:2905:LEU:HD12	1:C:2912:LEU:HD11	2.04	0.40
1:C:2953:GLU:OE1	1:C:2953:GLU:N	2.49	0.40
1:C:3344:GLN:HE22	1:C:3470:PHE:HD1	1.70	0.40
1:C:3446:TRP:HA	1:C:3452:PHE:HD2	1.87	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	4347/5035 (86%)	4258 (98%)	88 (2%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
1	C	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
1	D	4347/5035 (86%)	4257 (98%)	89 (2%)	1 (0%)	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
3	I	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	J	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	K	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	L	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	M	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	N	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
3	O	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
3	P	91/94 (97%)	82 (90%)	9 (10%)	0	100	100
All	All	18540/21324 (87%)	18125 (98%)	411 (2%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2948	ASP
1	D	2948	ASP
1	B	2948	ASP
1	C	2948	ASP

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	3808/4296 (89%)	3801 (100%)	7 (0%)	93	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	3808/4296 (89%)	3801 (100%)	7 (0%)	93 97
1	C	3808/4296 (89%)	3801 (100%)	7 (0%)	93 97
1	D	3808/4296 (89%)	3801 (100%)	7 (0%)	93 97
2	E	89/90 (99%)	89 (100%)	0	100 100
2	F	89/90 (99%)	89 (100%)	0	100 100
2	G	89/90 (99%)	89 (100%)	0	100 100
2	H	89/90 (99%)	89 (100%)	0	100 100
3	I	81/81 (100%)	81 (100%)	0	100 100
3	J	80/81 (99%)	79 (99%)	1 (1%)	69 86
3	K	81/81 (100%)	81 (100%)	0	100 100
3	L	80/81 (99%)	79 (99%)	1 (1%)	69 86
3	M	81/81 (100%)	81 (100%)	0	100 100
3	N	80/81 (99%)	79 (99%)	1 (1%)	69 86
3	O	81/81 (100%)	81 (100%)	0	100 100
3	P	80/81 (99%)	79 (99%)	1 (1%)	69 86
All	All	16232/18192 (89%)	16200 (100%)	32 (0%)	93 97

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	831	ARG
1	A	952	LYS
1	A	953	LYS
1	A	1973	ASN
1	A	2337	ARG
1	A	4582	ASP
1	A	4626	VAL
3	J	27	TYR
3	L	27	TYR
3	N	27	TYR
3	P	27	TYR
1	D	831	ARG
1	D	952	LYS
1	D	953	LYS
1	D	1973	ASN
1	D	2337	ARG
1	D	4582	ASP

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Mol	Chain	Res	Type
1	D	4626	VAL
1	B	831	ARG
1	B	952	LYS
1	B	953	LYS
1	B	1973	ASN
1	B	2337	ARG
1	B	4582	ASP
1	B	4626	VAL
1	C	831	ARG
1	C	952	LYS
1	C	953	LYS
1	C	1973	ASN
1	C	2337	ARG
1	C	4582	ASP
1	C	4626	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	878	ASN
1	A	2128	GLN
1	A	2689	HIS
1	A	3872	GLN
3	I	19	HIS
3	I	39	GLN
3	I	65	ASN
3	K	19	HIS
3	K	39	GLN
3	K	65	ASN
3	M	19	HIS
3	M	39	GLN
3	M	65	ASN
3	O	19	HIS
3	O	39	GLN
3	O	65	ASN
1	D	878	ASN
1	D	2128	GLN
1	D	2689	HIS
1	D	3872	GLN
1	B	878	ASN
1	B	2128	GLN
1	B	2689	HIS

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Mol	Chain	Res	Type
1	B	3872	GLN
1	C	878	ASN
1	C	2128	GLN
1	C	2689	HIS
1	C	3872	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PCW	C	5103	-	53,53,53	1.15	4 (7%)	59,61,61	2.36	9 (15%)
5	PCW	A	8003	-	53,53,53	1.17	4 (7%)	59,61,61	2.29	9 (15%)
5	PCW	D	5101	-	53,53,53	1.17	4 (7%)	59,61,61	2.29	9 (15%)
5	PCW	C	5101	-	53,53,53	1.17	4 (7%)	59,61,61	2.29	9 (15%)
5	PCW	B	8002	-	53,53,53	1.15	4 (7%)	59,61,61	2.36	9 (15%)
5	PCW	A	8002	-	53,53,53	1.16	4 (7%)	59,61,61	2.36	9 (15%)
5	PCW	D	5103	-	53,53,53	1.16	4 (7%)	59,61,61	2.36	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PCW	B	8003	-	53,53,53	1.17	4 (7%)	59,61,61	2.29	9 (15%)

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	PCW	C	5103	-	-	28/57/57/57	-
5	PCW	A	8003	-	-	21/57/57/57	-
5	PCW	D	5101	-	-	21/57/57/57	-
5	PCW	C	5101	-	-	21/57/57/57	-
5	PCW	B	8002	-	-	28/57/57/57	-
5	PCW	A	8002	-	-	28/57/57/57	-
5	PCW	D	5103	-	-	28/57/57/57	-
5	PCW	B	8003	-	-	21/57/57/57	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5103	PCW	O3-C11	3.10	1.42	1.33
5	A	8002	PCW	O3-C11	3.08	1.42	1.33
5	B	8002	PCW	O3-C11	3.08	1.42	1.33
5	C	5103	PCW	O3-C11	3.08	1.42	1.33
5	D	5101	PCW	O3-C11	3.07	1.42	1.33
5	A	8003	PCW	O3-C11	3.07	1.42	1.33
5	C	5101	PCW	O3-C11	3.07	1.42	1.33
5	B	8003	PCW	O3-C11	3.06	1.42	1.33
5	D	5101	PCW	O2-C31	2.93	1.42	1.34
5	B	8003	PCW	O2-C31	2.93	1.42	1.34
5	C	5101	PCW	O2-C31	2.93	1.42	1.34
5	A	8003	PCW	O2-C31	2.91	1.42	1.34
5	A	8002	PCW	O2-C31	2.78	1.42	1.34
5	D	5103	PCW	O2-C31	2.78	1.42	1.34
5	C	5103	PCW	O2-C31	2.75	1.42	1.34
5	B	8002	PCW	O2-C31	2.75	1.42	1.34
5	A	8002	PCW	O2-C2	-2.61	1.40	1.46
5	D	5103	PCW	O2-C2	-2.61	1.40	1.46
5	B	8002	PCW	O2-C2	-2.61	1.40	1.46
5	C	5103	PCW	O2-C2	-2.58	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8003	PCW	O2-C2	-2.48	1.40	1.46
5	D	5101	PCW	O2-C2	-2.48	1.40	1.46
5	B	8003	PCW	O2-C2	-2.47	1.40	1.46
5	C	5101	PCW	O2-C2	-2.47	1.40	1.46
5	C	5103	PCW	P-O4P	2.07	1.67	1.59
5	A	8002	PCW	P-O4P	2.06	1.67	1.59
5	B	8002	PCW	P-O4P	2.06	1.67	1.59
5	A	8003	PCW	P-O4P	2.05	1.67	1.59
5	D	5101	PCW	P-O4P	2.05	1.67	1.59
5	B	8003	PCW	P-O4P	2.05	1.67	1.59
5	D	5103	PCW	P-O4P	2.04	1.67	1.59
5	C	5101	PCW	P-O4P	2.03	1.67	1.59

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	5103	PCW	C8-N-C6	12.17	140.27	108.97
5	A	8002	PCW	C8-N-C6	12.15	140.21	108.97
5	B	8002	PCW	C8-N-C6	12.15	140.21	108.97
5	C	5103	PCW	C8-N-C6	12.14	140.19	108.97
5	B	8003	PCW	C8-N-C6	11.01	137.28	108.97
5	D	5101	PCW	C8-N-C6	11.01	137.28	108.97
5	C	5101	PCW	C8-N-C6	11.01	137.28	108.97
5	A	8003	PCW	C8-N-C6	11.00	137.25	108.97
5	A	8003	PCW	C7-N-C5	7.67	141.30	109.92
5	D	5101	PCW	C7-N-C5	7.67	141.29	109.92
5	C	5101	PCW	C7-N-C5	7.66	141.27	109.92
5	B	8003	PCW	C7-N-C5	7.66	141.27	109.92
5	A	8002	PCW	C7-N-C5	7.04	138.72	109.92
5	C	5103	PCW	C7-N-C5	7.04	138.72	109.92
5	B	8002	PCW	C7-N-C5	7.04	138.71	109.92
5	D	5103	PCW	C7-N-C5	7.03	138.69	109.92
5	D	5103	PCW	C8-N-C7	-5.43	95.01	108.97
5	A	8002	PCW	C8-N-C7	-5.43	95.02	108.97
5	C	5103	PCW	C8-N-C7	-5.43	95.02	108.97
5	B	8002	PCW	C8-N-C7	-5.40	95.08	108.97
5	C	5101	PCW	C8-N-C7	-5.09	95.89	108.97
5	D	5101	PCW	C8-N-C7	-5.09	95.90	108.97
5	A	8003	PCW	C8-N-C7	-5.07	95.93	108.97
5	B	8003	PCW	C8-N-C7	-5.07	95.93	108.97
5	B	8003	PCW	C7-N-C6	-4.93	96.30	108.97
5	C	5101	PCW	C7-N-C6	-4.92	96.33	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	5101	PCW	C7-N-C6	-4.92	96.33	108.97
5	A	8003	PCW	C7-N-C6	-4.90	96.37	108.97
5	B	8002	PCW	C7-N-C6	-4.79	96.66	108.97
5	A	8002	PCW	C7-N-C6	-4.79	96.66	108.97
5	D	5103	PCW	C7-N-C6	-4.79	96.66	108.97
5	C	5103	PCW	C7-N-C6	-4.78	96.69	108.97
5	B	8003	PCW	C21-C20-C19	4.07	155.93	124.73
5	A	8003	PCW	C21-C20-C19	4.06	155.91	124.73
5	D	5101	PCW	C21-C20-C19	4.06	155.88	124.73
5	C	5101	PCW	C21-C20-C19	4.06	155.86	124.73
5	A	8002	PCW	C21-C20-C19	3.90	154.65	124.73
5	D	5103	PCW	C21-C20-C19	3.90	154.65	124.73
5	B	8002	PCW	C21-C20-C19	3.90	154.65	124.73
5	C	5103	PCW	C21-C20-C19	3.89	154.59	124.73
5	B	8002	PCW	O2-C31-C32	3.73	119.54	111.50
5	C	5103	PCW	O2-C31-C32	3.73	119.53	111.50
5	A	8002	PCW	O2-C31-C32	3.72	119.52	111.50
5	D	5103	PCW	O2-C31-C32	3.70	119.48	111.50
5	A	8003	PCW	C8-N-C5	-3.46	95.75	109.92
5	D	5101	PCW	C8-N-C5	-3.45	95.81	109.92
5	C	5101	PCW	C8-N-C5	-3.44	95.82	109.92
5	B	8003	PCW	C8-N-C5	-3.44	95.83	109.92
5	A	8003	PCW	O2-C31-C32	3.31	118.64	111.50
5	D	5101	PCW	O2-C31-C32	3.30	118.62	111.50
5	B	8003	PCW	O2-C31-C32	3.29	118.59	111.50
5	C	5101	PCW	O2-C31-C32	3.29	118.59	111.50
5	B	8002	PCW	C8-N-C5	-3.26	96.57	109.92
5	D	5103	PCW	C8-N-C5	-3.26	96.59	109.92
5	A	8002	PCW	C8-N-C5	-3.25	96.61	109.92
5	C	5103	PCW	C8-N-C5	-3.25	96.61	109.92
5	C	5103	PCW	C6-N-C5	-2.62	99.18	109.92
5	B	8002	PCW	C6-N-C5	-2.62	99.19	109.92
5	A	8002	PCW	C6-N-C5	-2.62	99.19	109.92
5	D	5103	PCW	C6-N-C5	-2.62	99.20	109.92
5	B	8003	PCW	C6-N-C5	-2.51	99.63	109.92
5	A	8003	PCW	C6-N-C5	-2.51	99.64	109.92
5	D	5101	PCW	C6-N-C5	-2.51	99.64	109.92
5	C	5101	PCW	C6-N-C5	-2.51	99.65	109.92
5	C	5101	PCW	O3-C11-C12	2.49	119.73	111.91
5	A	8003	PCW	O3-C11-C12	2.49	119.71	111.91
5	D	5101	PCW	O3-C11-C12	2.47	119.66	111.91
5	B	8003	PCW	O3-C11-C12	2.46	119.62	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	8002	PCW	O3-C11-C12	2.28	119.06	111.91
5	C	5103	PCW	O3-C11-C12	2.28	119.06	111.91
5	A	8002	PCW	O3-C11-C12	2.27	119.03	111.91
5	D	5103	PCW	O3-C11-C12	2.26	119.00	111.91

There are no chirality outliers.

All (196) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8002	PCW	O4P-C4-C5-N
5	A	8003	PCW	O4P-C4-C5-N
5	D	5101	PCW	O4P-C4-C5-N
5	D	5103	PCW	O4P-C4-C5-N
5	B	8002	PCW	O4P-C4-C5-N
5	B	8003	PCW	O4P-C4-C5-N
5	C	5101	PCW	O4P-C4-C5-N
5	C	5103	PCW	O4P-C4-C5-N
5	A	8002	PCW	C13-C14-C15-C16
5	D	5103	PCW	C13-C14-C15-C16
5	B	8002	PCW	C13-C14-C15-C16
5	C	5103	PCW	C13-C14-C15-C16
5	A	8003	PCW	C11-C12-C13-C14
5	D	5101	PCW	C11-C12-C13-C14
5	B	8003	PCW	C11-C12-C13-C14
5	C	5101	PCW	C11-C12-C13-C14
5	A	8002	PCW	C1-O3P-P-O4P
5	D	5103	PCW	C1-O3P-P-O4P
5	B	8002	PCW	C1-O3P-P-O4P
5	C	5103	PCW	C1-O3P-P-O4P
5	A	8003	PCW	C12-C13-C14-C15
5	D	5101	PCW	C12-C13-C14-C15
5	B	8003	PCW	C12-C13-C14-C15
5	C	5101	PCW	C12-C13-C14-C15
5	A	8002	PCW	C44-C45-C46-C47
5	D	5103	PCW	C44-C45-C46-C47
5	B	8002	PCW	C44-C45-C46-C47
5	C	5103	PCW	C44-C45-C46-C47
5	A	8003	PCW	C44-C45-C46-C47
5	D	5101	PCW	C44-C45-C46-C47
5	B	8003	PCW	C44-C45-C46-C47
5	C	5101	PCW	C44-C45-C46-C47
5	A	8002	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	D	5103	PCW	C35-C36-C37-C38
5	B	8002	PCW	C35-C36-C37-C38
5	C	5103	PCW	C35-C36-C37-C38
5	A	8003	PCW	C20-C21-C22-C23
5	D	5101	PCW	C20-C21-C22-C23
5	B	8003	PCW	C20-C21-C22-C23
5	C	5101	PCW	C20-C21-C22-C23
5	A	8003	PCW	C14-C15-C16-C17
5	D	5101	PCW	C14-C15-C16-C17
5	B	8003	PCW	C14-C15-C16-C17
5	C	5101	PCW	C14-C15-C16-C17
5	A	8002	PCW	C11-C12-C13-C14
5	D	5103	PCW	C11-C12-C13-C14
5	B	8002	PCW	C11-C12-C13-C14
5	C	5103	PCW	C11-C12-C13-C14
5	A	8003	PCW	C41-C42-C43-C44
5	B	8003	PCW	C41-C42-C43-C44
5	D	5101	PCW	C41-C42-C43-C44
5	C	5101	PCW	C41-C42-C43-C44
5	A	8003	PCW	C16-C17-C18-C19
5	D	5101	PCW	C16-C17-C18-C19
5	B	8003	PCW	C16-C17-C18-C19
5	C	5101	PCW	C16-C17-C18-C19
5	A	8002	PCW	C32-C31-O2-C2
5	D	5103	PCW	C32-C31-O2-C2
5	B	8002	PCW	C32-C31-O2-C2
5	C	5103	PCW	C32-C31-O2-C2
5	A	8002	PCW	O31-C31-O2-C2
5	D	5103	PCW	O31-C31-O2-C2
5	B	8002	PCW	O31-C31-O2-C2
5	C	5103	PCW	O31-C31-O2-C2
5	A	8003	PCW	C2-C1-O3P-P
5	D	5101	PCW	C2-C1-O3P-P
5	B	8003	PCW	C2-C1-O3P-P
5	C	5101	PCW	C2-C1-O3P-P
5	A	8003	PCW	O3P-C1-C2-C3
5	D	5101	PCW	O3P-C1-C2-C3
5	B	8003	PCW	O3P-C1-C2-C3
5	C	5101	PCW	O3P-C1-C2-C3
5	A	8002	PCW	C40-C41-C42-C43
5	D	5103	PCW	C40-C41-C42-C43
5	B	8002	PCW	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
5	C	5103	PCW	C40-C41-C42-C43
5	C	5103	PCW	C41-C42-C43-C44
5	A	8002	PCW	C41-C42-C43-C44
5	D	5103	PCW	C41-C42-C43-C44
5	B	8002	PCW	C41-C42-C43-C44
5	A	8002	PCW	C21-C22-C23-C24
5	D	5103	PCW	C21-C22-C23-C24
5	B	8002	PCW	C21-C22-C23-C24
5	C	5103	PCW	C21-C22-C23-C24
5	A	8002	PCW	C12-C11-O3-C3
5	D	5103	PCW	C12-C11-O3-C3
5	B	8002	PCW	C12-C11-O3-C3
5	C	5103	PCW	C12-C11-O3-C3
5	A	8002	PCW	C24-C25-C26-C27
5	D	5103	PCW	C24-C25-C26-C27
5	B	8002	PCW	C24-C25-C26-C27
5	C	5103	PCW	C24-C25-C26-C27
5	B	8002	PCW	C33-C34-C35-C36
5	A	8002	PCW	C33-C34-C35-C36
5	D	5103	PCW	C33-C34-C35-C36
5	C	5103	PCW	C33-C34-C35-C36
5	A	8002	PCW	C1-C2-C3-O3
5	D	5103	PCW	C1-C2-C3-O3
5	B	8002	PCW	C1-C2-C3-O3
5	C	5103	PCW	C1-C2-C3-O3
5	A	8003	PCW	O3P-C1-C2-O2
5	D	5101	PCW	O3P-C1-C2-O2
5	B	8003	PCW	O3P-C1-C2-O2
5	C	5101	PCW	O3P-C1-C2-O2
5	A	8003	PCW	C21-C22-C23-C24
5	D	5101	PCW	C21-C22-C23-C24
5	B	8003	PCW	C21-C22-C23-C24
5	C	5101	PCW	C21-C22-C23-C24
5	C	5101	PCW	C19-C20-C21-C22
5	A	8002	PCW	O11-C11-O3-C3
5	D	5103	PCW	O11-C11-O3-C3
5	B	8002	PCW	O11-C11-O3-C3
5	C	5103	PCW	O11-C11-O3-C3
5	A	8003	PCW	C35-C36-C37-C38
5	D	5101	PCW	C35-C36-C37-C38
5	B	8003	PCW	C35-C36-C37-C38
5	C	5101	PCW	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	A	8003	PCW	C19-C20-C21-C22
5	D	5101	PCW	C19-C20-C21-C22
5	B	8003	PCW	C19-C20-C21-C22
5	A	8002	PCW	O2-C2-C3-O3
5	D	5103	PCW	O2-C2-C3-O3
5	B	8002	PCW	O2-C2-C3-O3
5	C	5103	PCW	O2-C2-C3-O3
5	D	5103	PCW	C32-C33-C34-C35
5	A	8002	PCW	C32-C33-C34-C35
5	B	8002	PCW	C32-C33-C34-C35
5	C	5103	PCW	C32-C33-C34-C35
5	A	8002	PCW	C1-O3P-P-O1P
5	A	8002	PCW	C1-O3P-P-O2P
5	A	8002	PCW	C4-O4P-P-O2P
5	D	5103	PCW	C1-O3P-P-O1P
5	D	5103	PCW	C1-O3P-P-O2P
5	D	5103	PCW	C4-O4P-P-O2P
5	B	8002	PCW	C1-O3P-P-O1P
5	B	8002	PCW	C1-O3P-P-O2P
5	B	8002	PCW	C4-O4P-P-O2P
5	C	5103	PCW	C1-O3P-P-O1P
5	C	5103	PCW	C1-O3P-P-O2P
5	C	5103	PCW	C4-O4P-P-O2P
5	A	8002	PCW	C2-C1-O3P-P
5	D	5103	PCW	C2-C1-O3P-P
5	B	8002	PCW	C2-C1-O3P-P
5	C	5103	PCW	C2-C1-O3P-P
5	A	8003	PCW	C4-C5-N-C8
5	D	5101	PCW	C4-C5-N-C8
5	B	8003	PCW	C4-C5-N-C8
5	C	5101	PCW	C4-C5-N-C8
5	A	8003	PCW	C13-C14-C15-C16
5	D	5101	PCW	C13-C14-C15-C16
5	B	8003	PCW	C13-C14-C15-C16
5	C	5101	PCW	C13-C14-C15-C16
5	A	8002	PCW	C25-C26-C27-C28
5	D	5103	PCW	C25-C26-C27-C28
5	B	8002	PCW	C25-C26-C27-C28
5	C	5103	PCW	C25-C26-C27-C28
5	A	8003	PCW	C40-C41-C42-C43
5	D	5101	PCW	C40-C41-C42-C43
5	B	8003	PCW	C40-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	5101	PCW	C40-C41-C42-C43
5	D	5103	PCW	C23-C24-C25-C26
5	B	8002	PCW	C23-C24-C25-C26
5	C	5103	PCW	C23-C24-C25-C26
5	A	8002	PCW	C23-C24-C25-C26
5	A	8003	PCW	C1-C2-O2-C31
5	D	5101	PCW	C1-C2-O2-C31
5	B	8003	PCW	C1-C2-O2-C31
5	C	5101	PCW	C1-C2-O2-C31
5	A	8002	PCW	C4-C5-N-C8
5	D	5103	PCW	C4-C5-N-C8
5	B	8002	PCW	C4-C5-N-C8
5	C	5103	PCW	C4-C5-N-C8
5	C	5103	PCW	C15-C16-C17-C18
5	B	8002	PCW	C15-C16-C17-C18
5	A	8002	PCW	C15-C16-C17-C18
5	D	5103	PCW	C15-C16-C17-C18
5	C	5101	PCW	C45-C46-C47-C48
5	D	5101	PCW	C45-C46-C47-C48
5	A	8003	PCW	C45-C46-C47-C48
5	B	8003	PCW	C45-C46-C47-C48
5	A	8002	PCW	C19-C20-C21-C22
5	D	5103	PCW	C19-C20-C21-C22
5	B	8002	PCW	C19-C20-C21-C22
5	C	5103	PCW	C19-C20-C21-C22
5	A	8002	PCW	C43-C44-C45-C46
5	D	5103	PCW	C43-C44-C45-C46
5	B	8002	PCW	C43-C44-C45-C46
5	C	5103	PCW	C43-C44-C45-C46
5	D	5101	PCW	C15-C16-C17-C18
5	A	8003	PCW	C15-C16-C17-C18
5	B	8003	PCW	C15-C16-C17-C18
5	C	5101	PCW	C15-C16-C17-C18
5	A	8003	PCW	C31-C32-C33-C34
5	D	5101	PCW	C31-C32-C33-C34
5	B	8003	PCW	C31-C32-C33-C34
5	C	5101	PCW	C31-C32-C33-C34

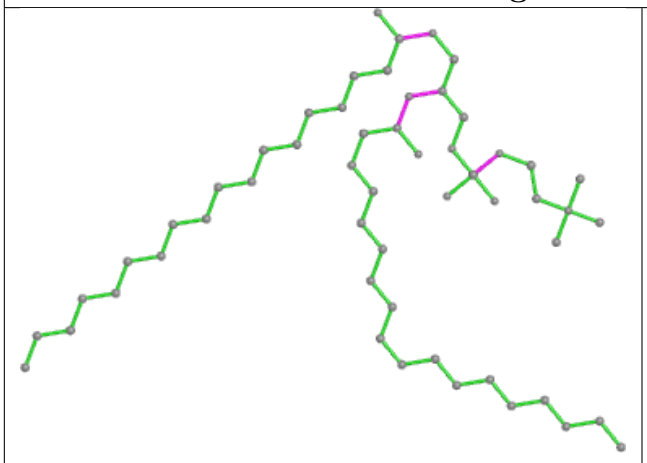
There are no ring outliers.

No monomer is involved in short contacts.

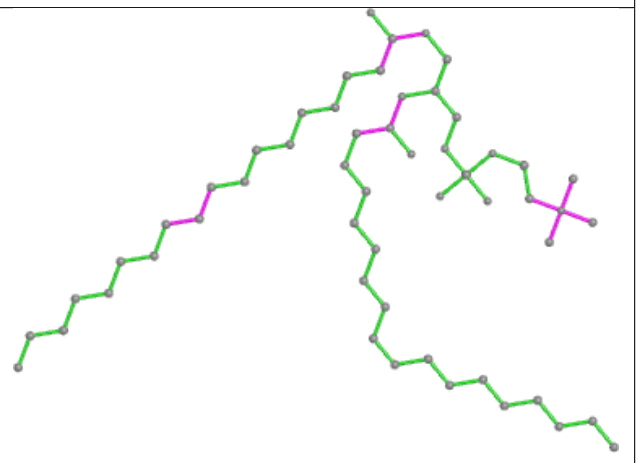
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

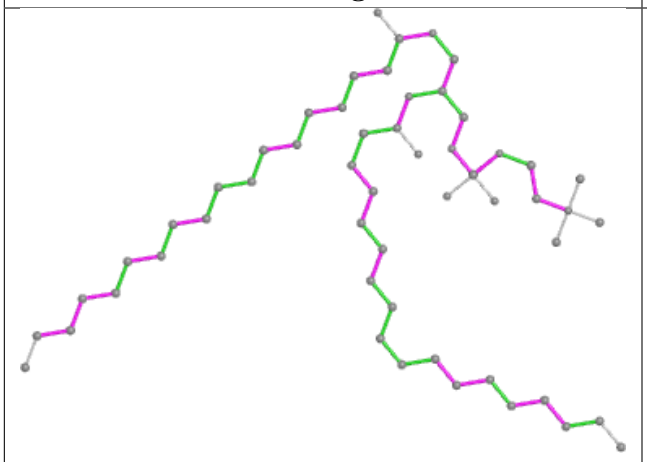
Ligand PCW C 5103



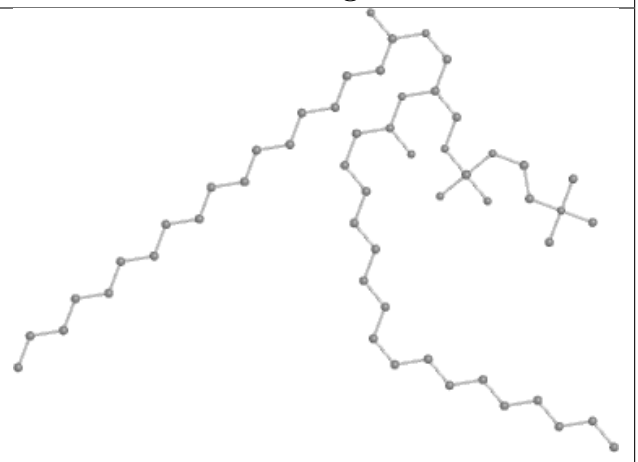
Bond lengths



Bond angles

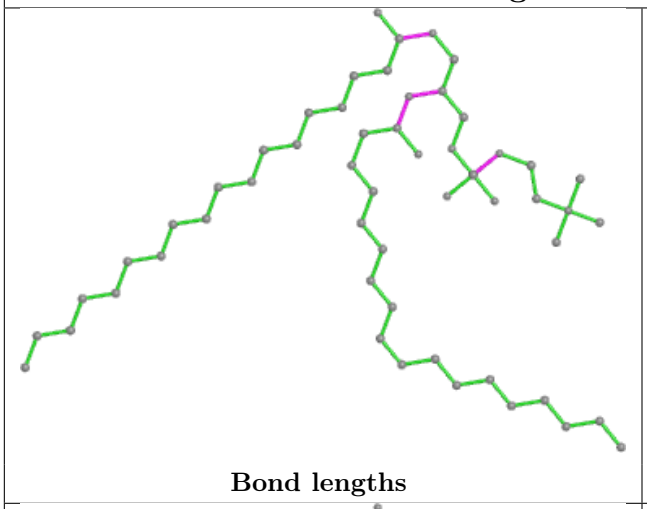


Torsions

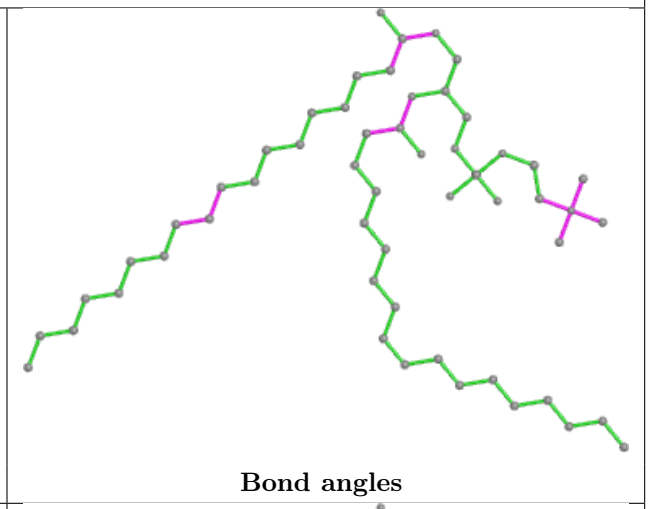


Rings

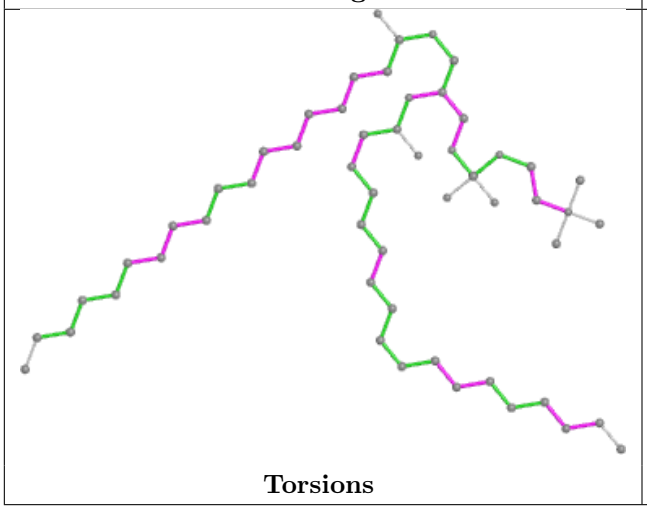
Ligand PCW A 8003



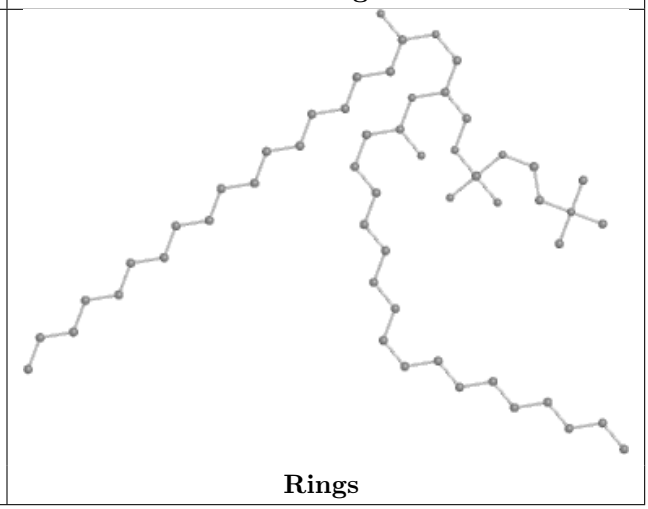
Bond lengths



Bond angles

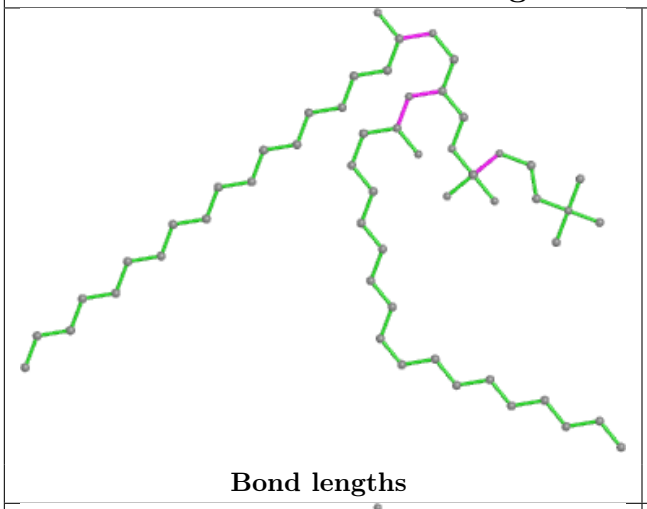


Torsions

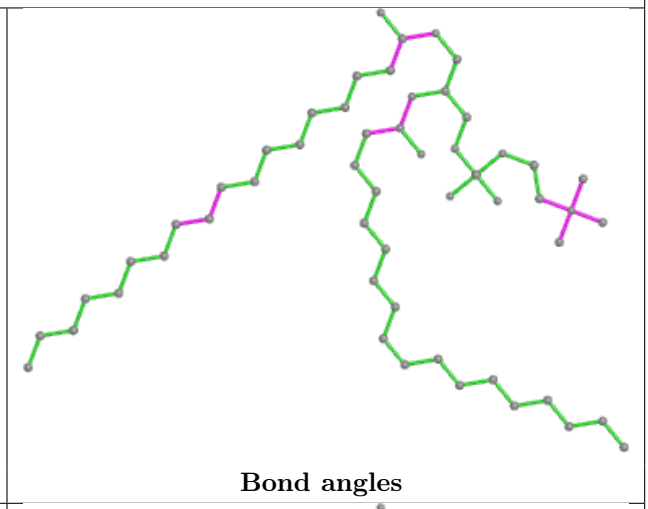


Rings

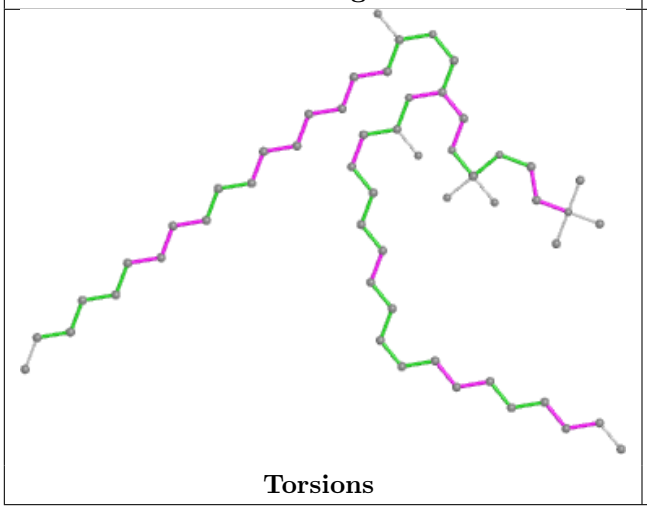
Ligand PCW D 5101



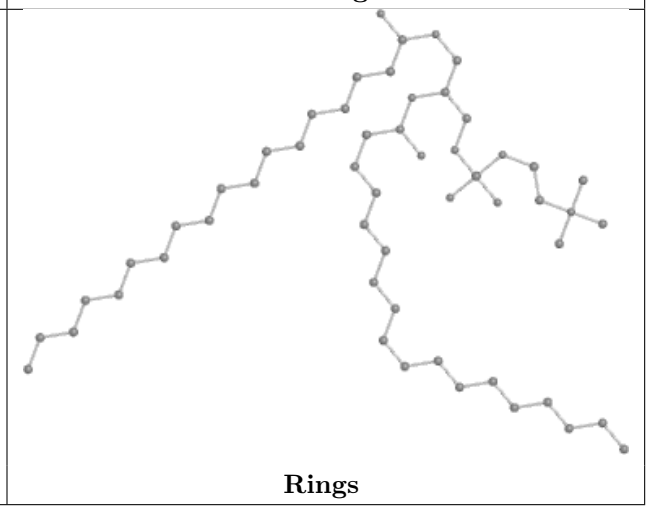
Bond lengths



Bond angles

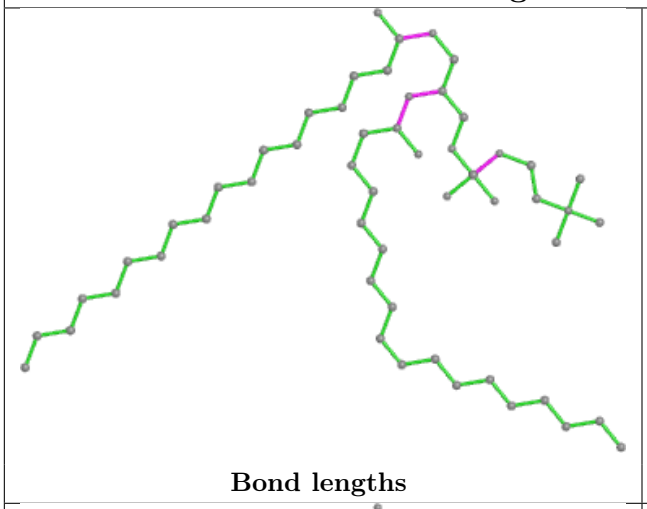


Torsions

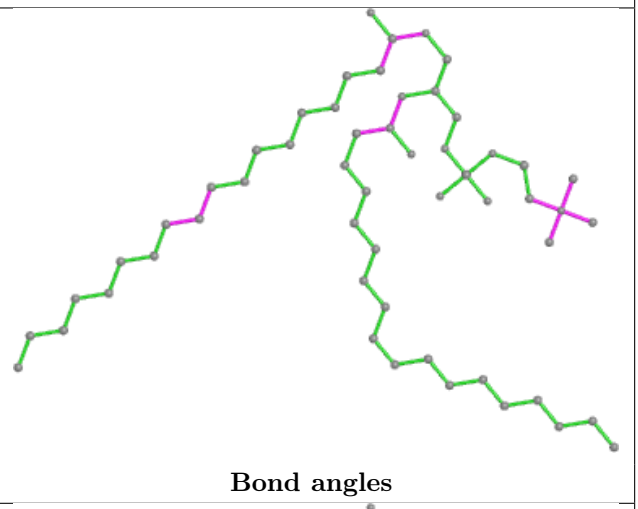


Rings

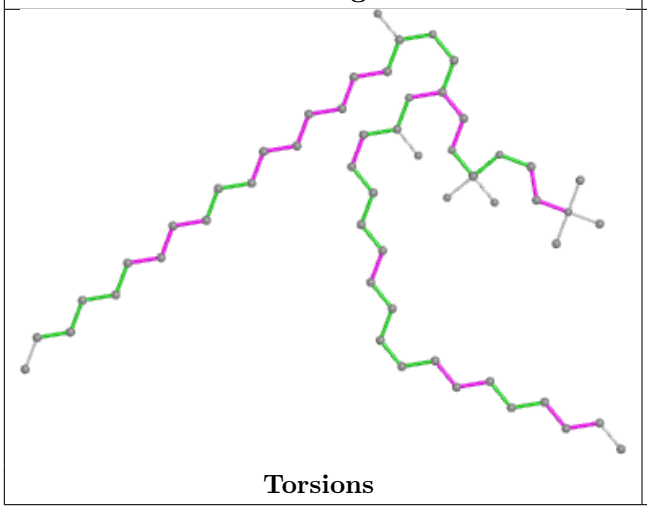
Ligand PCW C 5101



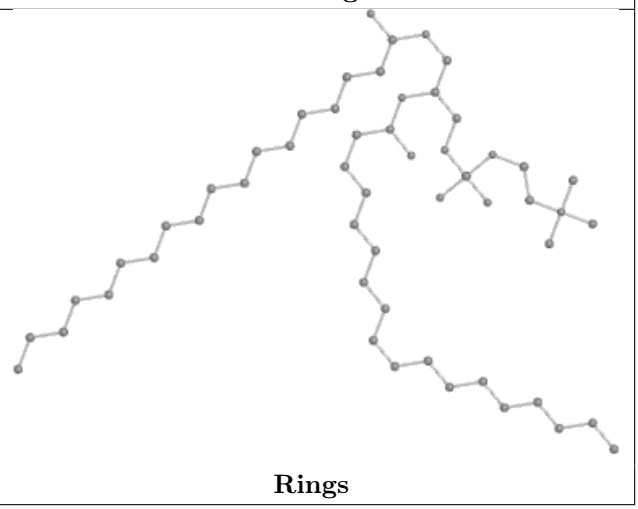
Bond lengths



Bond angles

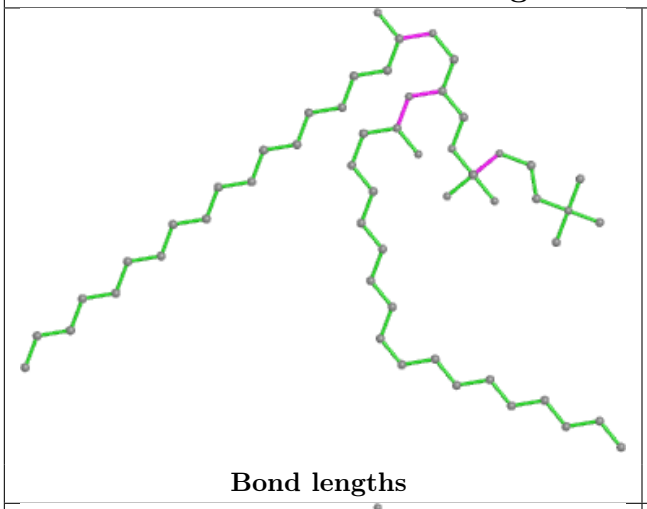


Torsions

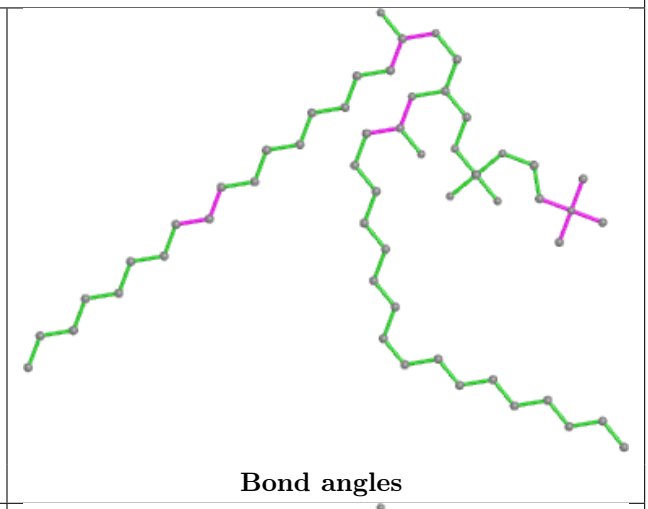


Rings

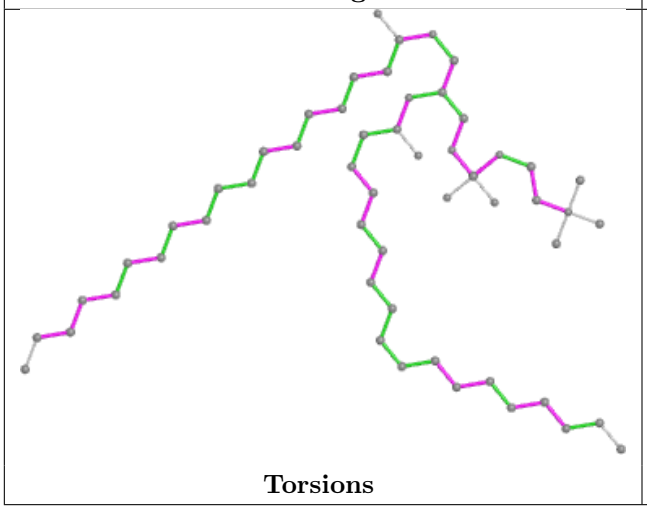
Ligand PCW B 8002



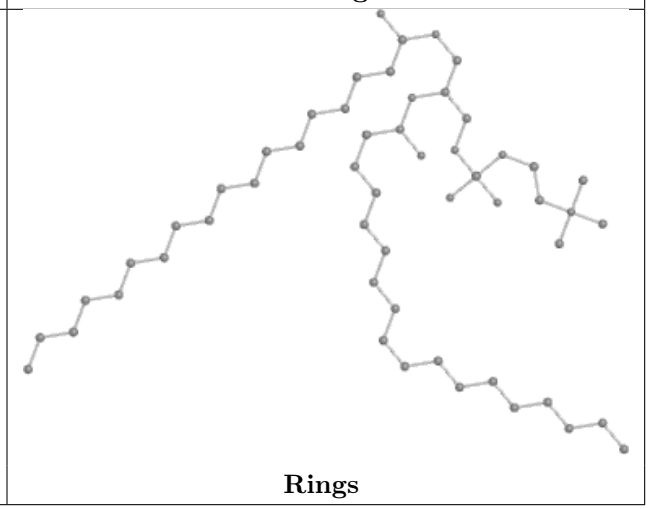
Bond lengths



Bond angles

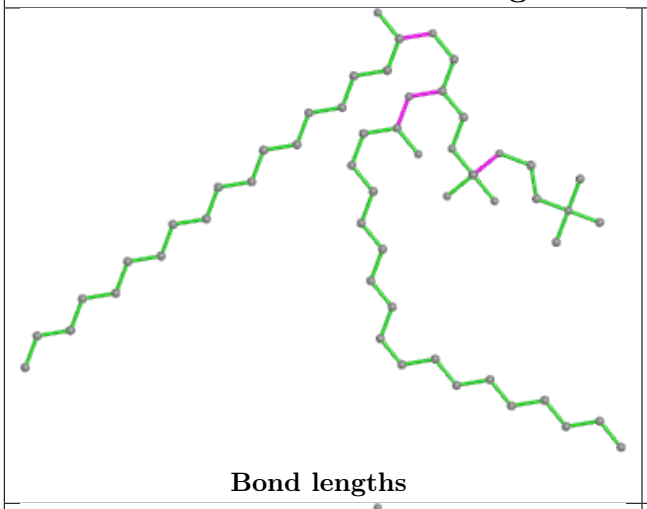


Torsions

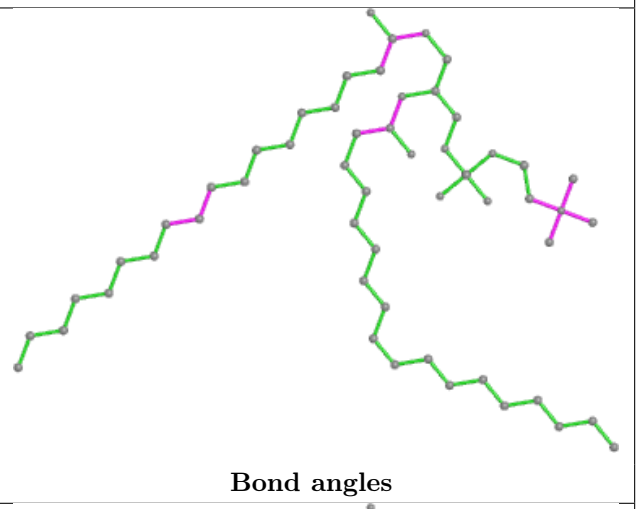


Rings

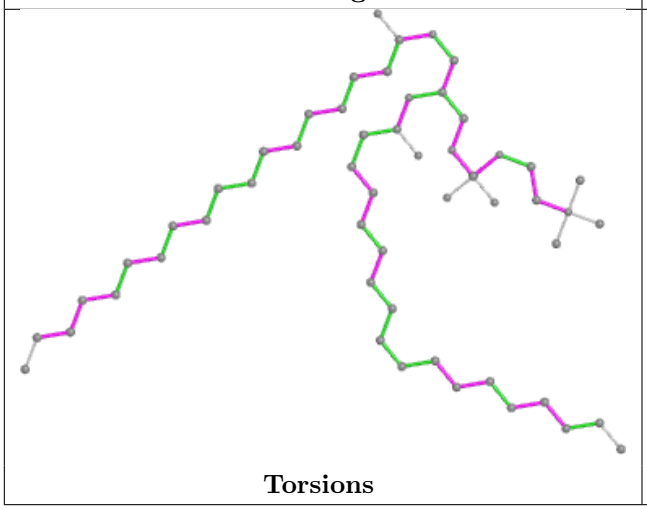
Ligand PCW A 8002



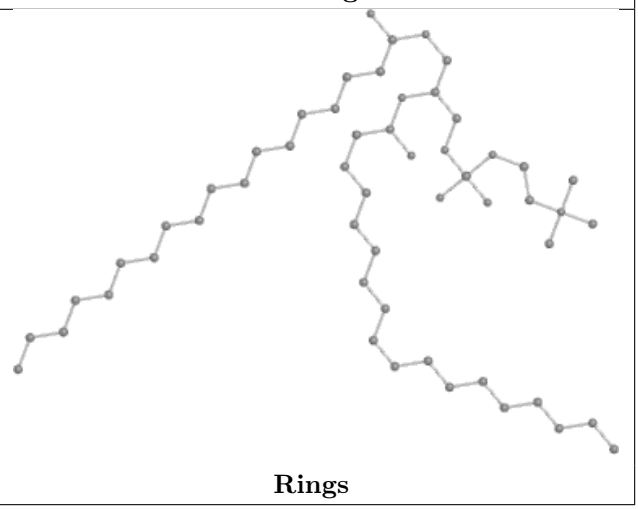
Bond lengths



Bond angles

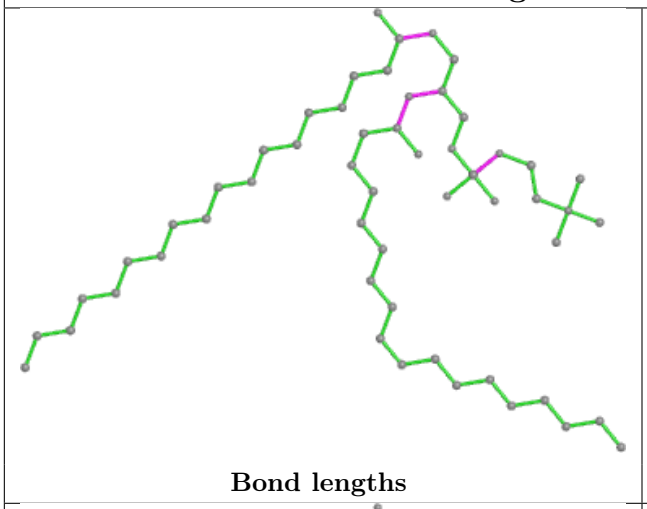


Torsions

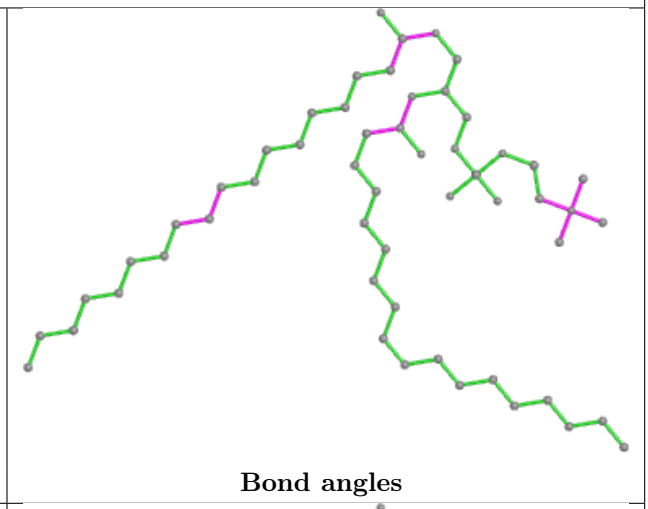


Rings

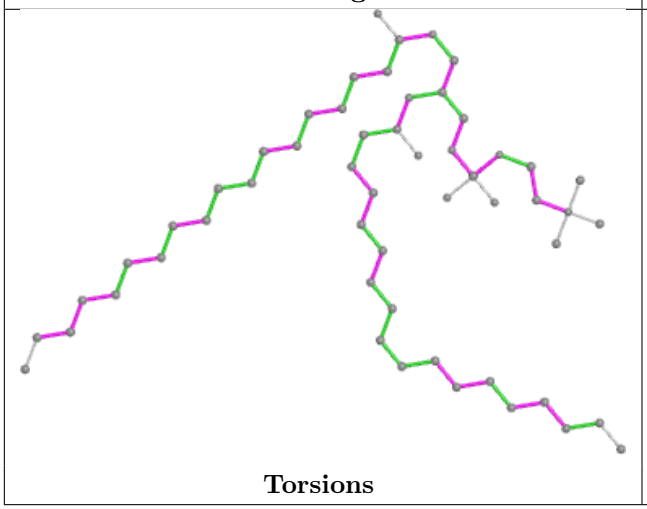
Ligand PCW D 5103



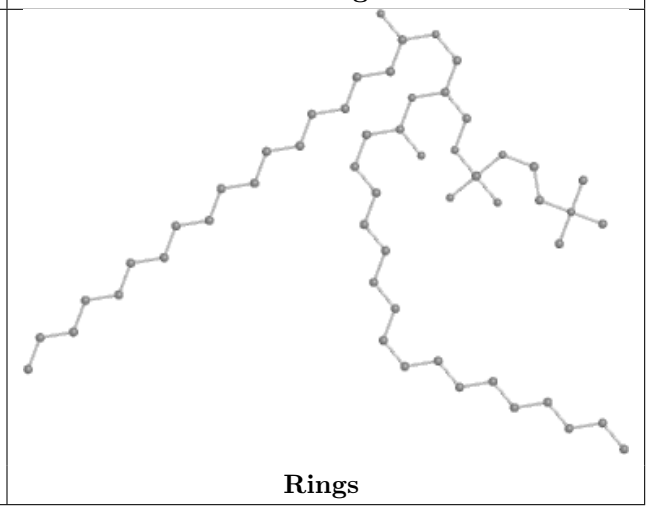
Bond lengths



Bond angles

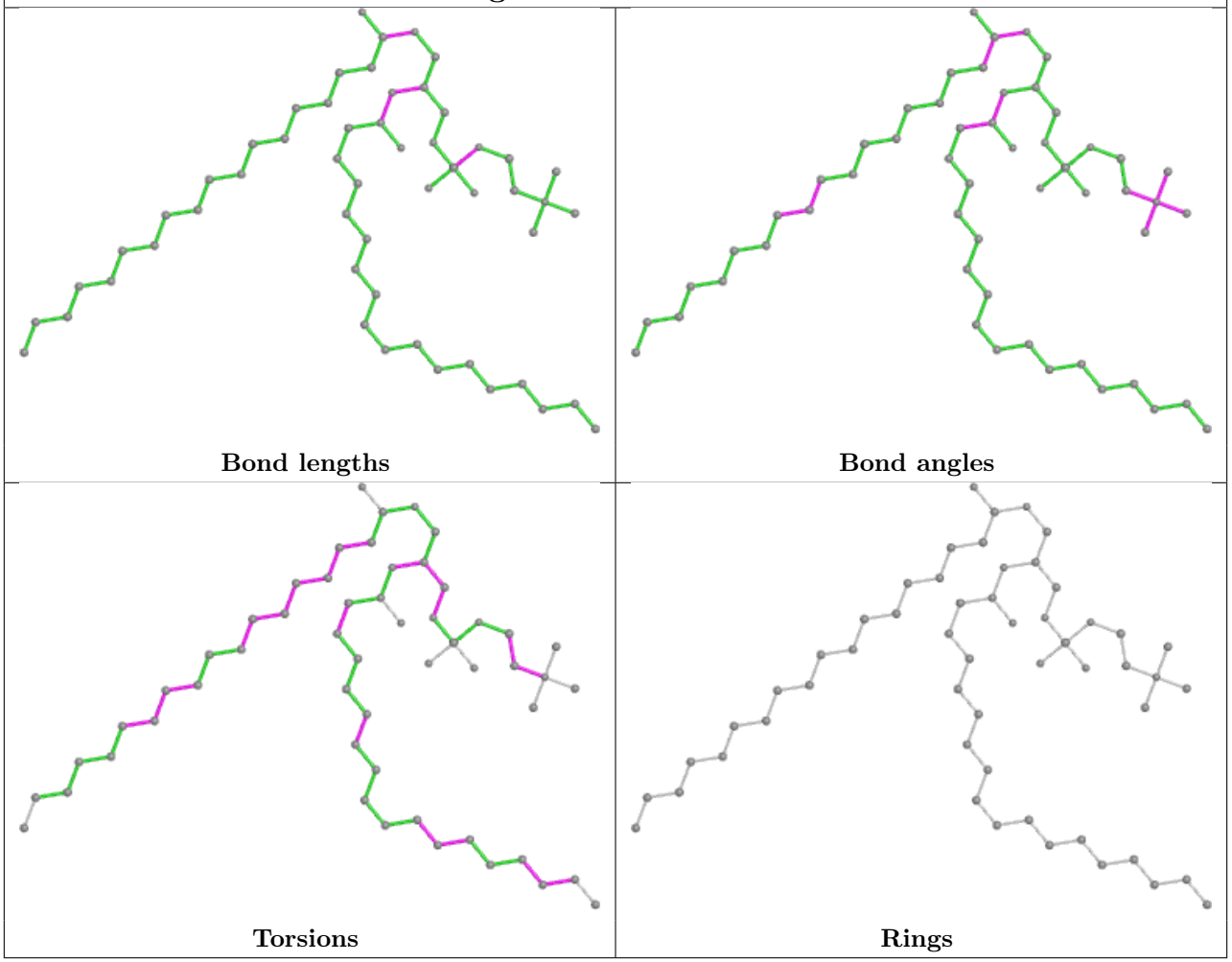


Torsions



Rings

Ligand PCW B 8003



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.

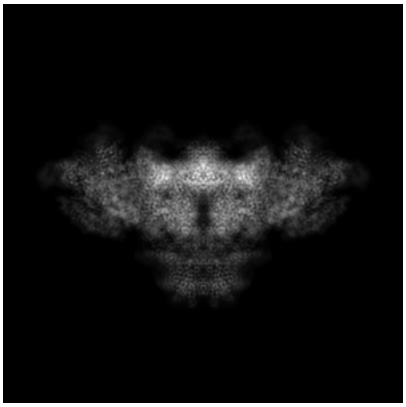
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43299. These allow visual inspection of the internal detail of the map and identification of artifacts.

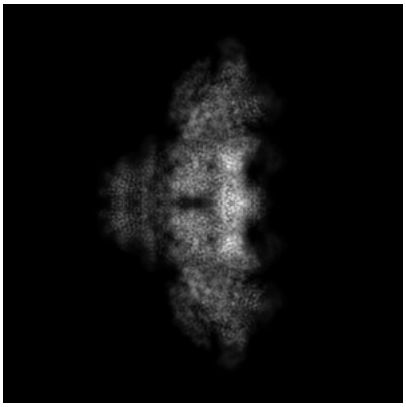
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

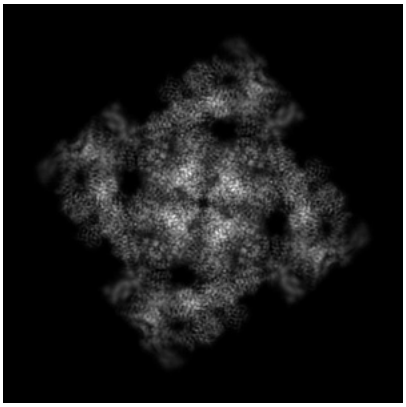
6.1.1 Primary map



X



Y



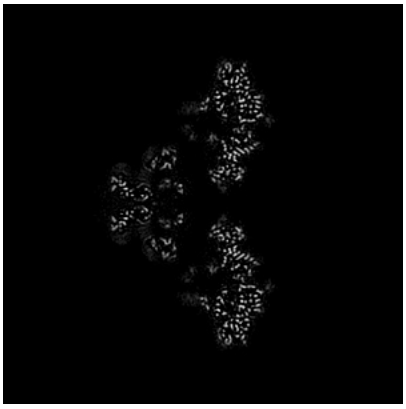
Z

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

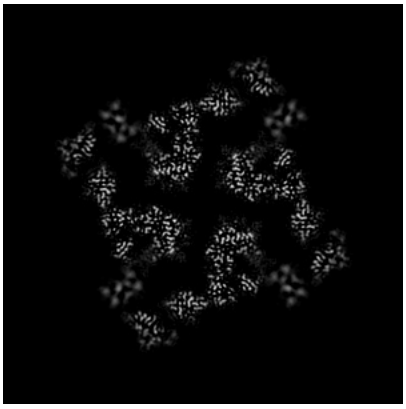
6.2 Central slices

6.2.1 Primary map

X Index: 256



Y Index: 256



Z Index: 256

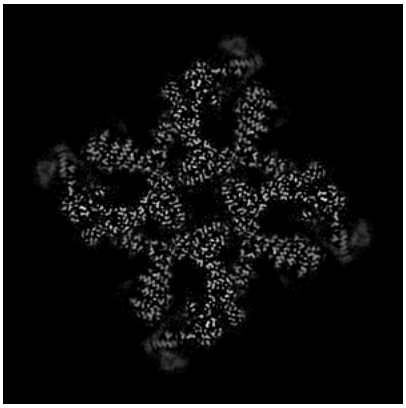
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 238

Y Index: 274

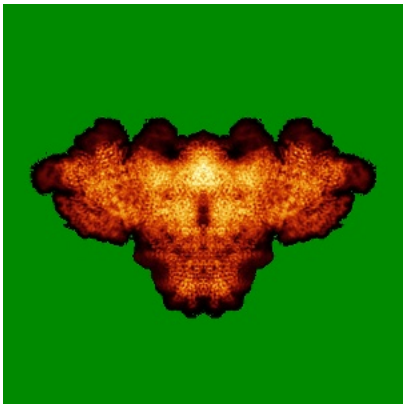


Z Index: 289

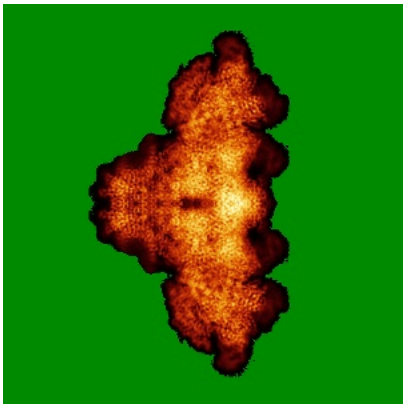
The images above show the largest variance slices of the map in three orthogonal directions.

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

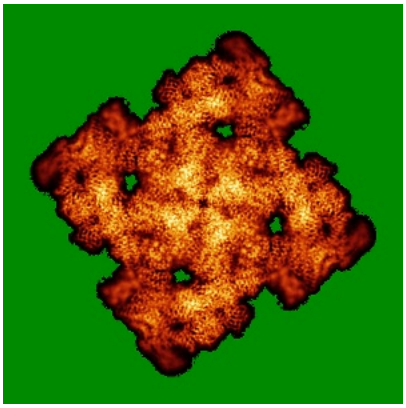
6.4.1 Primary map



X



Y

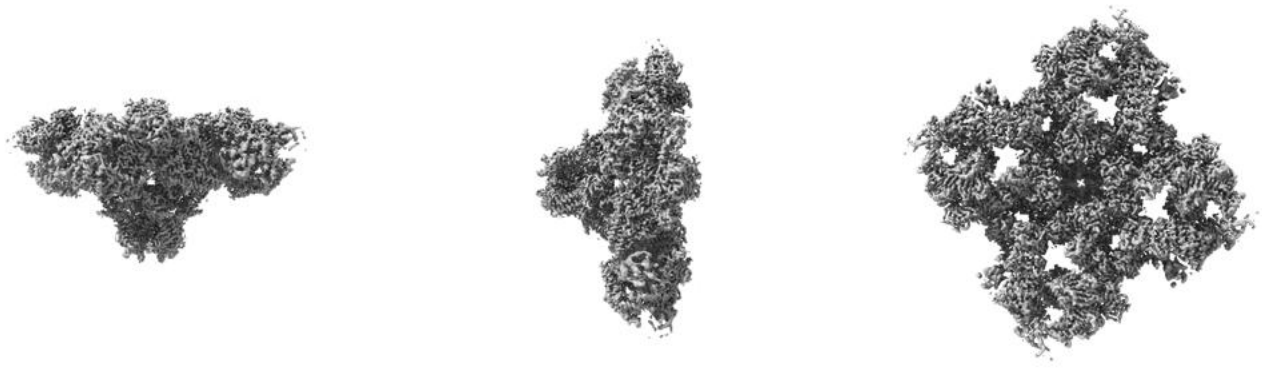


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

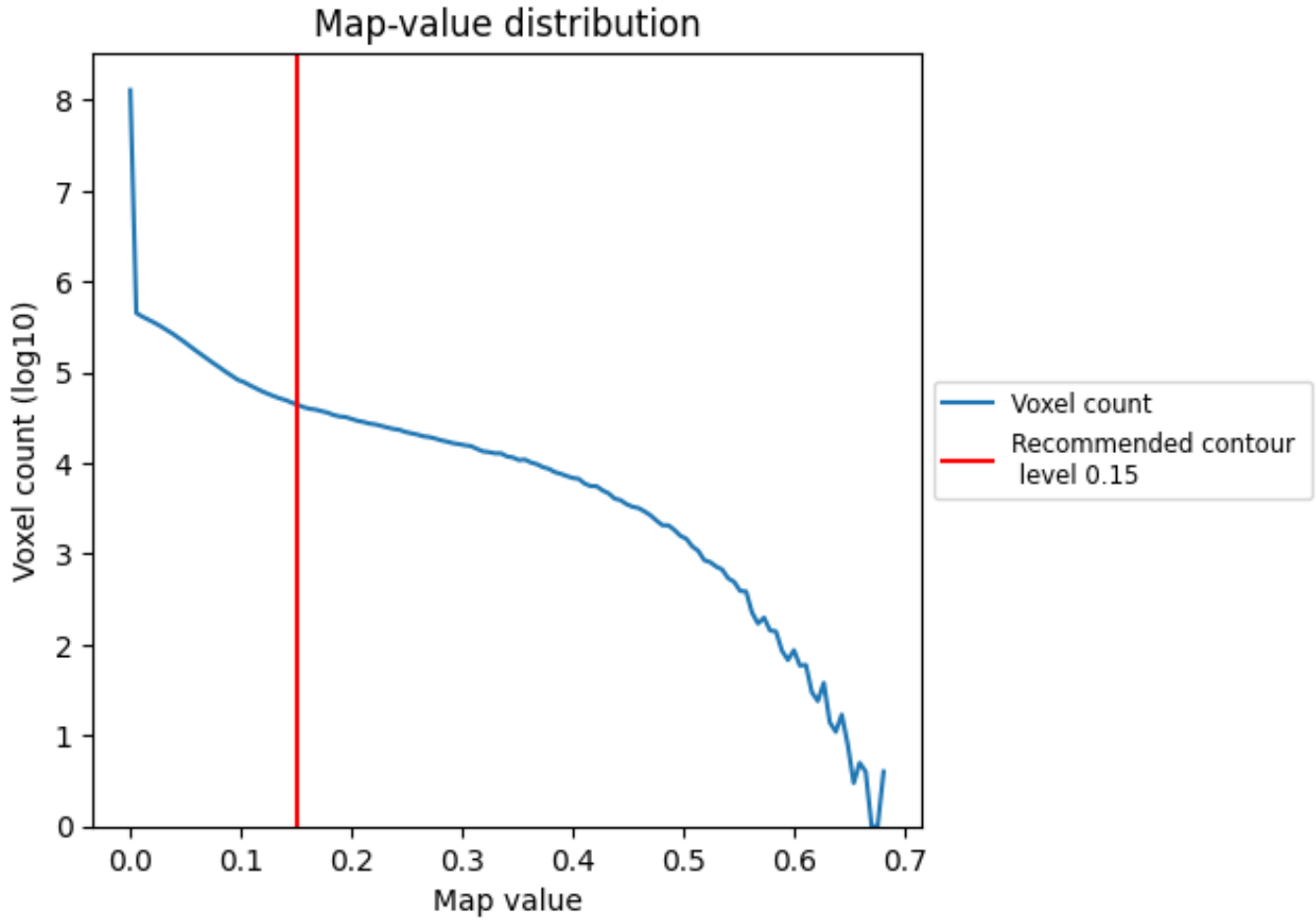
6.6 Mask visualisation (i)

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

7 Map analysis

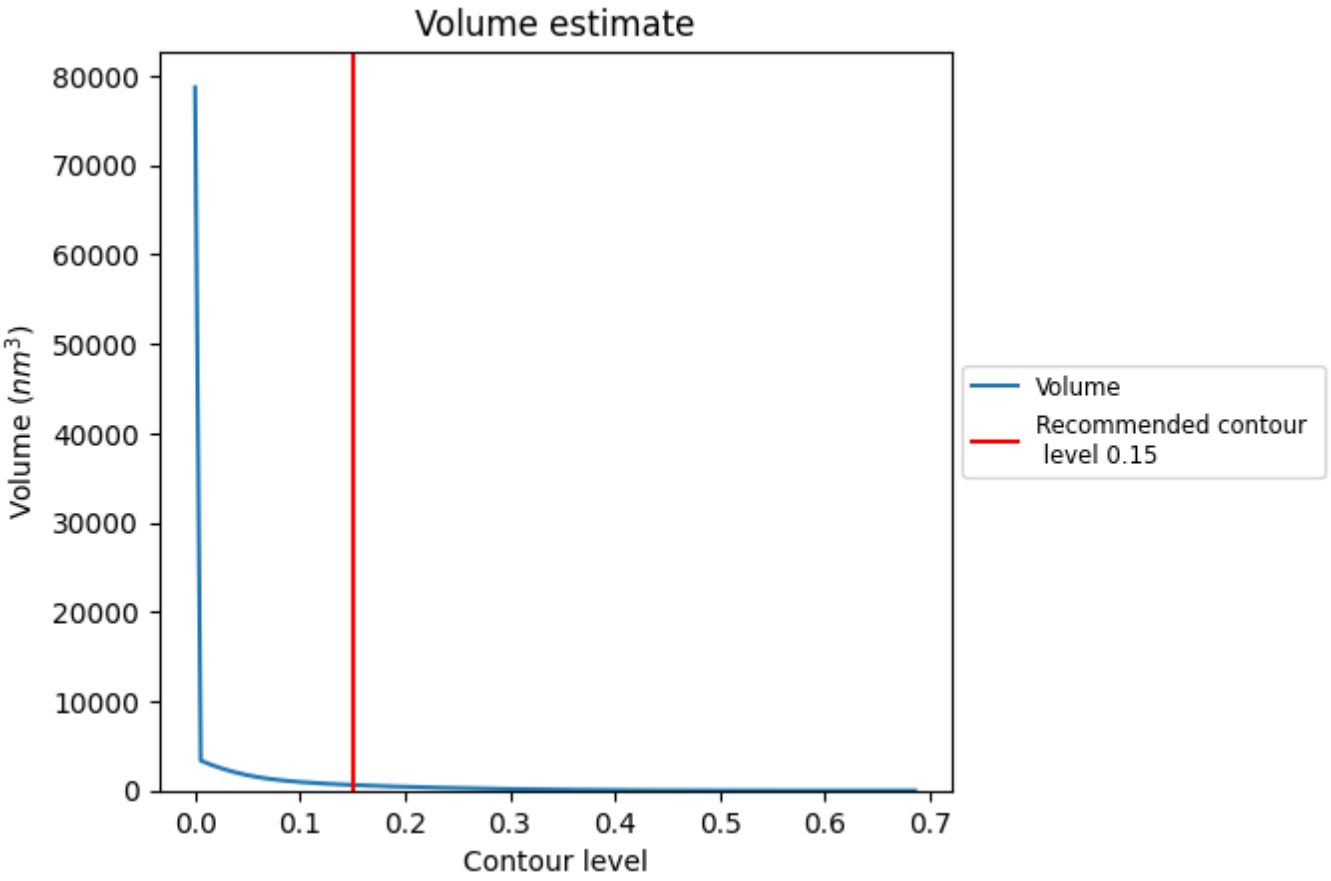
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

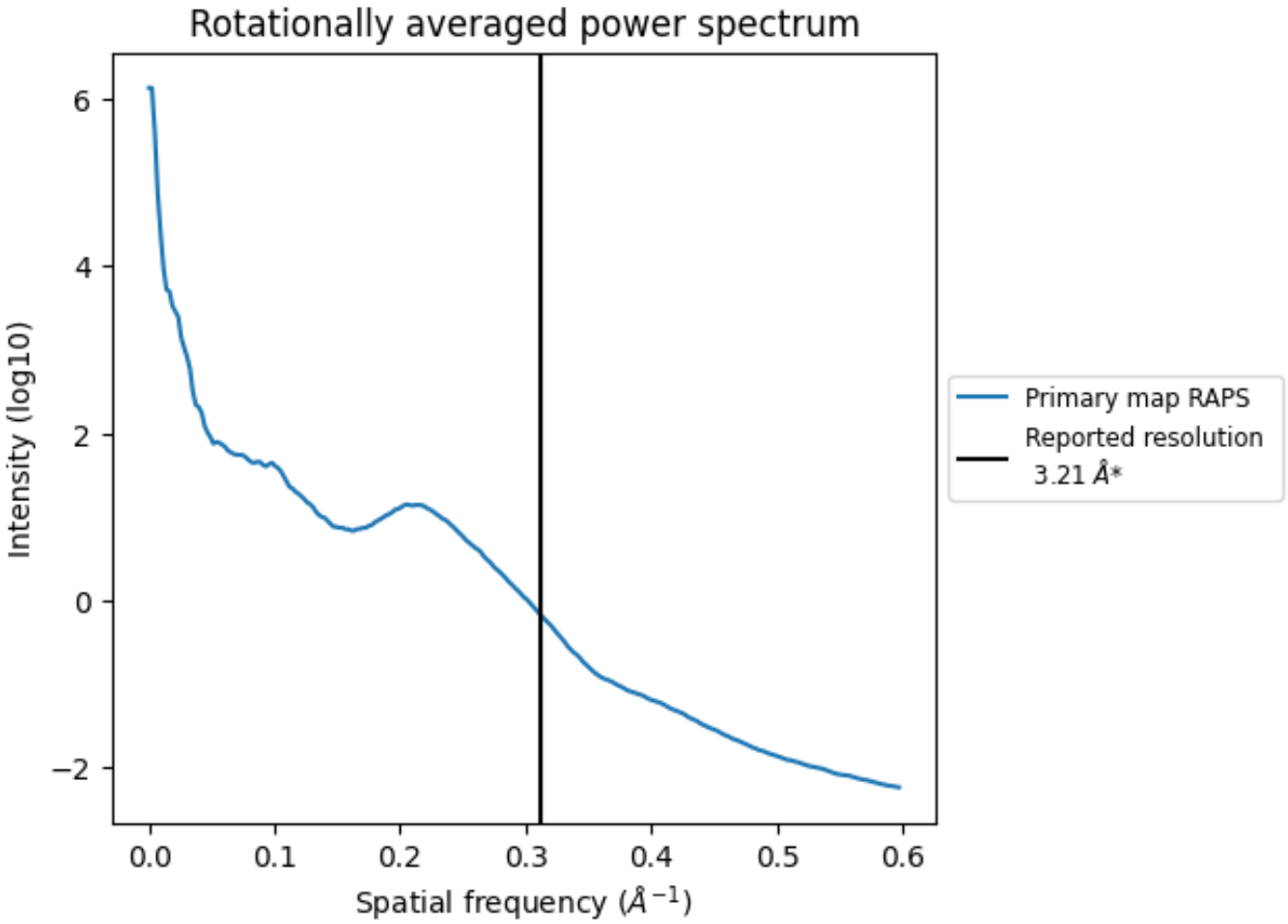
7.2 Volume estimate



The volume at the recommended contour level is 624 nm^3; this corresponds to an approximate mass of 564 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 0.312 $Å^{-1}$

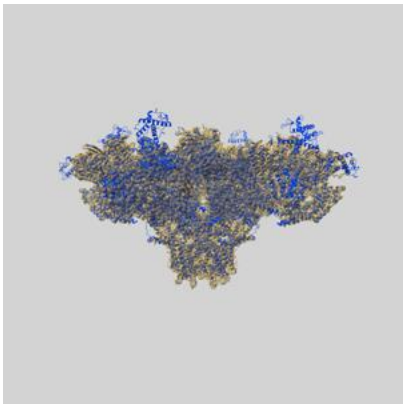
8 Fourier-Shell correlation (i)

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

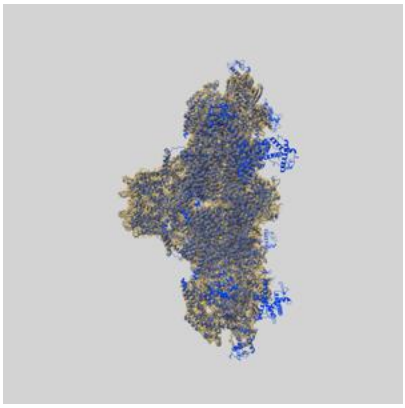
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43299 and PDB model 8VK3. Per-residue inclusion information can be found in section 3 on page 7.

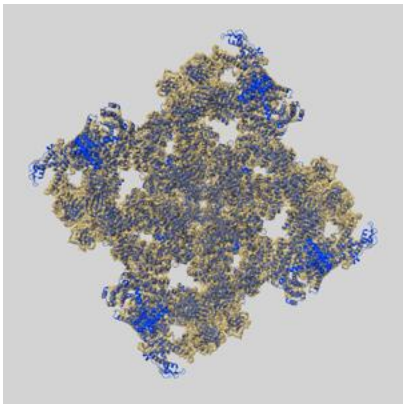
9.1 Map-model overlay



X



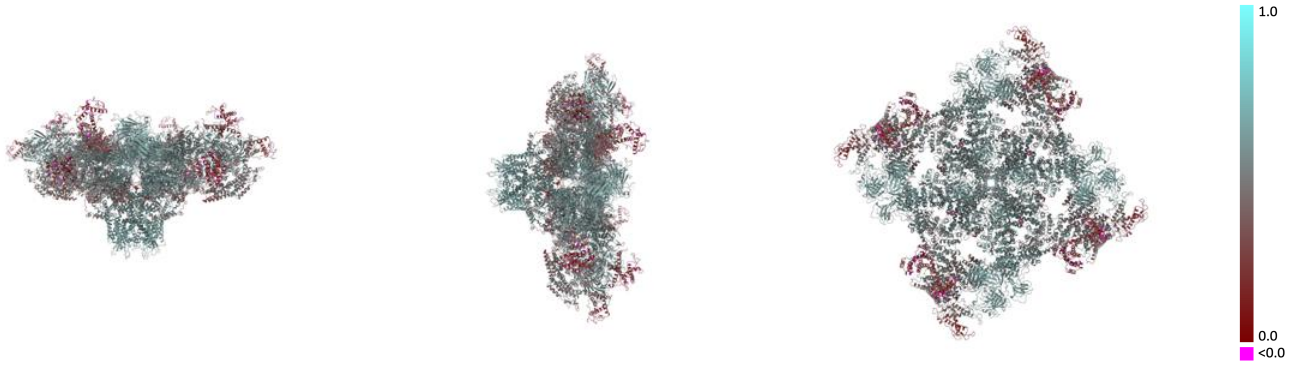
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

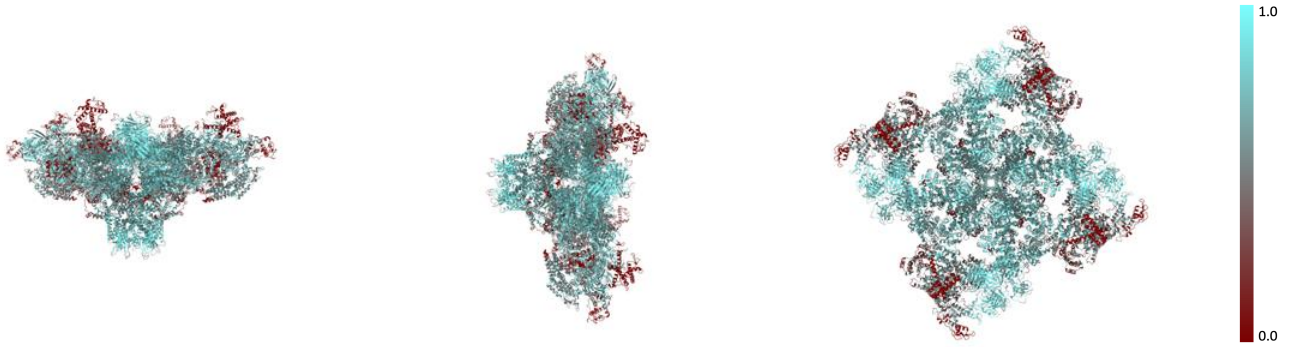
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

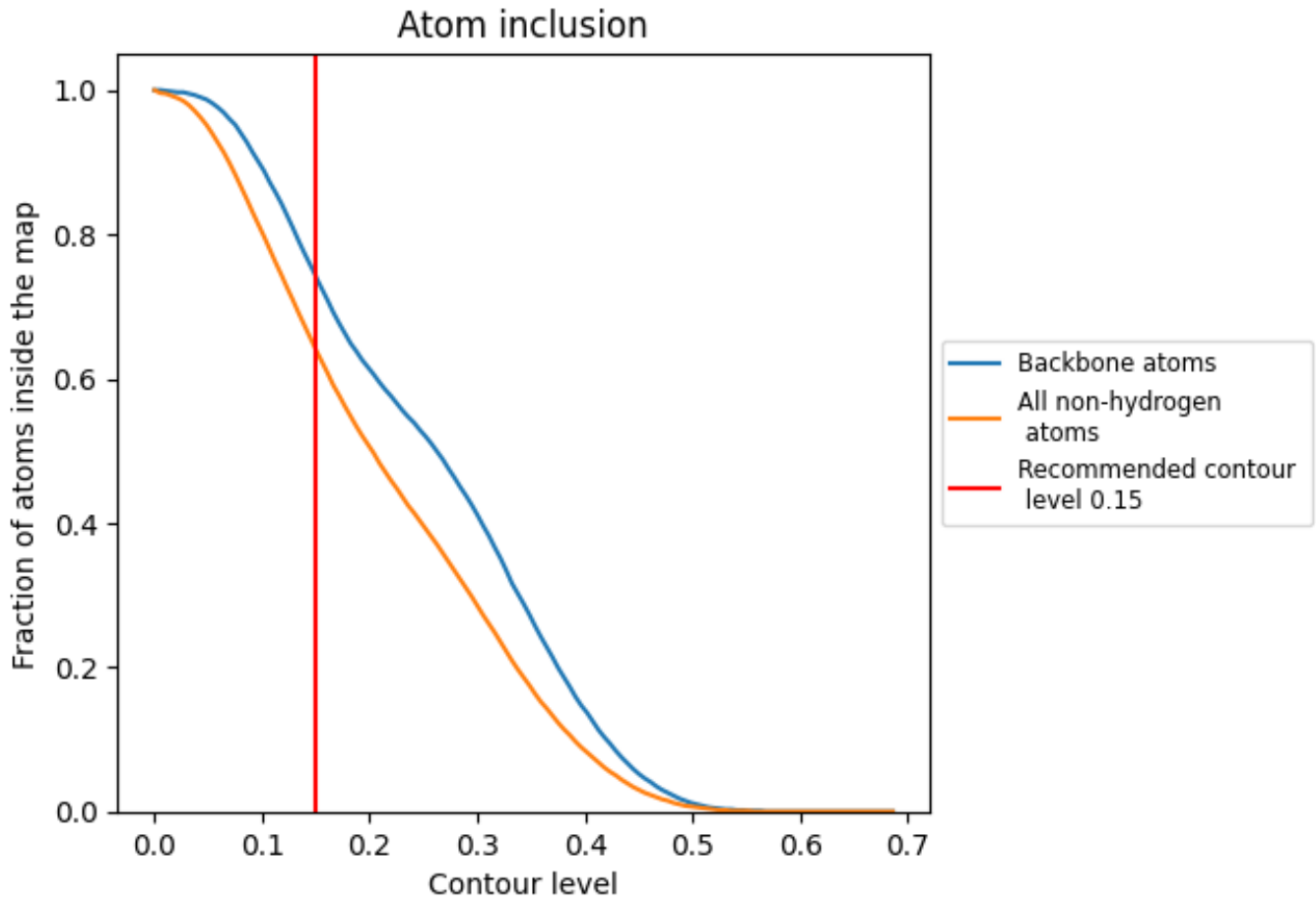
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6400	0.4910
A	0.6520	0.5030
B	0.6530	0.5020
C	0.6530	0.5020
D	0.6520	0.5030
E	0.7290	0.5660
F	0.7340	0.5630
G	0.7320	0.5630
H	0.7360	0.5630
I	0.3090	0.1620
J	0.2960	0.1670
K	0.3040	0.1620
L	0.2910	0.1640
M	0.3010	0.1640
N	0.2960	0.1680
O	0.3060	0.1590
P	0.2930	0.1660