Full wwPDB EM Validation Report ⓘ

Jun 30, 2024 – 02:49 PM EDT

PDB ID	:	8VJK
EMDB ID	:	EMD-43284
Title	:	Structure of mouse RyR1 (high-Ca2+/CFF/ATP dataset)
Authors	:	Weninger, G.; Marks, A.R.
Deposited on	:	2024-01-07
Resolution	:	2.92 Å(reported)

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

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

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

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

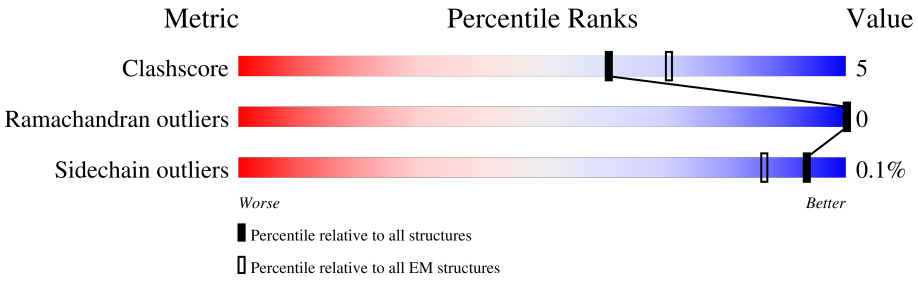
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.92 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	9% 77% 9% 13%
1	B	5035	9% 77% 9% 13%
1	C	5035	9% 77% 9% 13%
1	D	5035	9% 78% 9% 13%
2	E	108	82% 17%
2	F	108	85% 14%
2	G	108	84% 15%
2	H	108	81% 18%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 143248 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	4373	Total 34797	C 22132	N 5983	O 6445	S 237	0	0
1	B	4373	Total 34797	C 22132	N 5983	O 6445	S 237	0	0
1	C	4373	Total 34797	C 22132	N 5983	O 6445	S 237	0	0
1	D	4373	Total 34797	C 22132	N 5983	O 6445	S 237	0	0

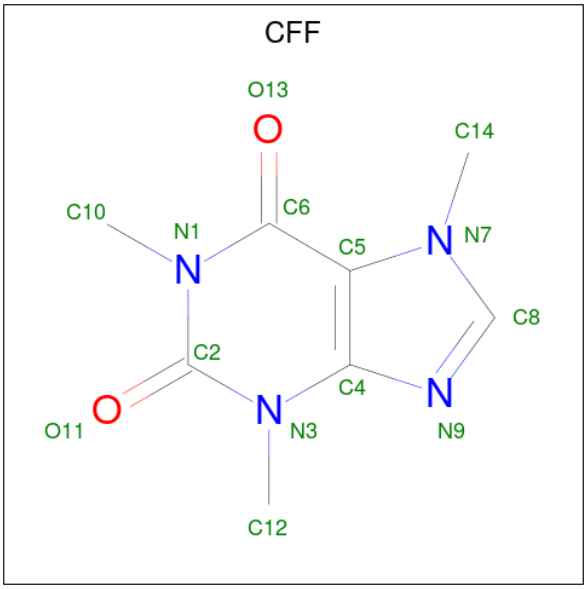
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

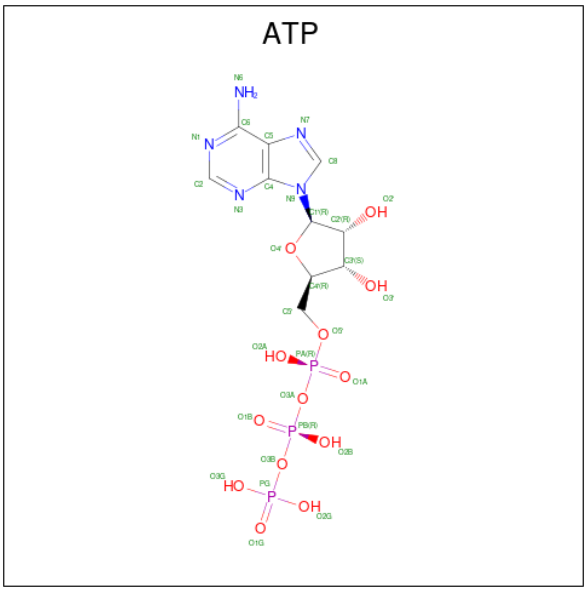
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	4	2	
4	B	1	Total	C	N	O	0
			14	8	4	2	
4	C	1	Total	C	N	O	0
			14	8	4	2	
4	D	1	Total	C	N	O	0
			14	8	4	2	

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



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

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

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

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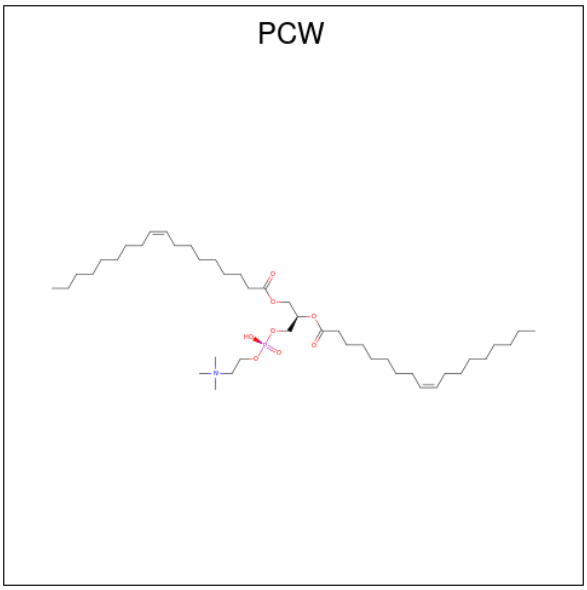
Mol	Chain	Residues	Atoms	AltConf
6	D	1	Total Ca 1 1	0

- Molecule 7 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



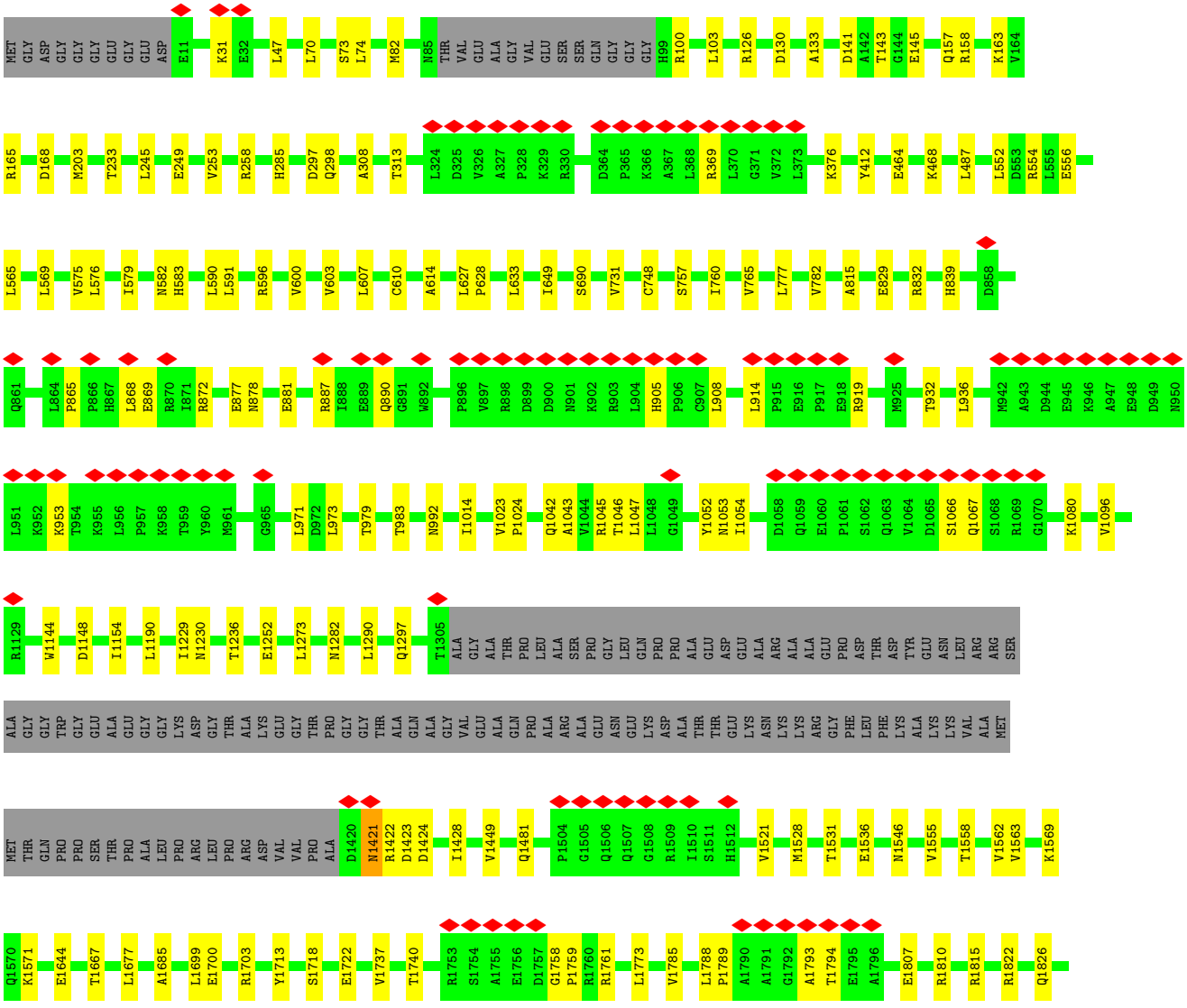
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O P 54 44 1 8 1	0
7	A	1	Total C N O P 54 44 1 8 1	0
7	B	1	Total C N O P 54 44 1 8 1	0
7	B	1	Total C N O P 54 44 1 8 1	0
7	C	1	Total C N O P 54 44 1 8 1	0
7	C	1	Total C N O P 54 44 1 8 1	0
7	D	1	Total C N O P 54 44 1 8 1	0
7	D	1	Total C N O P 54 44 1 8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

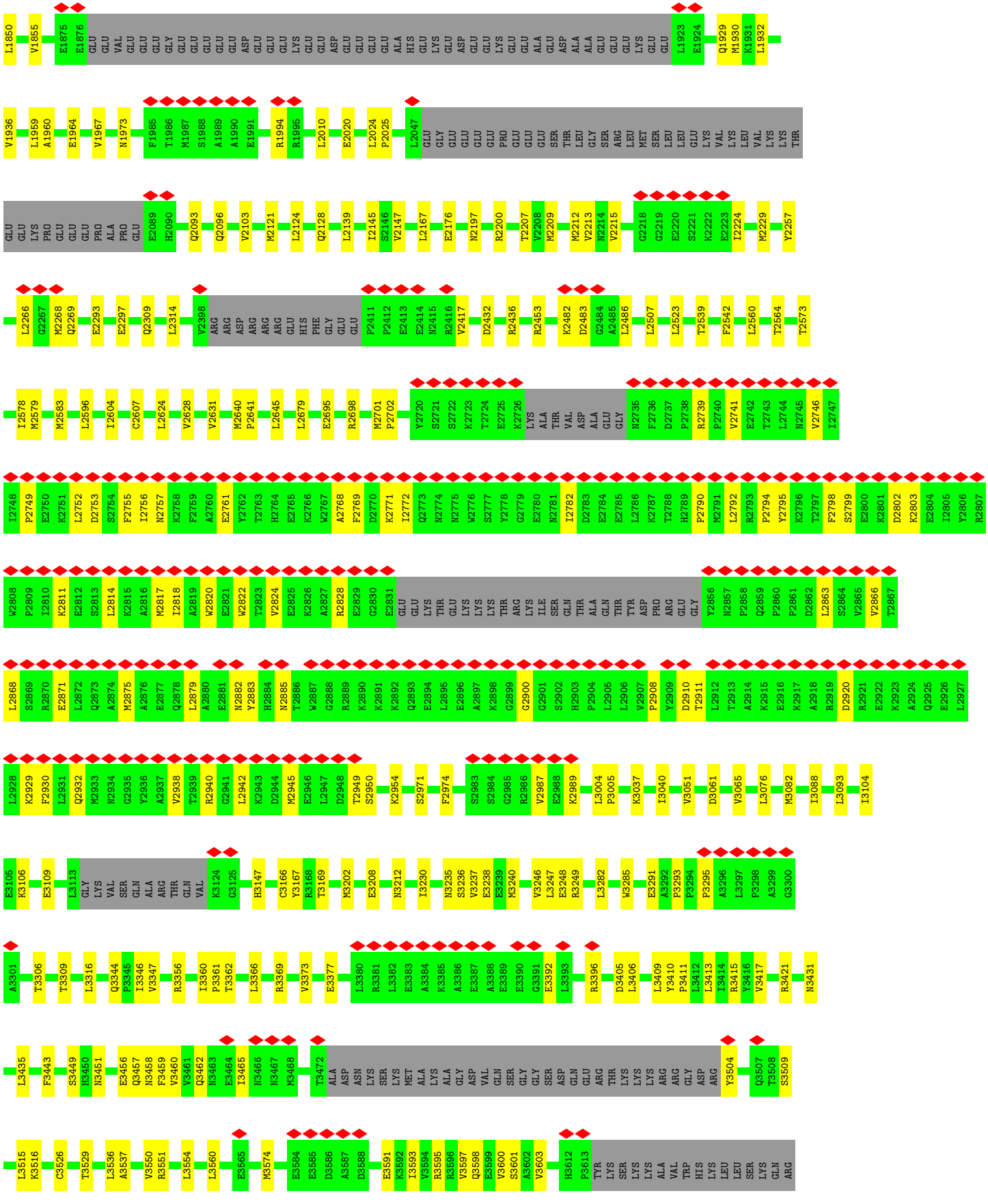
3 Residue-property plots (i)

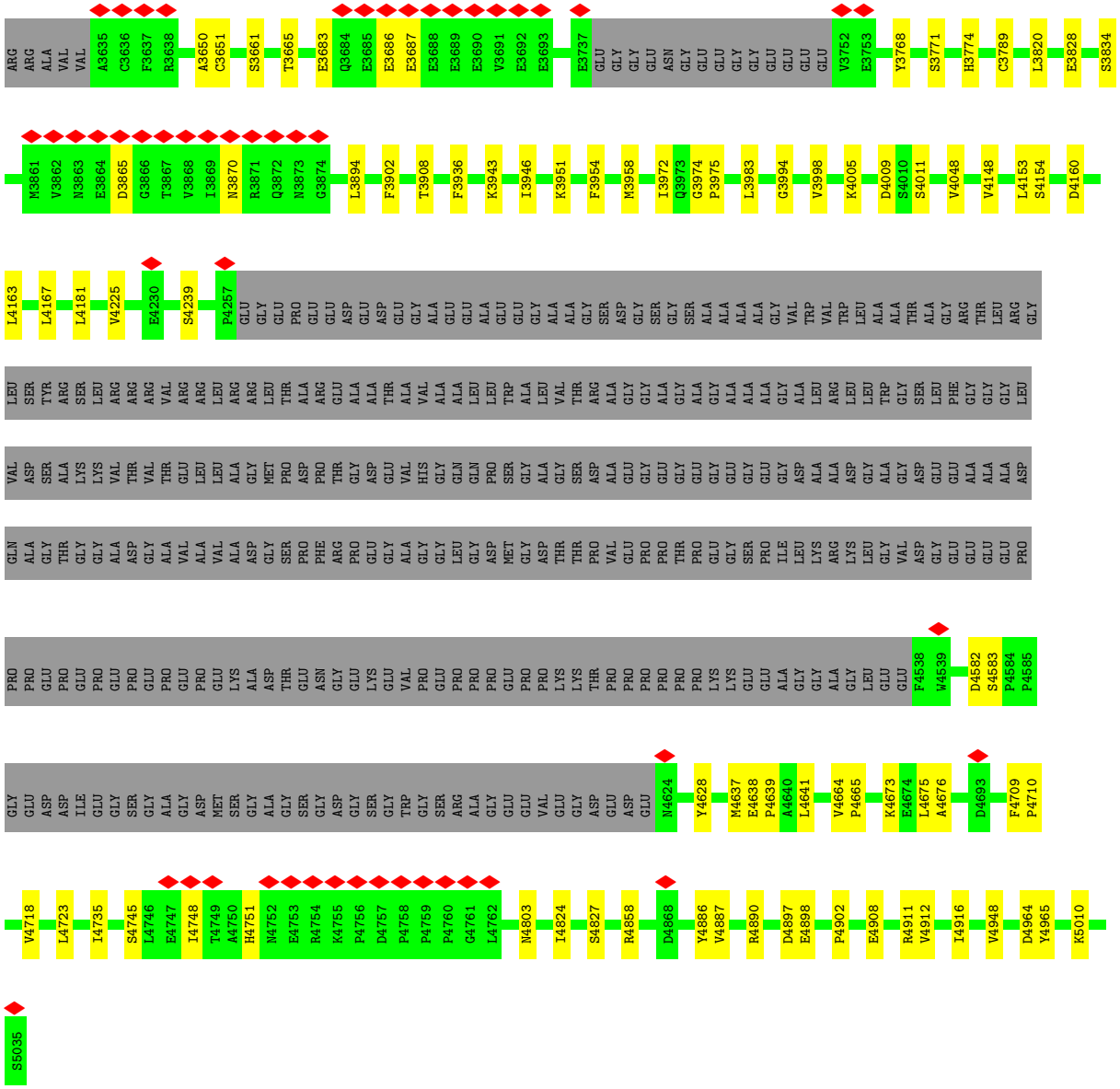
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Ryanodine receptor 1

Chain A:

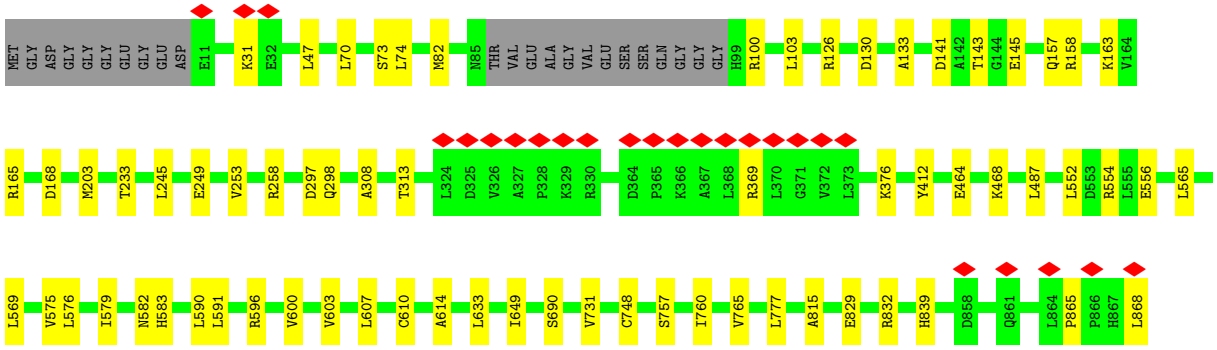


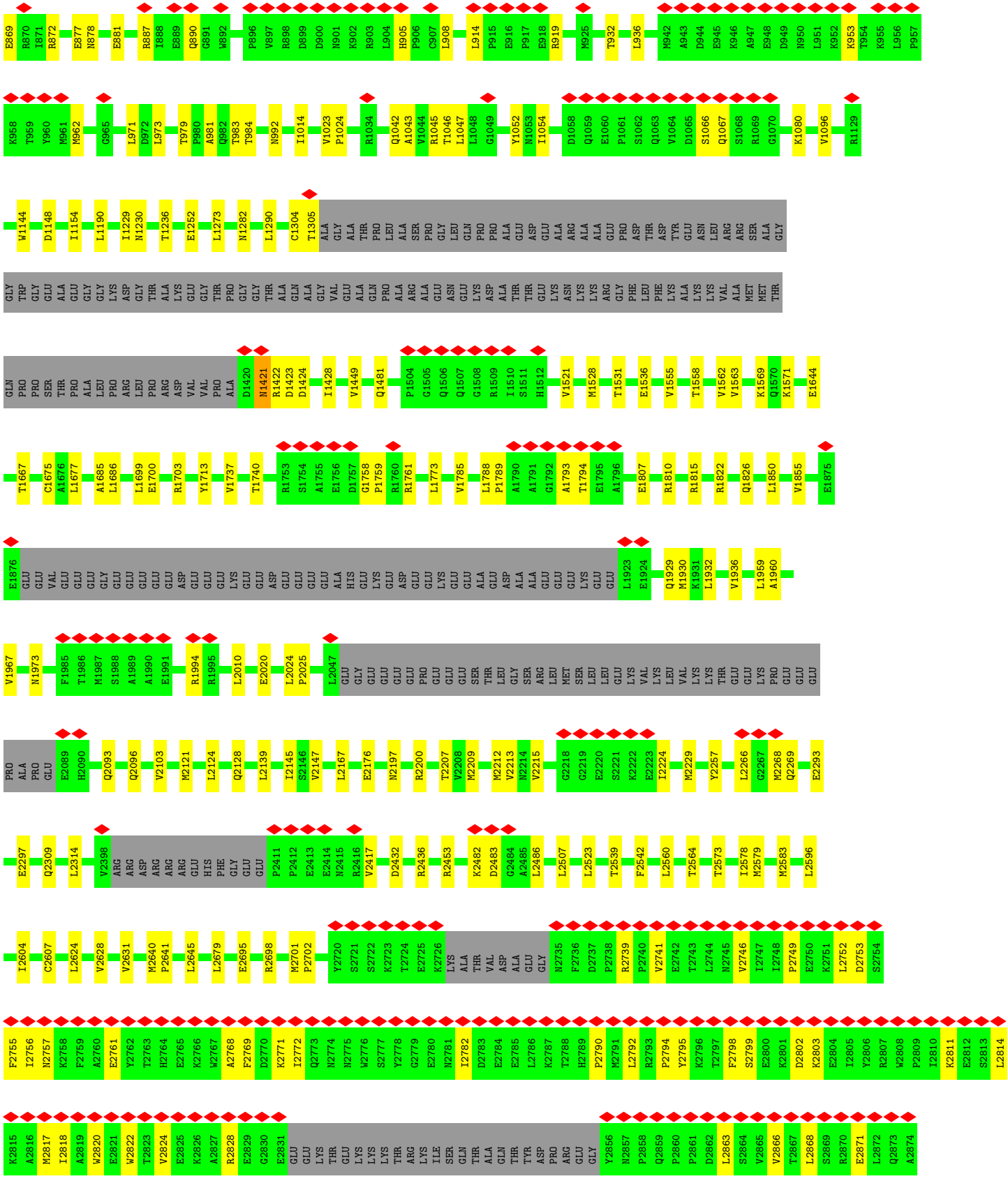


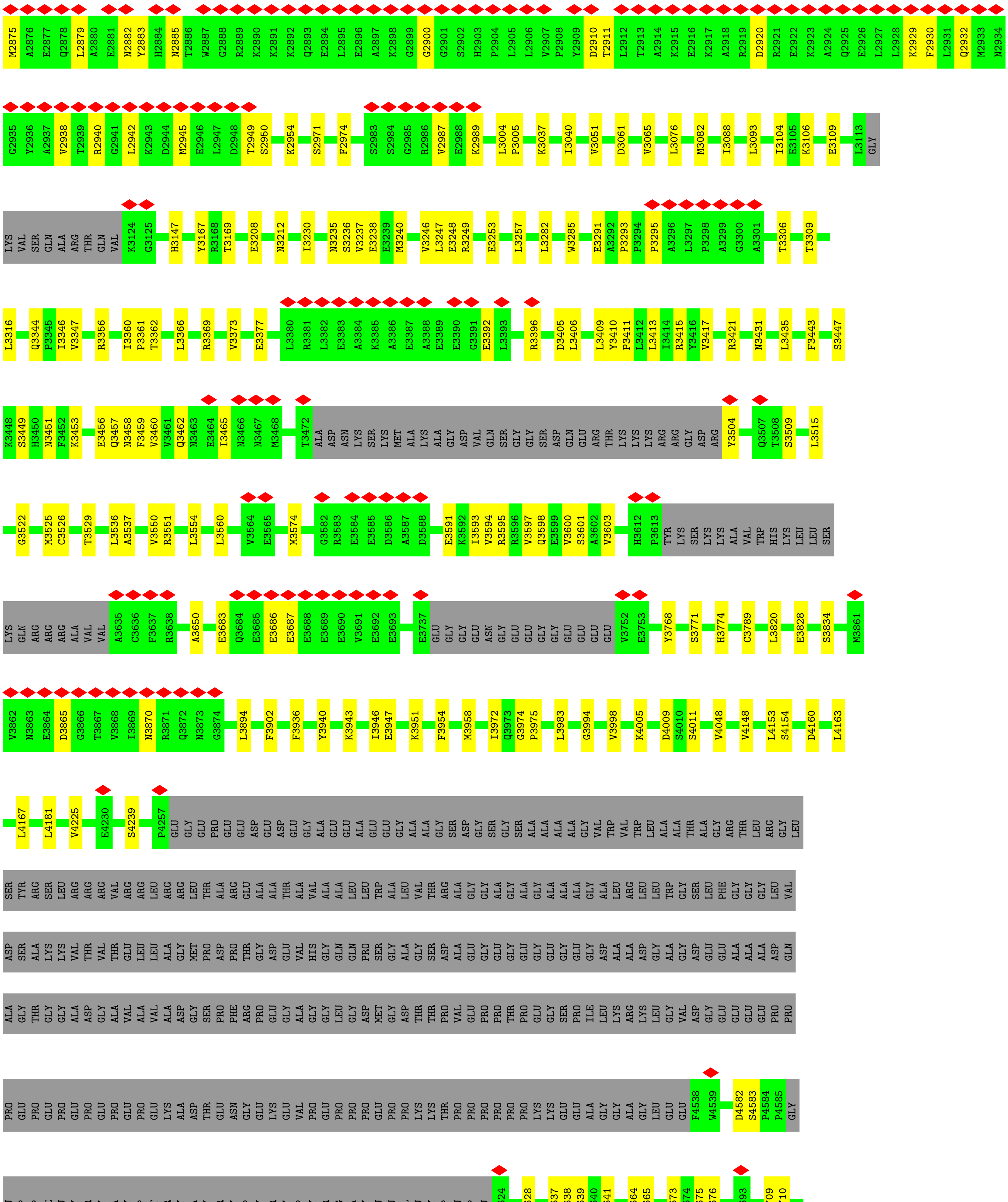


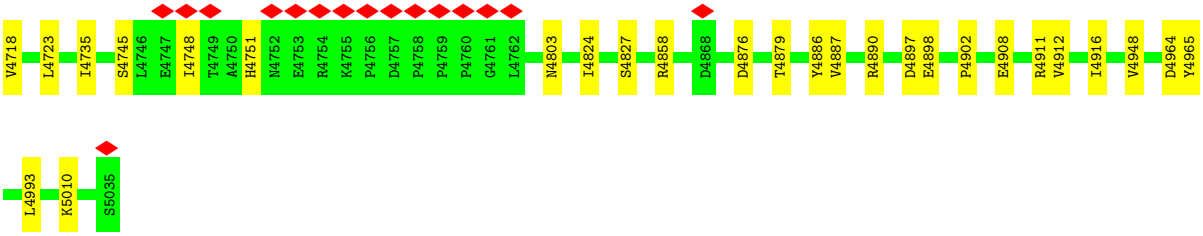
• Molecule 1: Ryanodine receptor 1

Chain B:



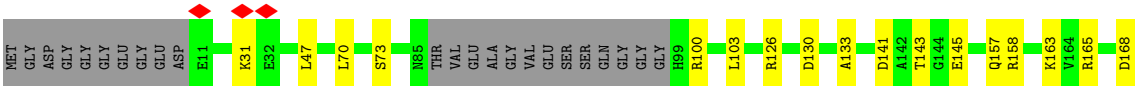

E869 R870 I871 R872 E877 N878 E881 R887 I888 E889 Q890 G891 W892 P896 V897 R898 D899 D900 N901 K902 R903 L904 H905 P906 C907 L908 L914 P915 E916 P917 E918 R919 M925 T932 L936 M942 A943 D944 E945 K946 A947 E948 D949 N950 L951 K952 K953 T954 K955 L956 P957
K958 T959 Y960 M961 M962 G965 L971 D972 L973 T979 P980 A981 Q982 T983 T984 N992 I1014 V1023 P1024 R1034 Q1042 A1043 V1044 R1045 T1046 L1047 L1048 G1049 Y1052 N1053 I1054 D1058 Q1059 E1060 P1061 S1062 Q1063 V1064 D1065 S1066 Q1067 S1068 R1069 G1070 K1080 V1096 R1129
W1144 D1148 I1154 L1190 I1229 N1230 T1236 E1252 L1273 N1282 L1290 C1304 T1305 ALA GLY ALA THR PRO LEU ALA SER PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP THR ASP TYR GLU ASN LEU ARG ARG SER ALA GLY
GLY TRP GLY GLU ALA GLU GLY GLY LYS ASP GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR ALA GLN ALA GLY VAL GLU ALA GLN PRO ALA ARG ALA GLU GLU ASN GLU GLY LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR
GLN PRO PRO PRO SER THR PRO ALA LEU PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423 D1424 I1428 V1449 Q1481 P1504 G1505 Q1506 Q1507 G1508 R1509 I1510 S1511 H1512 V1521 M1528 T1531 E1536 V1555 T1558 V1562 V1563 K1569 Q1570 K1571 E1644
T1667 C1675 A1676 L1677 A1685 L1686 L1699 E1700 R1703 Y1713 V1737 T1740 R1753 S1754 A1755 E1756 D1757 G1758 P1759 R1760 R1761 L1773 V1785 L1788 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 E1807 R1810 R1815 R1822 Q1826 L1850 V1855 E1875
E1876 GLU GLU VAL GLU GLU GLU GLY GLU GLU GLU GLU ASP 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 GLU LYS GLU GLU L1923 E1924 Q1929 M1930 K1931 L1932 V1936 L1959 A1960
V1967 N1973 F1985 T1986 M1987 S1988 A1989 A1990 E1991 R1994 R1995 L2010 E2020 L2024 P2025 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 Q2093 Q2096 V2103 M2121 L2124 Q2128 L2139 I2145 S2146 V2147 L2167 E2176 N2197 R2200 T2207 V2208 M2209 M2212 V2213 N2214 V2215 G2218 G2219 E2220 S2221 K2222 E2223 I2224 M2229 Y2257 L2266 G2267 M2268 Q2269 E2293
E2297 Q2309 L2314 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 N2415 R2416 V2417 D2432 R2436 R2453 K2482 D2483 G2484 A2485 L2486 L2507 L2523 T2539 F2542 L2560 T2564 T2573 I2578 M2579 M2583 L2596
I2604 C2607 L2624 V2628 V2631 M2640 P2641 L2645 L2679 E2695 R2698 M2701 P2702 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

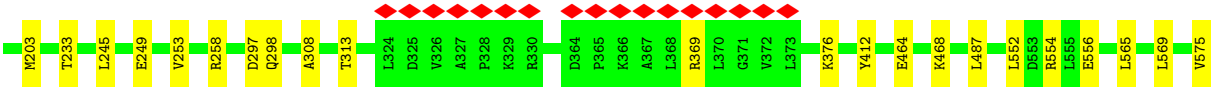


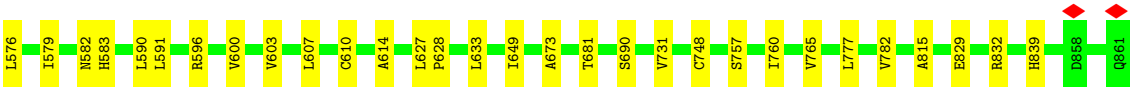


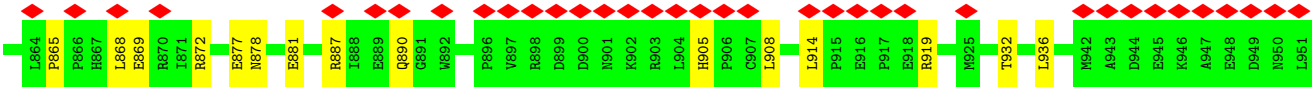
• Molecule 1: Ryanodine receptor 1

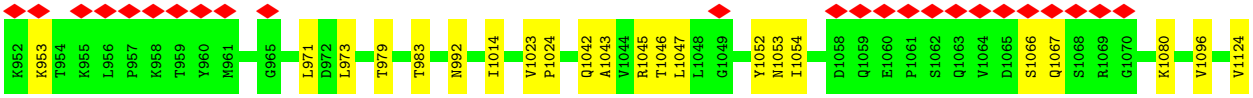
Chain C:

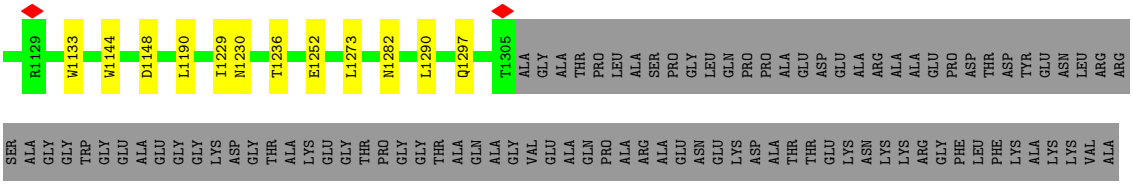


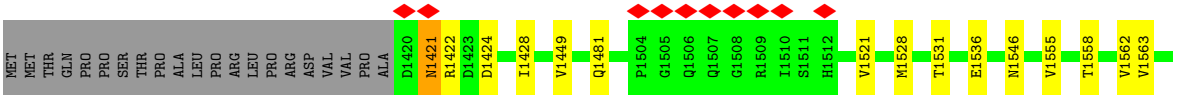


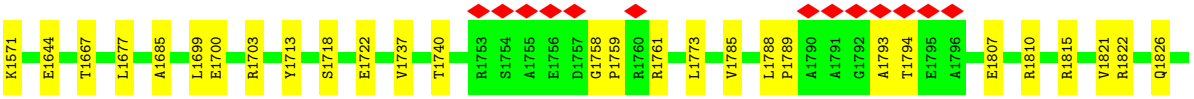


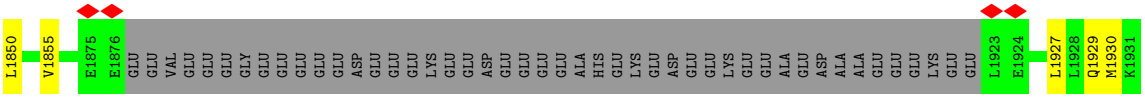


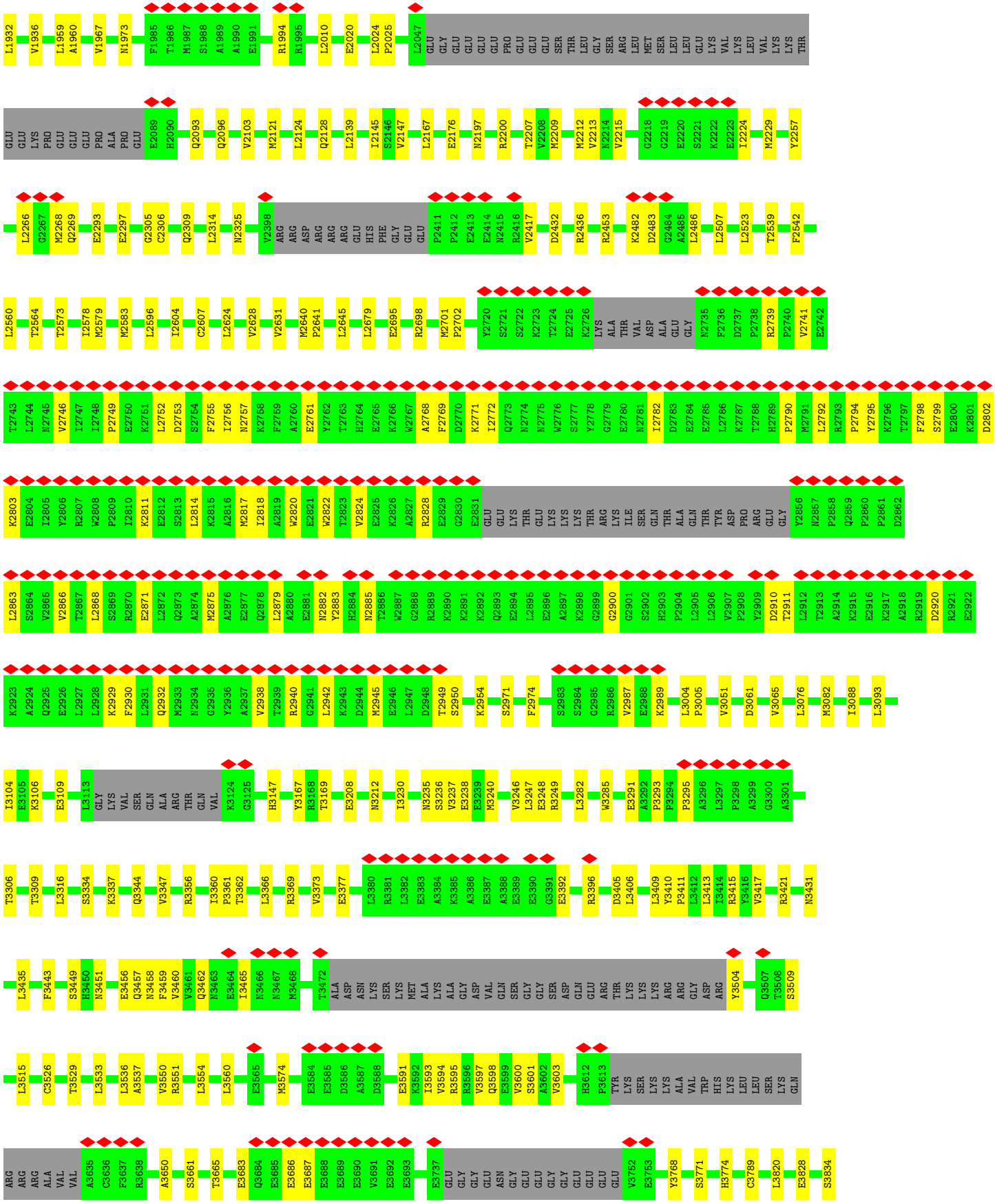


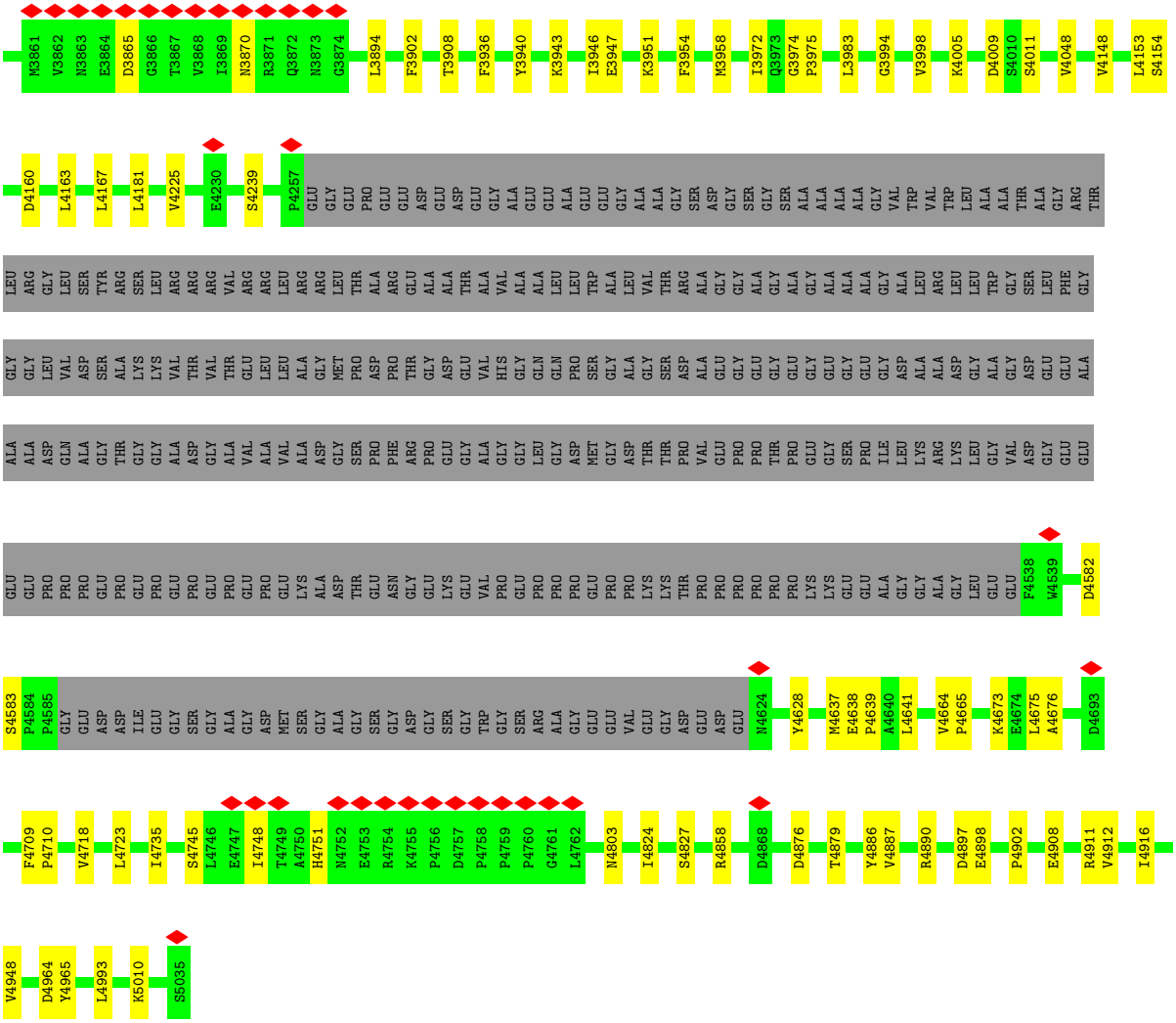






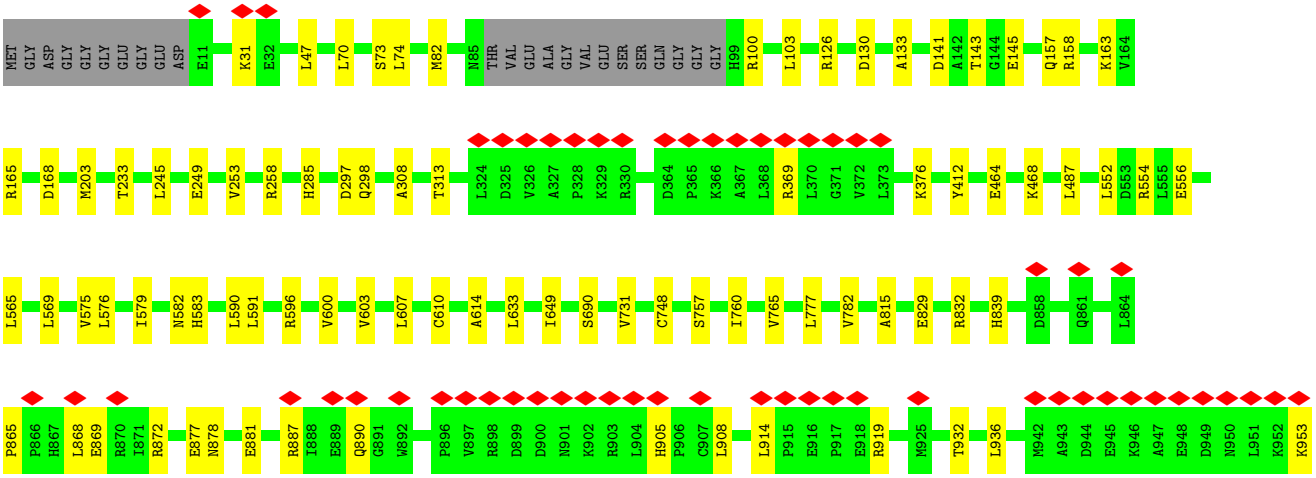


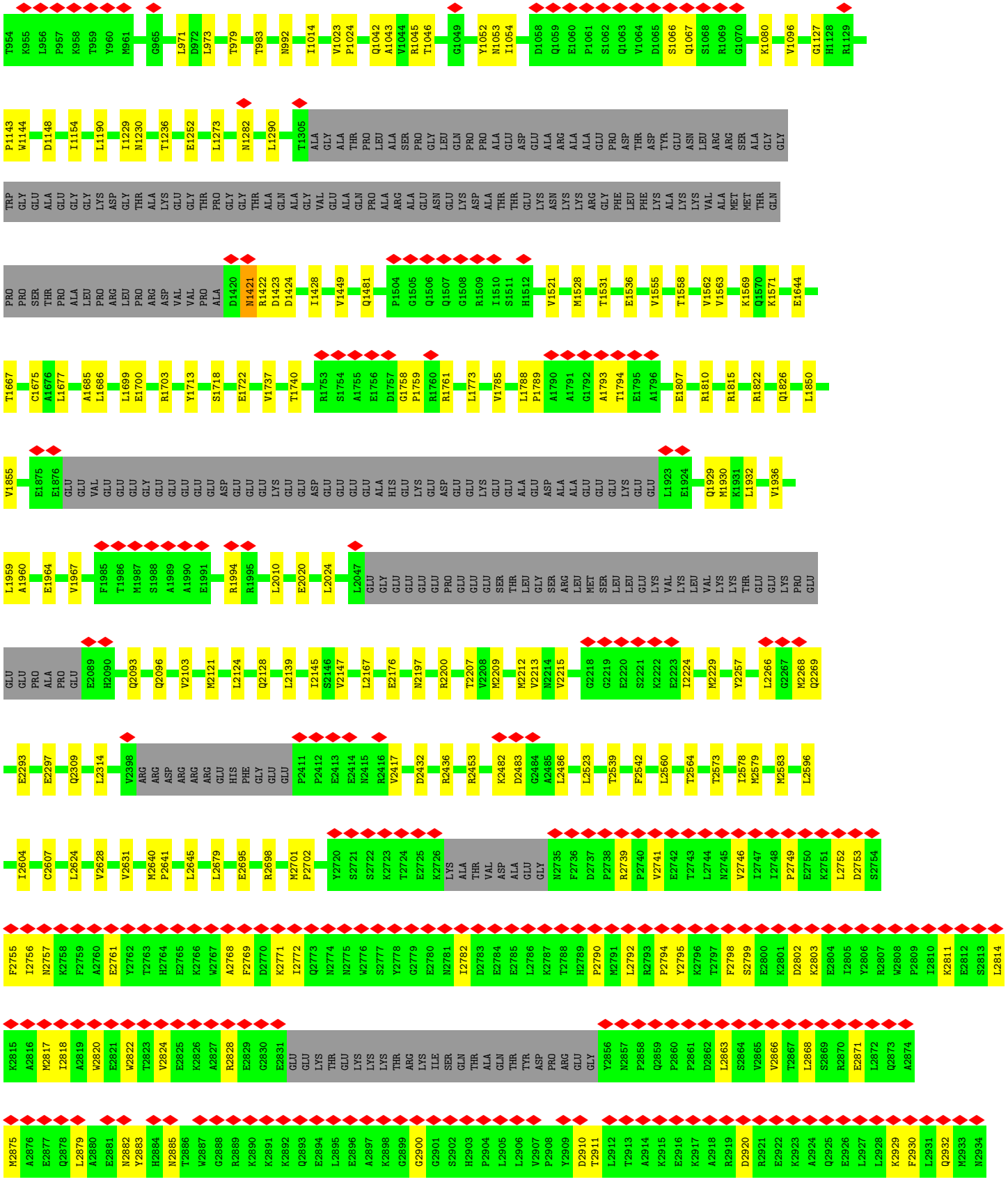


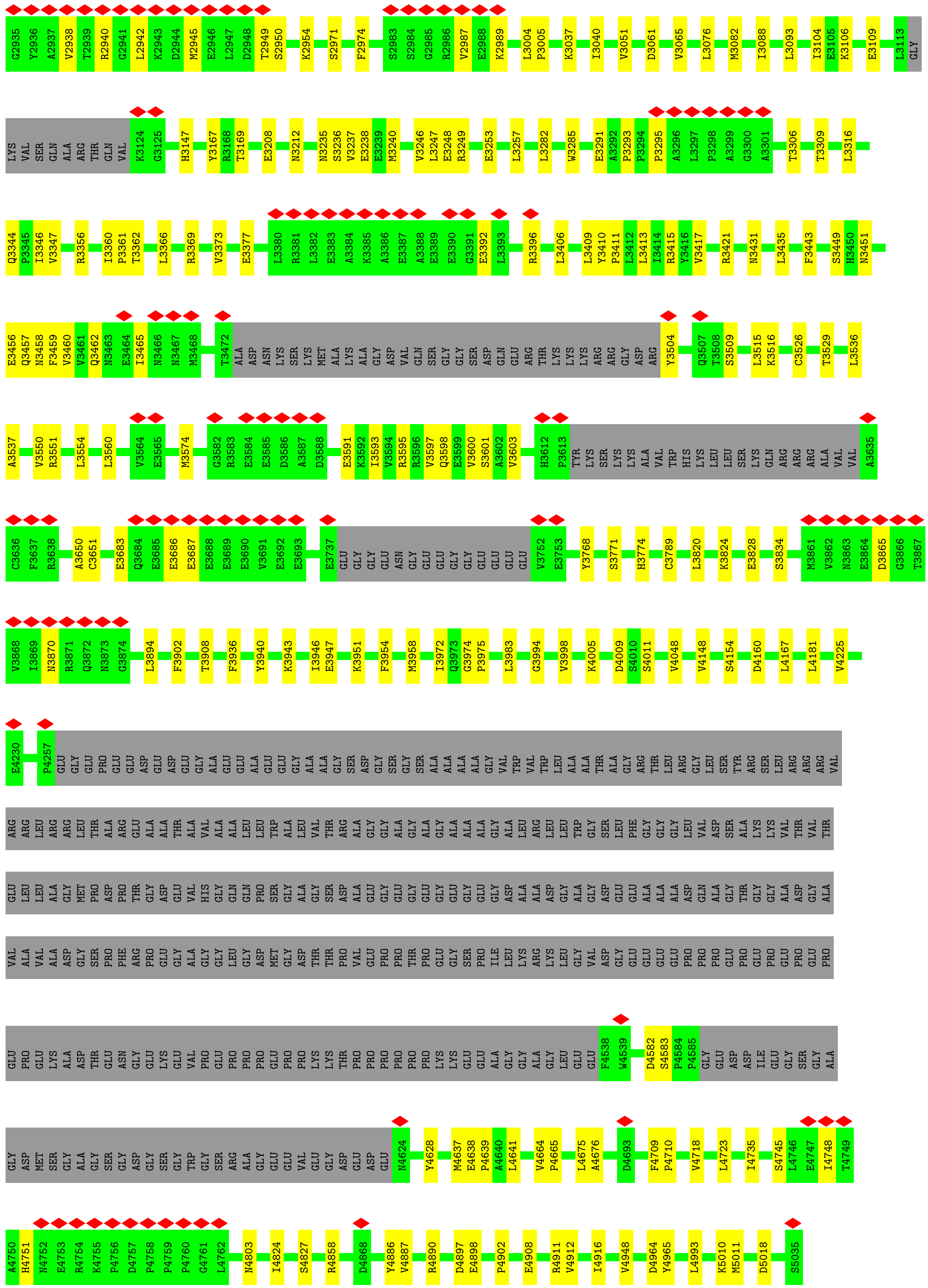


• Molecule 1: Ryanodine receptor 1

Chain D:




T954 K955 L956 P957 K958 T959 Y960 M961 G965 L971 D972 L973 T979 T983 N992 I1014 V1023 P1024 Q1042 A1043 V1044 R1045 T1046 G1049 Y1052 N1053 I1054 D1058 Q1059 E1060 P1061 S1062 Q1063 V1064 D1065 S1066 Q1067 S1068 R1069 G1070 K1080 V1096 G1127 H1128 R1129
P1143 W1144 D1148 I1154 L1190 I1229 N1230 T1236 E1252 L1273 N1282 L1290 T1305 ALA GLY ALA THR PRO LEU ALA SER PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP THR ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY
TRP GLY GLU ALA GLU GLY GLY LYS ASP GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR ALA GLN ALA GLY VAL GLU ALA GLN PRO ALA ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS VAL ALA MET MET THR GLN
PRO PRO SER THR PRO ALA LEU PRO PRO ARG LEU PRO ARG ASP VAL VAL PRO ALA D1420 N1421 R1422 D1423 D1424 I1428 V1449 Q1481 P1504 G1505 Q1506 Q1507 G1508 R1509 I1510 S1511 H1512 V1521 M1528 T1531 E1536 V1555 T1558 V1562 V1563 K1569 Q1570 K1571 E1644
T1667 C1675 A1676 L1677 A1685 L1686 L1699 E1700 R1703 Y1713 S1718 E1722 V1737 T1740 R1753 S1754 A1755 E1756 D1757 G1758 P1759 R1760 R1761 L1773 V1785 L1788 P1789 A1790 A1791 G1792 A1793 T1794 E1795 A1796 E1807 R1810 R1815 R1822 Q1826 L1850
V1855 E1875 E1876 GLU GLU VAL GLU GLU GLU GLY GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU ALA HIS GLU LYS GLU ASP GLU GLU LYS GLU GLU GLU ALA GLU ASP ALA ALA GLU GLU GLU GLU LYS GLU GLU L1923 E1924 Q1929 M1930 K1931 L1932 V1936
L1959 A1960 E1964 V1967 F1985 T1986 M1987 S1988 A1989 A1990 E1991 R1994 R1995 L2010 E2020 L2024 L2047 GLU GLY GLU 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 Q2093 Q2096 V2103 M2121 L2124 Q2128 L2139 I2145 S2146 V2147 L2167 E2176 N2197 R2200 T2207 V2208 M2209 M2212 V2213 N2214 V2215 G2218 G2219 E2220 S2221 K2222 E2223 I2224 M2229 Y2257 L2266 G2267 M2268 Q2269
E2293 E2297 Q2309 L2314 V2398 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2411 P2412 E2413 E2414 N2415 R2416 V2417 D2432 R2436 R2453 K2482 D2483 G2484 A2485 L2486 L2523 T2539 F2542 L2560 T2564 T2573 I2578 M2579 M2583 L2596
I2604 C2607 L2624 V2628 V2631 M2640 P2641 L2645 L2679 E2695 R2698 M2701 P2702 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 K2786 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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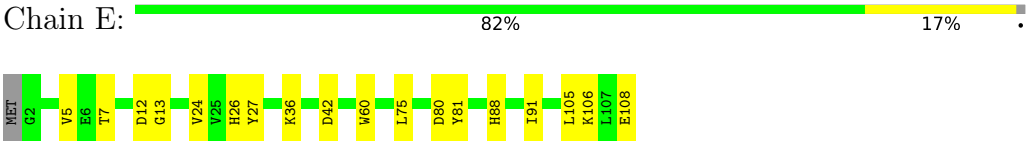
LYS VAL SER GLN ALA ARG THR GLN VAL K3124 G3125 H3147 Y3167 R3168 T3169 E3208 N3212 N3235 S3236 V3237 E3238 E3239 M3240 V3246 L3247 E3248 R3249 E3253 L3257 L3282 W3285 E3291 A3292 P3293 P3294 P3295 A3296 L3297 P3298 A3299 G3300 A3301 T3306 T3309 L3316
Q3344 P3345 I3346 V3347 R3356 I3360 P3361 T3362 L3366 R3369 V3373 E3377 L3380 R3381 L3382 E3383 A3384 K3385 A3386 E3387 A3388 E3389 E3390 G3391 E3392 L3393 R3396 L3406 L3409 Y3410 P3411 L3412 L3413 I3414 R3415 Y3416 V3417 R3421 N3431 L3435 F3443 S3449 H3450 N3451
E3456 Q3457 N3458 F3459 V3460 V3461 Q3462 N3463 E3464 I3465 N3466 N3467 M3468 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 Q3507 T3508 S3509 L3515 K3516 C3526 T3529 L3536
A3537 V3550 R3551 L3554 L3560 V3564 E3565 M3574 G3582 R3583 E3584 E3585 D3586 A3587 D3588 E3591 K3592 I3593 V3594 R3595 R3596 V3597 Q3598 E3599 V3600 S3601 A3602 V3603 H3612 P3613 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL A3635
C3636 F3637 R3638 A3650 C3651 E3683 Q3684 E3685 E3686 E3687 E3688 E3689 E3690 V3691 E3692 E3693 E3737 GLU GLY GLY GLU ASN GLY GLU GLU GLY GLY GLU GLU GLU GLU V3752 E3753 Y3768 S3771 H3774 C3789 L3820 K3824 E3828 S3834 M3861 V3862 N3863 E3864 D3865 G3866 T3867
V3868 I3869 N3870 R3871 Q3872 N3873 G3874 L3894 F3902 T3908 F3936 Y3940 K3943 I3946 E3947 K3951 F3954 M3958 I3972 Q3973 G3974 P3975 L3983 G3994 V3998 K4005 D4009 S4010 S4011 V4048 V4148 S4154 D4160 L4167 L4181 V4225
E4230 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 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 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 GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY 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 D4582 S4583 P4584 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 SER ARG ALA GLY GLU GLU VAL GLU GLY ASP GLU ASP GLU N4624 Y4628 M4637 E4638 P4639 A4640 L4641 V4664 P4665 L4675 A4676 D4693 F4709 P4710 V4718 L4723 I4735 S4745 L4746 E4747 I4748 T4749
A4750 H4751 N4752 E4753 R4754 K4755 P4756 D4757 P4758 P4759 P4760 G4761 L4762 N4803 I4824 S4827 R4858 D4868 Y4886 V4887 R4890 D4897 E4898 P4902 E4908 R4911 V4912 I4916 V4948 D4964 Y4965 L4993 K5010 M5011 D5018 S5035

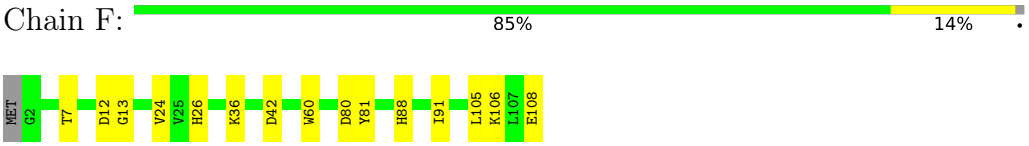
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E:



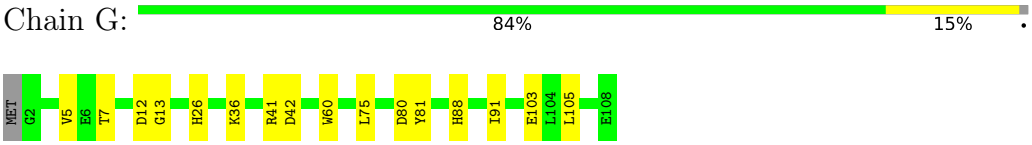
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



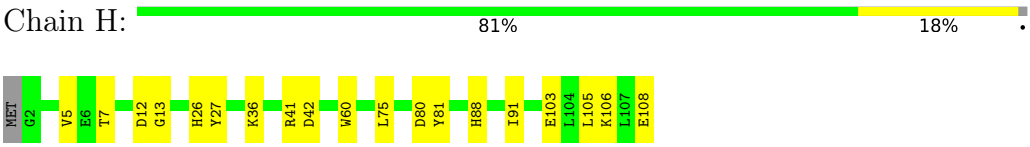
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:



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

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	292757	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	0.700	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	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, CA, CFF, PCW, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.25	0/35586	0.47	0/48203
1	B	0.25	0/35586	0.47	0/48203
1	C	0.25	0/35586	0.47	0/48203
1	D	0.25	0/35586	0.47	0/48203
2	E	0.26	0/847	0.49	0/1142
2	F	0.26	0/847	0.49	0/1142
2	G	0.25	0/847	0.49	0/1142
2	H	0.26	0/847	0.49	0/1142
All	All	0.25	0/145732	0.47	0/197380

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34797	0	34386	318	0
1	B	34797	0	34386	316	0
1	C	34797	0	34386	318	0
1	D	34797	0	34386	312	0
2	E	829	0	826	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	829	0	826	12	0
2	G	829	0	826	12	0
2	H	829	0	826	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	62	0	24	0	0
5	B	62	0	24	0	0
5	C	62	0	24	0	0
5	D	62	0	24	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	108	0	168	3	0
7	B	108	0	168	3	0
7	C	108	0	168	3	0
7	D	108	0	168	3	0
All	All	143248	0	141656	1300	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 5.

All (1300) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:CYS:SG	1:B:757:SER:OG	2.24	0.96
1:A:748:CYS:SG	1:A:757:SER:OG	2.24	0.95
1:C:748:CYS:SG	1:C:757:SER:OG	2.24	0.95
1:D:748:CYS:SG	1:D:757:SER:OG	2.24	0.93
1:D:3248:GLU:OE2	1:D:3249:ARG:NH1	2.10	0.85
1:B:3248:GLU:OE2	1:B:3249:ARG:NH1	2.10	0.84
1:A:3248:GLU:OE2	1:A:3249:ARG:NH1	2.10	0.84
1:C:3456:GLU:OE1	1:C:3509:SER:OG	1.96	0.84
1:C:3248:GLU:OE2	1:C:3249:ARG:NH1	2.10	0.84
1:A:3456:GLU:OE1	1:A:3509:SER:OG	1.96	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3456:GLU:OE1	1:B:3509:SER:OG	1.96	0.84
1:B:3208:GLU:OE2	1:B:3306:THR:OG1	1.97	0.83
1:D:3456:GLU:OE1	1:D:3509:SER:OG	1.96	0.83
1:A:3208:GLU:OE2	1:A:3306:THR:OG1	1.97	0.81
1:D:3208:GLU:OE2	1:D:3306:THR:OG1	1.97	0.81
1:C:3457:GLN:OE1	1:C:3504:TYR:N	2.15	0.80
1:C:3208:GLU:OE2	1:C:3306:THR:OG1	1.97	0.80
1:D:3457:GLN:OE1	1:D:3504:TYR:N	2.15	0.80
1:B:3457:GLN:OE1	1:B:3504:TYR:N	2.15	0.80
1:A:3457:GLN:OE1	1:A:3504:TYR:N	2.15	0.80
1:B:2167:LEU:HD11	1:B:2207:THR:HG23	1.65	0.79
1:C:2167:LEU:HD11	1:C:2207:THR:HG23	1.65	0.79
1:B:2596:LEU:HD21	1:B:2604:ILE:HD12	1.65	0.79
1:C:2596:LEU:HD21	1:C:2604:ILE:HD12	1.65	0.79
1:D:2167:LEU:HD11	1:D:2207:THR:HG23	1.65	0.79
1:A:2167:LEU:HD11	1:A:2207:THR:HG23	1.65	0.78
1:A:2596:LEU:HD21	1:A:2604:ILE:HD12	1.65	0.78
1:D:2596:LEU:HD21	1:D:2604:ILE:HD12	1.65	0.77
1:D:3946:ILE:O	1:D:3951:LYS:NZ	2.19	0.76
1:A:3946:ILE:O	1:A:3951:LYS:NZ	2.19	0.76
1:C:3946:ILE:O	1:C:3951:LYS:NZ	2.19	0.75
1:B:3946:ILE:O	1:B:3951:LYS:NZ	2.19	0.75
1:B:2213:VAL:HG11	1:B:2257:TYR:HE2	1.52	0.74
1:B:3560:LEU:HD23	1:B:3560:LEU:O	1.88	0.74
1:A:1930:MET:CE	1:A:1932:LEU:HD21	2.18	0.74
1:C:3560:LEU:O	1:C:3560:LEU:HD23	1.88	0.74
1:B:1930:MET:CE	1:B:1932:LEU:HD21	2.18	0.74
1:B:3593:ILE:O	1:B:3597:VAL:HG23	1.88	0.74
1:B:2866:VAL:O	1:B:2929:LYS:NZ	2.21	0.73
1:D:2866:VAL:O	1:D:2929:LYS:NZ	2.21	0.73
1:C:3593:ILE:O	1:C:3597:VAL:HG23	1.88	0.73
1:C:1930:MET:CE	1:C:1932:LEU:HD21	2.18	0.73
1:A:2866:VAL:O	1:A:2929:LYS:NZ	2.21	0.73
1:A:3560:LEU:HD23	1:A:3560:LEU:O	1.88	0.73
1:C:2213:VAL:HG11	1:C:2257:TYR:HE2	1.53	0.73
1:D:2645:LEU:HD13	1:D:2679:LEU:HD21	1.71	0.73
1:C:2564:THR:HG22	1:C:2607:CYS:HA	1.71	0.73
1:A:2213:VAL:HG11	1:A:2257:TYR:HE2	1.53	0.73
1:A:2645:LEU:HD13	1:A:2679:LEU:HD21	1.71	0.73
1:D:1930:MET:CE	1:D:1932:LEU:HD21	2.18	0.73
1:A:3593:ILE:O	1:A:3597:VAL:HG23	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2866:VAL:O	1:C:2929:LYS:NZ	2.21	0.72
1:D:3560:LEU:HD23	1:D:3560:LEU:O	1.88	0.72
1:D:3593:ILE:O	1:D:3597:VAL:HG23	1.88	0.72
1:D:2564:THR:HG22	1:D:2607:CYS:HA	1.71	0.72
1:B:2564:THR:HG22	1:B:2607:CYS:HA	1.71	0.72
1:A:2564:THR:HG22	1:A:2607:CYS:HA	1.71	0.72
1:B:2645:LEU:HD13	1:B:2679:LEU:HD21	1.71	0.72
1:D:2949:THR:O	1:D:2954:LYS:NZ	2.22	0.72
1:D:2213:VAL:HG11	1:D:2257:TYR:HE2	1.53	0.71
1:C:2645:LEU:HD13	1:C:2679:LEU:HD21	1.71	0.71
1:D:1930:MET:HE2	1:D:1932:LEU:HD21	1.73	0.71
1:D:3943:LYS:O	1:D:4005:LYS:NZ	2.23	0.71
1:B:2482:LYS:HD2	1:B:2483:ASP:H	1.56	0.71
1:A:2573:THR:HG22	1:A:2573:THR:O	1.91	0.71
1:B:3356:ARG:NH2	1:B:3431:ASN:OD1	2.24	0.70
1:C:2482:LYS:HD2	1:C:2483:ASP:H	1.56	0.70
1:C:2573:THR:HG22	1:C:2573:THR:O	1.91	0.70
1:C:3943:LYS:O	1:C:4005:LYS:NZ	2.23	0.70
1:B:2573:THR:HG22	1:B:2573:THR:O	1.91	0.70
1:C:3356:ARG:NH2	1:C:3431:ASN:OD1	2.24	0.70
1:A:3356:ARG:NH2	1:A:3431:ASN:OD1	2.24	0.70
1:B:3943:LYS:O	1:B:4005:LYS:NZ	2.23	0.70
1:D:3356:ARG:NH2	1:D:3431:ASN:OD1	2.24	0.70
1:A:3943:LYS:O	1:A:4005:LYS:NZ	2.23	0.70
1:D:2573:THR:O	1:D:2573:THR:HG22	1.91	0.69
1:A:2482:LYS:HD2	1:A:2483:ASP:H	1.56	0.69
1:D:2197:ASN:OD1	1:D:2200:ARG:NH2	2.26	0.69
1:D:2482:LYS:HD2	1:D:2483:ASP:H	1.56	0.69
1:A:1930:MET:HE2	1:A:1932:LEU:HD21	1.75	0.69
1:A:2949:THR:O	1:A:2954:LYS:NZ	2.22	0.68
1:D:2828:ARG:NH2	1:D:2932:GLN:O	2.27	0.68
1:A:2828:ARG:NH2	1:A:2932:GLN:O	2.26	0.68
1:B:2828:ARG:NH2	1:B:2932:GLN:O	2.26	0.68
1:C:2828:ARG:NH2	1:C:2932:GLN:O	2.26	0.68
1:A:2197:ASN:OD1	1:A:2200:ARG:NH2	2.26	0.68
1:C:2197:ASN:OD1	1:C:2200:ARG:NH2	2.26	0.68
1:A:157:GLN:OE1	1:A:158:ARG:NH1	2.27	0.68
1:B:2949:THR:O	1:B:2954:LYS:NZ	2.22	0.68
1:C:157:GLN:OE1	1:C:158:ARG:NH1	2.27	0.68
1:D:157:GLN:OE1	1:D:158:ARG:NH1	2.27	0.68
1:B:2197:ASN:OD1	1:B:2200:ARG:NH2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2949:THR:O	1:C:2954:LYS:NZ	2.22	0.67
2:G:26:HIS:ND1	2:G:105:LEU:HD11	2.09	0.67
1:B:157:GLN:OE1	1:B:158:ARG:NH1	2.27	0.67
2:F:26:HIS:ND1	2:F:105:LEU:HD11	2.09	0.66
1:B:73:SER:O	1:B:100:ARG:NH1	2.29	0.66
1:C:2560:LEU:O	1:C:2564:THR:HG23	1.96	0.66
1:D:2560:LEU:O	1:D:2564:THR:HG23	1.96	0.66
1:A:73:SER:O	1:A:100:ARG:NH1	2.29	0.66
1:A:3344:GLN:O	1:A:3347:VAL:HG12	1.96	0.66
1:B:2560:LEU:O	1:B:2564:THR:HG23	1.96	0.66
1:C:3344:GLN:O	1:C:3347:VAL:HG12	1.96	0.66
1:D:73:SER:O	1:D:100:ARG:NH1	2.29	0.66
1:D:3515:LEU:HD11	1:D:3603:VAL:HG13	1.78	0.66
1:C:3515:LEU:HD11	1:C:3603:VAL:HG13	1.78	0.65
1:D:3344:GLN:O	1:D:3347:VAL:HG12	1.96	0.65
1:C:73:SER:O	1:C:100:ARG:NH1	2.29	0.65
2:H:26:HIS:ND1	2:H:105:LEU:HD11	2.10	0.65
1:A:2560:LEU:O	1:A:2564:THR:HG23	1.96	0.65
1:B:3344:GLN:O	1:B:3347:VAL:HG12	1.96	0.65
1:A:2010:LEU:HD22	1:A:2024:LEU:HD13	1.79	0.65
1:C:2010:LEU:HD22	1:C:2024:LEU:HD13	1.79	0.65
1:A:3515:LEU:HD11	1:A:3603:VAL:HG13	1.79	0.65
1:B:3515:LEU:HD11	1:B:3603:VAL:HG13	1.78	0.65
1:D:2010:LEU:HD22	1:D:2024:LEU:HD13	1.79	0.64
1:B:2209:MET:O	1:B:2213:VAL:HG13	1.97	0.64
1:C:2209:MET:O	1:C:2213:VAL:HG13	1.97	0.64
1:A:2209:MET:O	1:A:2213:VAL:HG13	1.97	0.64
1:C:3972:ILE:HG21	1:C:3983:LEU:HD12	1.79	0.64
1:B:2010:LEU:HD22	1:B:2024:LEU:HD13	1.79	0.64
1:D:1043:ALA:O	1:D:1046:THR:OG1	2.15	0.64
1:B:141:ASP:OD1	1:B:143:THR:OG1	2.10	0.64
2:H:36:LYS:NZ	2:H:42:ASP:OD2	2.30	0.64
1:B:3285:TRP:O	1:B:3306:THR:HG21	1.99	0.63
1:A:1236:THR:OG1	1:A:1703:ARG:NH1	2.32	0.63
1:C:1236:THR:OG1	1:C:1703:ARG:NH1	2.32	0.63
1:D:2209:MET:O	1:D:2213:VAL:HG13	1.97	0.63
1:A:3285:TRP:O	1:A:3306:THR:HG21	1.99	0.63
1:B:869:GLU:OE2	1:B:872:ARG:NH2	2.32	0.63
1:D:1236:THR:OG1	1:D:1703:ARG:NH1	2.32	0.63
1:B:3972:ILE:HG21	1:B:3983:LEU:HD12	1.79	0.63
1:D:869:GLU:OE2	1:D:872:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3972:ILE:HG21	1:A:3983:LEU:HD12	1.79	0.63
2:E:26:HIS:CE1	2:E:105:LEU:HD11	2.33	0.63
2:G:88:HIS:ND1	2:G:91:ILE:HD13	2.14	0.63
1:C:869:GLU:OE2	1:C:872:ARG:NH2	2.32	0.63
1:D:3972:ILE:HG21	1:D:3983:LEU:HD12	1.79	0.63
1:A:869:GLU:OE2	1:A:872:ARG:NH2	2.32	0.63
2:H:88:HIS:ND1	2:H:91:ILE:HD13	2.14	0.63
2:E:106:LYS:NZ	2:E:108:GLU:OE1	2.32	0.62
1:B:3366:LEU:HD11	1:B:3409:LEU:HD12	1.81	0.62
1:C:865:PRO:HD2	1:C:868:LEU:HD12	1.82	0.62
1:B:1236:THR:OG1	1:B:1703:ARG:NH1	2.32	0.62
1:C:3285:TRP:O	1:C:3306:THR:HG21	1.99	0.62
1:D:3285:TRP:O	1:D:3306:THR:HG21	1.99	0.62
1:A:582:ASN:OD1	1:A:583:HIS:N	2.33	0.62
1:A:3366:LEU:HD11	1:A:3409:LEU:HD12	1.82	0.62
1:A:4858:ARG:NH1	1:D:4628:TYR:OH	2.32	0.62
2:E:26:HIS:ND1	2:E:105:LEU:HD11	2.14	0.62
1:D:582:ASN:OD1	1:D:583:HIS:N	2.33	0.62
2:F:88:HIS:ND1	2:F:91:ILE:HD13	2.14	0.62
1:B:1043:ALA:O	1:B:1046:THR:OG1	2.15	0.62
1:B:582:ASN:OD1	1:B:583:HIS:N	2.33	0.62
1:B:1930:MET:HE2	1:B:1932:LEU:HD21	1.81	0.62
2:G:36:LYS:NZ	2:G:42:ASP:OD2	2.33	0.61
2:H:80:ASP:OD1	2:H:81:TYR:N	2.33	0.61
1:D:865:PRO:HD2	1:D:868:LEU:HD12	1.82	0.61
1:B:4628:TYR:OH	1:C:4858:ARG:NH1	2.32	0.61
1:B:865:PRO:HD2	1:B:868:LEU:HD12	1.82	0.61
2:F:80:ASP:OD1	2:F:81:TYR:N	2.33	0.61
2:F:106:LYS:NZ	2:F:108:GLU:OE1	2.31	0.61
1:C:4628:TYR:OH	1:D:4858:ARG:NH1	2.33	0.61
1:C:2817:MET:SD	1:C:2879:LEU:HD11	2.41	0.61
1:C:4908:GLU:O	1:C:4912:VAL:HG13	2.01	0.61
2:E:88:HIS:ND1	2:E:91:ILE:HD13	2.15	0.61
1:B:4908:GLU:O	1:B:4912:VAL:HG13	2.01	0.61
1:C:582:ASN:OD1	1:C:583:HIS:N	2.33	0.61
1:D:4824:ILE:O	1:D:4827:SER:OG	2.12	0.61
1:A:2817:MET:SD	1:A:2879:LEU:HD11	2.41	0.61
1:B:2817:MET:SD	1:B:2879:LEU:HD11	2.41	0.61
1:C:3366:LEU:HD11	1:C:3409:LEU:HD12	1.82	0.61
2:G:80:ASP:OD1	2:G:81:TYR:N	2.33	0.61
1:A:865:PRO:HD2	1:A:868:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1422:ARG:O	1:A:1571:LYS:NZ	2.34	0.61
2:F:36:LYS:NZ	2:F:42:ASP:OD2	2.33	0.61
1:D:2817:MET:SD	1:D:2879:LEU:HD11	2.41	0.61
1:C:1422:ARG:O	1:C:1571:LYS:NZ	2.34	0.60
1:D:3366:LEU:HD11	1:D:3409:LEU:HD12	1.81	0.60
1:B:2215:VAL:HG11	1:B:2229:MET:CE	2.32	0.60
1:D:1422:ARG:O	1:D:1571:LYS:NZ	2.34	0.60
1:D:2215:VAL:HG11	1:D:2229:MET:CE	2.32	0.60
1:C:1930:MET:HE2	1:C:1932:LEU:HD21	1.82	0.60
2:E:80:ASP:OD1	2:E:81:TYR:N	2.33	0.60
1:B:4009:ASP:OD2	1:B:4011:SER:OG	2.20	0.60
1:B:1422:ARG:O	1:B:1571:LYS:NZ	2.34	0.60
1:C:2215:VAL:HG11	1:C:2229:MET:CE	2.32	0.60
1:A:3347:VAL:HG11	1:A:3415:ARG:HB2	1.84	0.60
1:C:4824:ILE:O	1:C:4827:SER:OG	2.12	0.60
1:D:4009:ASP:OD2	1:D:4011:SER:OG	2.19	0.60
1:B:2741:VAL:HG21	1:B:2820:TRP:NE1	2.17	0.60
1:B:4675:LEU:HD23	1:B:4709:PHE:HE1	1.67	0.60
1:C:1043:ALA:O	1:C:1046:THR:OG1	2.15	0.60
1:A:2215:VAL:HG11	1:A:2229:MET:CE	2.32	0.60
1:A:2753:ASP:HA	1:A:2756:ILE:HD12	1.84	0.60
1:C:887:ARG:NH2	1:C:890:GLN:OE1	2.35	0.60
1:C:2753:ASP:HA	1:C:2756:ILE:HD12	1.84	0.60
1:A:4628:TYR:OH	1:B:4858:ARG:NH1	2.35	0.60
1:A:4675:LEU:HD23	1:A:4709:PHE:HE1	1.67	0.60
1:D:1449:VAL:HG22	1:D:1555:VAL:HG23	1.84	0.60
1:D:4908:GLU:O	1:D:4912:VAL:HG13	2.01	0.60
1:B:3865:ASP:OD2	1:B:3870:ASN:ND2	2.36	0.59
1:D:2741:VAL:HG21	1:D:2820:TRP:NE1	2.17	0.59
1:B:3347:VAL:HG11	1:B:3415:ARG:HB2	1.84	0.59
1:C:4009:ASP:OD2	1:C:4011:SER:OG	2.19	0.59
1:A:887:ARG:NH2	1:A:890:GLN:OE1	2.35	0.59
1:A:1043:ALA:O	1:A:1046:THR:OG1	2.15	0.59
2:H:106:LYS:NZ	2:H:108:GLU:OE1	2.34	0.59
1:C:905:HIS:HB3	1:C:908:LEU:HD12	1.85	0.59
1:C:2741:VAL:HG21	1:C:2820:TRP:HE1	1.67	0.59
1:B:2753:ASP:HA	1:B:2756:ILE:HD12	1.84	0.59
1:C:2756:ILE:HD13	1:C:2811:LYS:HG2	1.85	0.59
1:D:2753:ASP:HA	1:D:2756:ILE:HD12	1.84	0.59
1:D:3347:VAL:HG11	1:D:3415:ARG:HB2	1.84	0.59
1:A:2741:VAL:HG21	1:A:2820:TRP:HE1	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4908:GLU:O	1:A:4912:VAL:HG13	2.01	0.59
1:C:1449:VAL:HG22	1:C:1555:VAL:HG23	1.84	0.59
1:C:3347:VAL:HG11	1:C:3415:ARG:HB2	1.84	0.59
1:C:245:LEU:HD22	1:C:376:LYS:NZ	2.18	0.59
1:D:887:ARG:NH2	1:D:890:GLN:OE1	2.35	0.59
1:D:2293:GLU:O	1:D:2297:GLU:HG3	2.03	0.59
1:A:2741:VAL:HG21	1:A:2820:TRP:NE1	2.17	0.59
1:C:2293:GLU:O	1:C:2297:GLU:HG3	2.03	0.59
1:B:245:LEU:HD22	1:B:376:LYS:NZ	2.18	0.59
1:A:2293:GLU:O	1:A:2297:GLU:HG3	2.03	0.59
1:A:2453:ARG:NH2	1:B:145:GLU:OE1	2.34	0.59
1:A:4009:ASP:OD2	1:A:4011:SER:OG	2.19	0.59
1:A:245:LEU:HD22	1:A:376:LYS:NZ	2.18	0.58
1:A:3865:ASP:OD2	1:A:3870:ASN:ND2	2.36	0.58
1:B:905:HIS:HB3	1:B:908:LEU:HD12	1.85	0.58
1:B:2741:VAL:HG21	1:B:2820:TRP:HE1	1.67	0.58
1:B:2756:ILE:HD13	1:B:2811:LYS:HG2	1.85	0.58
1:C:249:GLU:HB3	1:C:253:VAL:HG11	1.85	0.58
1:C:4675:LEU:HD23	1:C:4709:PHE:HE1	1.67	0.58
1:D:4675:LEU:HD23	1:D:4709:PHE:HE1	1.67	0.58
1:A:905:HIS:HB3	1:A:908:LEU:HD12	1.85	0.58
1:B:2293:GLU:O	1:B:2297:GLU:HG3	2.03	0.58
1:A:249:GLU:HB3	1:A:253:VAL:HG11	1.85	0.58
1:A:1449:VAL:HG22	1:A:1555:VAL:HG23	1.84	0.58
1:B:2453:ARG:NH2	1:C:145:GLU:OE1	2.37	0.58
1:C:2741:VAL:HG21	1:C:2820:TRP:NE1	2.17	0.58
1:A:829:GLU:OE2	1:A:832:ARG:NH1	2.37	0.58
1:B:829:GLU:OE2	1:B:832:ARG:NH1	2.37	0.58
1:C:1421:ASN:O	1:C:1421:ASN:ND2	2.36	0.58
1:C:3865:ASP:OD2	1:C:3870:ASN:ND2	2.36	0.58
1:A:2756:ILE:HD13	1:A:2811:LYS:HG2	1.85	0.58
1:D:829:GLU:OE2	1:D:832:ARG:NH1	2.37	0.58
1:D:1421:ASN:ND2	1:D:1421:ASN:O	2.36	0.58
1:D:3865:ASP:OD2	1:D:3870:ASN:ND2	2.36	0.58
1:A:1421:ASN:O	1:A:1421:ASN:ND2	2.36	0.58
1:B:887:ARG:NH2	1:B:890:GLN:OE1	2.35	0.58
1:D:249:GLU:HB3	1:D:253:VAL:HG11	1.85	0.58
1:C:829:GLU:OE2	1:C:832:ARG:NH1	2.37	0.58
1:D:905:HIS:HB3	1:D:908:LEU:HD12	1.85	0.58
1:D:2756:ILE:HD13	1:D:2811:LYS:HG2	1.85	0.58
1:D:245:LEU:HD22	1:D:376:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1421:ASN:ND2	1:B:1421:ASN:O	2.36	0.58
1:B:249:GLU:HB3	1:B:253:VAL:HG11	1.85	0.57
1:B:1449:VAL:HG22	1:B:1555:VAL:HG23	1.84	0.57
1:B:3082:MET:CE	1:B:3093:LEU:HD23	2.35	0.57
1:D:2741:VAL:HG21	1:D:2820:TRP:HE1	1.67	0.57
1:A:3235:ASN:OD1	1:A:3236:SER:N	2.37	0.57
1:B:1932:LEU:HD22	1:B:1936:VAL:HG11	1.87	0.57
1:B:2792:LEU:O	1:B:2792:LEU:HD23	2.05	0.57
1:D:2749:PRO:HD2	1:D:2752:LEU:HD12	1.87	0.57
1:A:145:GLU:OE1	1:D:2453:ARG:NH2	2.36	0.57
1:A:3551:ARG:NH1	1:A:3598:GLN:OE1	2.38	0.57
1:C:3082:MET:CE	1:C:3093:LEU:HD23	2.35	0.57
1:C:3235:ASN:OD1	1:C:3236:SER:N	2.37	0.57
1:D:103:LEU:HD23	1:D:163:LYS:HA	1.87	0.57
1:D:1932:LEU:HD22	1:D:1936:VAL:HG11	1.86	0.57
1:A:103:LEU:HD23	1:A:163:LYS:HA	1.87	0.57
1:B:4890:ARG:NH1	1:C:4897:ASP:OD1	2.38	0.57
1:A:2749:PRO:HD2	1:A:2752:LEU:HD12	1.87	0.57
1:A:3972:ILE:CG2	1:A:3983:LEU:HD12	2.35	0.57
1:D:3235:ASN:OD1	1:D:3236:SER:N	2.37	0.57
1:B:3235:ASN:OD1	1:B:3236:SER:N	2.37	0.57
1:D:2792:LEU:HD23	1:D:2792:LEU:O	2.05	0.57
1:C:2792:LEU:HD23	1:C:2792:LEU:O	2.05	0.56
1:A:2523:LEU:HD21	1:A:2583:MET:SD	2.45	0.56
1:A:4676:ALA:HB1	1:A:4718:VAL:HG21	1.87	0.56
1:A:4897:ASP:OD1	1:D:4890:ARG:NH1	2.39	0.56
1:C:103:LEU:HD23	1:C:163:LYS:HA	1.87	0.56
1:C:649:ILE:HG23	1:C:815:ALA:HB3	1.87	0.56
1:C:2523:LEU:HD21	1:C:2583:MET:SD	2.45	0.56
1:C:3551:ARG:NH1	1:C:3598:GLN:OE1	2.38	0.56
1:D:141:ASP:OD1	1:D:143:THR:OG1	2.10	0.56
1:A:2792:LEU:HD23	1:A:2792:LEU:O	2.05	0.56
1:A:3082:MET:CE	1:A:3093:LEU:HD23	2.35	0.56
1:B:3551:ARG:NH1	1:B:3598:GLN:OE1	2.38	0.56
1:B:3396:ARG:NH2	1:B:3451:ASN:OD1	2.39	0.56
1:C:3972:ILE:CG2	1:C:3983:LEU:HD12	2.35	0.56
1:D:2523:LEU:HD21	1:D:2583:MET:SD	2.45	0.56
1:D:3551:ARG:NH1	1:D:3598:GLN:OE1	2.38	0.56
1:C:2453:ARG:NH2	1:D:145:GLU:OE1	2.37	0.56
1:D:4676:ALA:HB1	1:D:4718:VAL:HG21	1.87	0.56
1:B:103:LEU:HD23	1:B:163:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1562:VAL:HG12	1:C:1563:VAL:HG13	1.88	0.56
1:C:1932:LEU:HD22	1:C:1936:VAL:HG11	1.86	0.56
1:C:2749:PRO:HD2	1:C:2752:LEU:HD12	1.87	0.56
1:D:3082:MET:CE	1:D:3093:LEU:HD23	2.35	0.56
1:D:3396:ARG:NH2	1:D:3451:ASN:OD1	2.39	0.56
1:D:3972:ILE:CG2	1:D:3983:LEU:HD12	2.35	0.56
1:A:2820:TRP:CZ2	1:A:2882:ASN:ND2	2.74	0.56
1:B:649:ILE:HG23	1:B:815:ALA:HB3	1.87	0.56
1:C:4890:ARG:NH1	1:D:4897:ASP:OD1	2.39	0.56
1:D:2820:TRP:CZ2	1:D:2882:ASN:ND2	2.74	0.56
1:A:1967:VAL:HG21	1:A:3650:ALA:HB1	1.88	0.56
1:B:3236:SER:OG	1:B:3238:GLU:OE1	2.24	0.56
1:C:233:THR:HG21	1:C:253:VAL:HG21	1.88	0.56
1:A:233:THR:HG21	1:A:253:VAL:HG21	1.88	0.56
1:A:649:ILE:HG23	1:A:815:ALA:HB3	1.87	0.56
1:B:2749:PRO:HD2	1:B:2752:LEU:HD12	1.87	0.56
1:B:2820:TRP:CZ2	1:B:2882:ASN:ND2	2.74	0.56
1:B:3972:ILE:CG2	1:B:3983:LEU:HD12	2.35	0.56
1:C:4676:ALA:HB1	1:C:4718:VAL:HG21	1.87	0.56
1:B:2523:LEU:HD21	1:B:2583:MET:SD	2.45	0.55
1:C:2820:TRP:CZ2	1:C:2882:ASN:ND2	2.74	0.55
1:D:649:ILE:HG23	1:D:815:ALA:HB3	1.87	0.55
1:D:3529:THR:HG23	1:D:3574:MET:CE	2.36	0.55
1:A:3529:THR:HG23	1:A:3574:MET:CE	2.36	0.55
1:B:1967:VAL:HG21	1:B:3650:ALA:HB1	1.88	0.55
1:C:1967:VAL:HG21	1:C:3650:ALA:HB1	1.88	0.55
1:C:3396:ARG:NH2	1:C:3451:ASN:OD1	2.39	0.55
1:A:1932:LEU:HD22	1:A:1936:VAL:HG11	1.86	0.55
1:A:3236:SER:OG	1:A:3238:GLU:OE1	2.24	0.55
1:A:3377:GLU:OE1	1:A:3449:SER:OG	2.20	0.55
1:A:3396:ARG:NH2	1:A:3451:ASN:OD1	2.39	0.55
1:B:130:ASP:OD2	1:B:133:ALA:N	2.40	0.55
1:B:4676:ALA:HB1	1:B:4718:VAL:HG21	1.87	0.55
1:B:4745:SER:HA	1:B:4748:ILE:HG22	1.89	0.55
1:D:1773:LEU:HD11	1:D:2145:ILE:HD11	1.89	0.55
1:A:4745:SER:HA	1:A:4748:ILE:HG22	1.88	0.55
1:C:3529:THR:HG23	1:C:3574:MET:HE3	1.88	0.55
1:A:1773:LEU:HD11	1:A:2145:ILE:HD11	1.89	0.55
1:B:3529:THR:HG23	1:B:3574:MET:CE	2.36	0.55
1:C:130:ASP:OD2	1:C:133:ALA:N	2.40	0.55
1:D:2820:TRP:HZ3	1:D:2879:LEU:HD22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3282:LEU:HD12	1:A:3316:LEU:HD22	1.89	0.55
1:C:2987:VAL:HG12	1:C:2989:LYS:H	1.72	0.55
1:D:1967:VAL:HG21	1:D:3650:ALA:HB1	1.88	0.55
1:C:3236:SER:OG	1:C:3238:GLU:OE1	2.24	0.55
1:C:4964:ASP:OD1	1:C:4965:TYR:N	2.40	0.55
1:D:2987:VAL:HG12	1:D:2989:LYS:H	1.72	0.55
1:D:3236:SER:OG	1:D:3238:GLU:OE1	2.24	0.55
1:D:4745:SER:HA	1:D:4748:ILE:HG22	1.88	0.55
1:A:130:ASP:OD2	1:A:133:ALA:N	2.40	0.54
1:A:2987:VAL:HG12	1:A:2989:LYS:H	1.72	0.54
1:B:1562:VAL:HG12	1:B:1563:VAL:HG13	1.88	0.54
1:D:130:ASP:OD2	1:D:133:ALA:N	2.40	0.54
1:D:1562:VAL:HG12	1:D:1563:VAL:HG13	1.88	0.54
1:D:3282:LEU:HD12	1:D:3316:LEU:HD22	1.89	0.54
2:E:12:ASP:OD1	2:E:13:GLY:N	2.40	0.54
1:D:2875:MET:O	1:D:2879:LEU:HD23	2.08	0.54
1:A:2971:SER:HA	1:A:2974:PHE:CE1	2.43	0.54
2:E:7:THR:HG23	2:E:7:THR:O	2.08	0.54
2:F:12:ASP:OD1	2:F:13:GLY:N	2.40	0.54
1:B:2820:TRP:HZ3	1:B:2879:LEU:HD22	1.72	0.54
1:C:3282:LEU:HD12	1:C:3316:LEU:HD22	1.89	0.54
1:C:3529:THR:HG23	1:C:3574:MET:CE	2.37	0.54
1:D:233:THR:HG21	1:D:253:VAL:HG21	1.88	0.54
1:D:4964:ASP:OD1	1:D:4965:TYR:N	2.40	0.54
1:A:3661:SER:O	1:A:3665:THR:OG1	2.16	0.54
1:A:4890:ARG:NH1	1:B:4897:ASP:OD1	2.40	0.54
1:B:233:THR:HG21	1:B:253:VAL:HG21	1.88	0.54
1:C:1930:MET:HE3	1:C:1932:LEU:HD21	1.88	0.54
1:A:1562:VAL:HG12	1:A:1563:VAL:HG13	1.88	0.54
2:G:12:ASP:OD1	2:G:13:GLY:N	2.40	0.54
2:H:12:ASP:OD1	2:H:13:GLY:N	2.40	0.54
1:B:2987:VAL:HG12	1:B:2989:LYS:H	1.72	0.54
1:B:3282:LEU:HD12	1:B:3316:LEU:HD22	1.89	0.54
1:C:2096:GLN:HA	1:C:2128:GLN:HE21	1.72	0.54
1:A:2096:GLN:HA	1:A:2128:GLN:HE21	1.72	0.54
1:B:2096:GLN:HA	1:B:2128:GLN:HE21	1.72	0.54
1:A:2820:TRP:HZ3	1:A:2879:LEU:HD22	1.72	0.54
1:C:1773:LEU:HD11	1:C:2145:ILE:HD11	1.89	0.54
1:C:2820:TRP:HZ3	1:C:2879:LEU:HD22	1.72	0.54
1:A:2875:MET:O	1:A:2879:LEU:HD23	2.08	0.54
1:B:1558:THR:HG22	1:B:1558:THR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1700:GLU:OE2	1:C:1815:ARG:NH2	2.41	0.54
1:D:2755:PHE:CD2	1:D:2814:LEU:HD11	2.43	0.54
1:A:1994:ARG:NH2	1:A:2020:GLU:OE1	2.41	0.54
1:B:1793:ALA:O	1:B:1794:THR:OG1	2.24	0.54
1:C:3377:GLU:OE1	1:C:3449:SER:OG	2.20	0.54
1:D:2096:GLN:HA	1:D:2128:GLN:HE21	1.72	0.54
1:A:412:TYR:HB2	1:A:487:LEU:HD21	1.90	0.54
1:B:552:LEU:HB3	1:B:590:LEU:HD11	1.90	0.54
1:B:4964:ASP:OD1	1:B:4965:TYR:N	2.40	0.54
1:C:1994:ARG:NH2	1:C:2020:GLU:OE1	2.41	0.54
1:B:1773:LEU:HD11	1:B:2145:ILE:HD11	1.89	0.53
1:C:1558:THR:HG22	1:C:1558:THR:O	2.08	0.53
1:C:2875:MET:O	1:C:2879:LEU:HD23	2.08	0.53
1:C:4745:SER:HA	1:C:4748:ILE:HG22	1.88	0.53
1:D:1700:GLU:OE2	1:D:1815:ARG:NH2	2.41	0.53
1:A:552:LEU:HB3	1:A:590:LEU:HD11	1.90	0.53
1:A:1558:THR:O	1:A:1558:THR:HG22	2.08	0.53
1:A:4964:ASP:OD1	1:A:4965:TYR:N	2.40	0.53
1:C:2971:SER:HA	1:C:2974:PHE:CE1	2.43	0.53
1:D:1994:ARG:NH2	1:D:2020:GLU:OE1	2.41	0.53
1:D:2824:VAL:HG22	1:D:2938:VAL:HG22	1.91	0.53
1:D:2971:SER:HA	1:D:2974:PHE:CE1	2.43	0.53
1:B:2822:TRP:CZ3	1:B:2875:MET:HG3	2.44	0.53
1:B:2971:SER:HA	1:B:2974:PHE:CE1	2.43	0.53
1:C:2755:PHE:CD2	1:C:2814:LEU:HD11	2.43	0.53
1:C:2822:TRP:CZ3	1:C:2875:MET:HG3	2.44	0.53
1:C:3661:SER:O	1:C:3665:THR:OG1	2.16	0.53
1:A:2755:PHE:CD2	1:A:2814:LEU:HD11	2.43	0.53
1:D:412:TYR:HB2	1:D:487:LEU:HD21	1.90	0.53
1:D:2266:LEU:O	1:D:2269:GLN:NE2	2.41	0.53
1:B:2875:MET:O	1:B:2879:LEU:HD23	2.08	0.53
1:A:4902:PRO:HB3	1:A:4911:ARG:HG2	1.90	0.53
1:C:1793:ALA:O	1:C:1794:THR:OG1	2.24	0.53
1:D:4154:SER:HB2	1:D:4167:LEU:HD11	1.91	0.53
1:A:249:GLU:OE1	1:A:258:ARG:NH2	2.42	0.53
1:A:2824:VAL:HG22	1:A:2938:VAL:HG22	1.91	0.53
1:B:1994:ARG:NH2	1:B:2020:GLU:OE1	2.41	0.53
1:C:552:LEU:HB3	1:C:590:LEU:HD11	1.90	0.53
1:C:2824:VAL:HG22	1:C:2938:VAL:HG22	1.91	0.53
1:A:4154:SER:HB2	1:A:4167:LEU:HD11	1.91	0.53
2:F:7:THR:HG23	2:F:7:THR:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:OE1	1:B:258:ARG:NH2	2.42	0.53
1:A:4887:VAL:HG12	1:A:4898:GLU:HG3	1.91	0.53
1:B:2755:PHE:CD2	1:B:2814:LEU:HD11	2.43	0.53
1:B:4902:PRO:HB3	1:B:4911:ARG:HG2	1.90	0.53
1:C:249:GLU:OE1	1:C:258:ARG:NH2	2.42	0.53
1:D:1558:THR:O	1:D:1558:THR:HG22	2.08	0.53
1:D:4902:PRO:HB3	1:D:4911:ARG:HG2	1.90	0.53
1:A:4675:LEU:HD23	1:A:4709:PHE:CE1	2.45	0.52
1:B:1761:ARG:NH2	1:B:2093:GLN:O	2.41	0.52
1:C:979:THR:O	1:C:983:THR:HG23	2.09	0.52
1:D:2822:TRP:CZ3	1:D:2875:MET:HG3	2.44	0.52
1:C:4154:SER:HB2	1:C:4167:LEU:HD11	1.91	0.52
1:B:412:TYR:HB2	1:B:487:LEU:HD21	1.90	0.52
1:B:4154:SER:HB2	1:B:4167:LEU:HD11	1.91	0.52
1:B:4887:VAL:HG12	1:B:4898:GLU:HG3	1.91	0.52
1:D:249:GLU:OE1	1:D:258:ARG:NH2	2.42	0.52
1:D:552:LEU:HB3	1:D:590:LEU:HD11	1.90	0.52
1:A:2822:TRP:CZ3	1:A:2875:MET:HG3	2.43	0.52
1:B:3082:MET:HE2	1:B:3093:LEU:HD23	1.92	0.52
1:C:4902:PRO:HB3	1:C:4911:ARG:HG2	1.90	0.52
1:D:1761:ARG:NH2	1:D:2093:GLN:O	2.41	0.52
1:B:2739:ARG:O	1:B:2885:ASN:ND2	2.43	0.52
1:B:2824:VAL:HG22	1:B:2938:VAL:HG22	1.91	0.52
1:D:4675:LEU:HD23	1:D:4709:PHE:CE1	2.45	0.52
1:A:1685:ALA:HA	2:E:91:ILE:HD11	1.90	0.52
1:B:979:THR:O	1:B:983:THR:HG23	2.09	0.52
1:B:2266:LEU:O	1:B:2269:GLN:NE2	2.41	0.52
1:B:3377:GLU:OE1	1:B:3449:SER:OG	2.20	0.52
1:C:412:TYR:HB2	1:C:487:LEU:HD21	1.90	0.52
1:C:4675:LEU:HD23	1:C:4709:PHE:CE1	2.45	0.52
1:D:4887:VAL:HG12	1:D:4898:GLU:HG3	1.91	0.52
1:D:3212:ASN:ND2	1:D:3237:VAL:HG21	2.25	0.52
2:G:7:THR:HG23	2:G:7:THR:O	2.09	0.52
1:C:4887:VAL:HG12	1:C:4898:GLU:HG3	1.91	0.52
1:D:979:THR:O	1:D:983:THR:HG23	2.09	0.52
1:A:1700:GLU:OE2	1:A:1815:ARG:NH2	2.41	0.52
1:C:2739:ARG:O	1:C:2885:ASN:ND2	2.43	0.52
1:D:3347:VAL:HG11	1:D:3415:ARG:CB	2.41	0.52
1:A:2266:LEU:O	1:A:2269:GLN:NE2	2.41	0.51
2:H:7:THR:HG23	2:H:7:THR:O	2.09	0.51
1:C:3347:VAL:HG11	1:C:3415:ARG:CB	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1930:MET:HE3	1:B:1932:LEU:HD21	1.90	0.51
1:C:1761:ARG:NH2	1:C:2093:GLN:O	2.41	0.51
1:D:3828:GLU:OE1	1:D:3828:GLU:N	2.38	0.51
1:A:3347:VAL:HG11	1:A:3415:ARG:CB	2.41	0.51
1:B:3347:VAL:HG11	1:B:3415:ARG:CB	2.41	0.51
1:B:4675:LEU:HD23	1:B:4709:PHE:CE1	2.44	0.51
1:C:141:ASP:OD1	1:C:143:THR:OG1	2.10	0.51
1:B:932:THR:O	1:B:936:LEU:HD23	2.10	0.51
1:B:3212:ASN:ND2	1:B:3237:VAL:HG21	2.25	0.51
1:A:70:LEU:HD21	1:A:203:MET:CE	2.41	0.51
1:A:932:THR:O	1:A:936:LEU:HD23	2.10	0.51
1:C:70:LEU:HD21	1:C:203:MET:CE	2.41	0.51
1:D:2739:ARG:O	1:D:2885:ASN:ND2	2.43	0.51
1:A:2739:ARG:O	1:A:2885:ASN:ND2	2.43	0.51
1:A:3529:THR:HG23	1:A:3574:MET:HE3	1.93	0.51
1:B:70:LEU:HD21	1:B:203:MET:CE	2.41	0.51
1:B:3104:ILE:HD13	1:B:3169:THR:HG23	1.93	0.51
1:C:3212:ASN:ND2	1:C:3237:VAL:HG21	2.25	0.51
1:D:2795:TYR:HA	1:D:2798:PHE:HB2	1.93	0.51
1:D:3104:ILE:HD13	1:D:3169:THR:HG23	1.93	0.51
1:A:3212:ASN:ND2	1:A:3237:VAL:HG21	2.25	0.51
1:B:3392:GLU:OE2	1:B:3396:ARG:NH2	2.44	0.51
1:C:297:ASP:OD1	1:C:298:GLN:N	2.44	0.51
1:D:3529:THR:HG23	1:D:3574:MET:HE3	1.91	0.51
1:A:979:THR:O	1:A:983:THR:HG23	2.09	0.51
1:C:3828:GLU:OE1	1:C:3828:GLU:N	2.38	0.51
1:A:3104:ILE:HD13	1:A:3169:THR:HG23	1.93	0.51
1:C:3104:ILE:HD13	1:C:3169:THR:HG23	1.93	0.51
1:C:3392:GLU:OE2	1:C:3396:ARG:NH2	2.44	0.51
1:A:554:ARG:NE	1:A:556:GLU:OE2	2.41	0.50
1:C:1481:GLN:HG2	1:C:1481:GLN:O	2.11	0.50
1:C:596:ARG:NH1	1:C:1644:GLU:OE2	2.44	0.50
1:C:932:THR:O	1:C:936:LEU:HD23	2.10	0.50
1:C:2266:LEU:O	1:C:2269:GLN:NE2	2.41	0.50
1:C:4225:VAL:HG11	1:C:4948:VAL:HA	1.94	0.50
1:A:2795:TYR:HA	1:A:2798:PHE:HB2	1.93	0.50
1:B:2795:TYR:HA	1:B:2798:PHE:HB2	1.93	0.50
1:C:2795:TYR:HA	1:C:2798:PHE:HB2	1.93	0.50
1:D:70:LEU:HD21	1:D:203:MET:CE	2.41	0.50
1:D:932:THR:O	1:D:936:LEU:HD23	2.10	0.50
1:A:1252:GLU:OE1	1:A:1252:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4824:ILE:O	1:A:4827:SER:OG	2.12	0.50
1:C:253:VAL:HG23	1:C:258:ARG:HG3	1.94	0.50
1:D:1273:LEU:HD22	1:D:1290:LEU:HD11	1.93	0.50
1:A:297:ASP:OD1	1:A:298:GLN:N	2.44	0.50
1:B:297:ASP:OD1	1:B:298:GLN:N	2.44	0.50
1:B:3529:THR:HG23	1:B:3574:MET:HE3	1.93	0.50
1:C:3082:MET:HE2	1:C:3093:LEU:HD23	1.94	0.50
1:D:253:VAL:HG23	1:D:258:ARG:HG3	1.94	0.50
1:A:3392:GLU:OE2	1:A:3396:ARG:NH2	2.44	0.50
2:E:5:VAL:HG22	2:E:75:LEU:CD2	2.42	0.50
1:D:1481:GLN:O	1:D:1481:GLN:HG2	2.11	0.50
1:D:3377:GLU:OE1	1:D:3449:SER:OG	2.20	0.50
1:A:1273:LEU:HD22	1:A:1290:LEU:HD11	1.93	0.50
1:B:1481:GLN:O	1:B:1481:GLN:HG2	2.12	0.50
1:B:4824:ILE:O	1:B:4827:SER:OG	2.12	0.50
1:D:1252:GLU:N	1:D:1252:GLU:OE1	2.45	0.50
1:D:3291:GLU:OE1	1:D:3309:THR:OG1	2.29	0.50
1:A:3291:GLU:OE1	1:A:3309:THR:OG1	2.29	0.50
1:B:253:VAL:HG23	1:B:258:ARG:HG3	1.94	0.50
1:B:1700:GLU:OE2	1:B:1815:ARG:NH2	2.41	0.50
1:B:4225:VAL:HG11	1:B:4948:VAL:HA	1.94	0.50
1:D:297:ASP:OD1	1:D:298:GLN:N	2.44	0.50
1:D:4637:MET:O	1:D:4641:LEU:N	2.41	0.50
1:C:1252:GLU:OE1	1:C:1252:GLU:N	2.45	0.50
1:C:1273:LEU:HD22	1:C:1290:LEU:HD11	1.93	0.50
1:A:253:VAL:HG23	1:A:258:ARG:HG3	1.94	0.49
1:A:2176:GLU:HG3	1:A:2229:MET:HB2	1.94	0.49
1:A:4225:VAL:HG11	1:A:4948:VAL:HA	1.94	0.49
1:B:1252:GLU:N	1:B:1252:GLU:OE1	2.45	0.49
1:B:1273:LEU:HD22	1:B:1290:LEU:HD11	1.93	0.49
1:B:1737:VAL:HG13	1:B:1737:VAL:O	2.12	0.49
1:C:2176:GLU:HG3	1:C:2229:MET:HB2	1.94	0.49
1:C:3291:GLU:OE1	1:C:3309:THR:OG1	2.29	0.49
1:C:3683:GLU:O	1:C:3687:GLU:OE1	2.30	0.49
2:G:5:VAL:HG22	2:G:75:LEU:CD2	2.42	0.49
2:H:5:VAL:HG22	2:H:75:LEU:CD2	2.42	0.49
1:B:1758:GLY:N	1:B:1759:PRO:CD	2.75	0.49
1:B:3291:GLU:OE1	1:B:3309:THR:OG1	2.29	0.49
1:B:3683:GLU:O	1:B:3687:GLU:OE1	2.30	0.49
1:D:2757:ASN:O	1:D:2761:GLU:OE1	2.31	0.49
1:D:3392:GLU:OE2	1:D:3396:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3686:GLU:N	1:B:3686:GLU:OE1	2.46	0.49
1:D:4582:ASP:OD1	1:D:4583:SER:N	2.45	0.49
1:A:1737:VAL:O	1:A:1737:VAL:HG13	2.12	0.49
1:A:1758:GLY:N	1:A:1759:PRO:CD	2.75	0.49
1:A:2757:ASN:O	1:A:2761:GLU:OE1	2.31	0.49
1:B:596:ARG:NH1	1:B:1644:GLU:OE2	2.44	0.49
1:B:1788:LEU:HD12	1:B:1789:PRO:HD2	1.94	0.49
1:B:4582:ASP:OD1	1:B:4583:SER:N	2.45	0.49
1:C:1758:GLY:N	1:C:1759:PRO:CD	2.75	0.49
1:C:1788:LEU:HD12	1:C:1789:PRO:HD2	1.94	0.49
1:D:2176:GLU:HG3	1:D:2229:MET:HB2	1.95	0.49
1:B:2176:GLU:HG3	1:B:2229:MET:HB2	1.94	0.49
1:C:1737:VAL:HG13	1:C:1737:VAL:O	2.12	0.49
1:C:4582:ASP:OD1	1:C:4583:SER:N	2.45	0.49
1:A:1481:GLN:O	1:A:1481:GLN:HG2	2.11	0.49
1:B:4709:PHE:HB3	1:B:4710:PRO:HD3	1.95	0.49
1:D:3366:LEU:HD11	1:D:3409:LEU:CD1	2.42	0.49
1:D:4048:VAL:HG11	1:D:4160:ASP:OD2	2.13	0.49
1:D:596:ARG:NH1	1:D:1644:GLU:OE2	2.44	0.49
1:D:3686:GLU:N	1:D:3686:GLU:OE1	2.46	0.49
1:A:596:ARG:NH1	1:A:1644:GLU:OE2	2.44	0.49
1:A:2799:SER:O	1:A:2802:ASP:OD1	2.31	0.49
1:A:3366:LEU:HD11	1:A:3409:LEU:CD1	2.42	0.49
1:A:4637:MET:O	1:A:4641:LEU:N	2.41	0.49
1:B:554:ARG:NE	1:B:556:GLU:OE2	2.41	0.49
1:B:2799:SER:O	1:B:2802:ASP:OD1	2.31	0.49
1:C:3366:LEU:HD11	1:C:3409:LEU:CD1	2.42	0.49
1:C:4709:PHE:HB3	1:C:4710:PRO:HD3	1.95	0.49
1:D:1737:VAL:HG13	1:D:1737:VAL:O	2.12	0.49
1:D:1758:GLY:N	1:D:1759:PRO:CD	2.75	0.49
1:A:3212:ASN:HD22	1:A:3237:VAL:HG21	1.78	0.49
1:C:2799:SER:O	1:C:2802:ASP:OD1	2.31	0.49
1:D:2799:SER:O	1:D:2802:ASP:OD1	2.31	0.49
1:C:2752:LEU:HB3	1:C:2814:LEU:HD13	1.94	0.49
1:D:2949:THR:HG23	1:D:2950:SER:H	1.78	0.49
1:A:3082:MET:HE1	1:A:3093:LEU:HD23	1.95	0.48
1:B:3212:ASN:HD22	1:B:3237:VAL:HG21	1.78	0.48
1:B:3366:LEU:HD11	1:B:3409:LEU:CD1	2.42	0.48
1:C:3686:GLU:OE1	1:C:3686:GLU:N	2.46	0.48
1:C:4048:VAL:HG11	1:C:4160:ASP:OD2	2.13	0.48
1:D:1788:LEU:HD12	1:D:1789:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2949:THR:HG23	1:D:2950:SER:N	2.28	0.48
7:A:8007:PCW:H232	7:A:8007:PCW:H20	1.72	0.48
1:B:4048:VAL:HG11	1:B:4160:ASP:OD2	2.13	0.48
1:C:1424:ASP:O	1:C:1428:ILE:HG22	2.13	0.48
1:D:3683:GLU:O	1:D:3687:GLU:OE1	2.30	0.48
1:D:4709:PHE:HB3	1:D:4710:PRO:HD3	1.95	0.48
1:A:839:HIS:CD2	1:A:1096:VAL:HG21	2.48	0.48
1:A:2949:THR:HG23	1:A:2950:SER:H	1.78	0.48
1:A:4048:VAL:HG11	1:A:4160:ASP:OD2	2.13	0.48
1:A:4582:ASP:OD1	1:A:4583:SER:N	2.45	0.48
2:G:91:ILE:HD11	1:C:1685:ALA:HA	1.95	0.48
1:C:2757:ASN:O	1:C:2761:GLU:OE1	2.31	0.48
1:C:3212:ASN:HD22	1:C:3237:VAL:HG21	1.78	0.48
1:D:1793:ALA:O	1:D:1794:THR:OG1	2.24	0.48
1:D:2752:LEU:HB3	1:D:2814:LEU:HD13	1.94	0.48
1:D:2871:GLU:OE1	1:D:2875:MET:HE1	2.12	0.48
1:A:2949:THR:HG23	1:A:2950:SER:N	2.28	0.48
2:F:91:ILE:HD11	1:B:1685:ALA:HA	1.95	0.48
1:B:839:HIS:CD2	1:B:1096:VAL:HG21	2.48	0.48
1:C:839:HIS:CD2	1:C:1096:VAL:HG21	2.48	0.48
1:D:839:HIS:CD2	1:D:1096:VAL:HG21	2.48	0.48
1:D:4225:VAL:HG11	1:D:4948:VAL:HA	1.94	0.48
1:D:4803:ASN:ND2	7:D:5101:PCW:O3P	2.47	0.48
1:A:1424:ASP:O	1:A:1428:ILE:HG22	2.13	0.48
1:A:3686:GLU:N	1:A:3686:GLU:OE1	2.46	0.48
1:A:3683:GLU:O	1:A:3687:GLU:OE1	2.30	0.48
1:B:2782:ILE:HG23	1:B:2790:PRO:CD	2.44	0.48
1:C:2949:THR:HG23	1:C:2950:SER:N	2.28	0.48
1:A:1788:LEU:HD12	1:A:1789:PRO:HD2	1.94	0.48
1:A:3526:CYS:SG	1:A:3600:VAL:HG21	2.54	0.48
1:B:2949:THR:HG23	1:B:2950:SER:H	1.78	0.48
1:C:3526:CYS:SG	1:C:3600:VAL:HG21	2.54	0.48
1:A:3936:PHE:HE2	1:A:3954:PHE:CD1	2.32	0.48
1:A:4709:PHE:HB3	1:A:4710:PRO:HD3	1.95	0.48
1:B:2752:LEU:HB3	1:B:2814:LEU:HD13	1.94	0.48
1:B:2757:ASN:O	1:B:2761:GLU:OE1	2.31	0.48
1:A:4886:TYR:HA	1:B:4916:ILE:HD11	1.95	0.48
1:B:2949:THR:HG23	1:B:2950:SER:N	2.28	0.48
1:C:2640:MET:HB3	1:C:2641:PRO:HD3	1.96	0.48
1:C:2782:ILE:HG23	1:C:2790:PRO:CD	2.44	0.48
1:C:4637:MET:O	1:C:4641:LEU:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2814:LEU:HA	1:D:2817:MET:HE2	1.96	0.48
1:D:3526:CYS:SG	1:D:3600:VAL:HG21	2.54	0.48
1:C:3936:PHE:HE2	1:C:3954:PHE:CD1	2.32	0.47
1:D:3936:PHE:HE2	1:D:3954:PHE:CD1	2.32	0.47
1:A:2752:LEU:HB3	1:A:2814:LEU:HD13	1.94	0.47
1:A:2782:ILE:HG23	1:A:2790:PRO:CD	2.44	0.47
2:H:26:HIS:CE1	2:H:105:LEU:HD11	2.49	0.47
1:B:1424:ASP:O	1:B:1428:ILE:HG22	2.13	0.47
1:C:2949:THR:HG23	1:C:2950:SER:H	1.78	0.47
1:D:554:ARG:NE	1:D:556:GLU:OE2	2.41	0.47
2:H:91:ILE:HD11	1:D:1685:ALA:HA	1.95	0.47
1:B:4886:TYR:HA	1:C:4916:ILE:HD11	1.96	0.47
1:D:2755:PHE:HD2	1:D:2814:LEU:HD11	1.80	0.47
1:A:2640:MET:HB3	1:A:2641:PRO:HD3	1.96	0.47
1:C:4886:TYR:HA	1:D:4916:ILE:HD11	1.96	0.47
1:D:2213:VAL:HG11	1:D:2257:TYR:CE2	2.42	0.47
1:A:4916:ILE:HD11	1:D:4886:TYR:HA	1.97	0.47
2:F:26:HIS:CE1	2:F:105:LEU:HD11	2.49	0.47
1:B:3366:LEU:HD13	1:B:3406:LEU:HD23	1.96	0.47
1:B:3936:PHE:HE2	1:B:3954:PHE:CD1	2.32	0.47
1:C:3366:LEU:HD13	1:C:3406:LEU:HD23	1.96	0.47
1:D:2782:ILE:HG23	1:D:2790:PRO:CD	2.44	0.47
1:A:3828:GLU:OE1	1:A:3828:GLU:N	2.38	0.47
1:A:2224:ILE:HD11	1:A:2268:MET:SD	2.54	0.47
1:B:165:ARG:N	1:B:168:ASP:OD2	2.48	0.47
1:B:878:ASN:HD22	1:B:1046:THR:HG21	1.80	0.47
1:B:3526:CYS:SG	1:B:3600:VAL:HG21	2.54	0.47
1:C:2103:VAL:HG13	1:C:2121:MET:HB2	1.97	0.47
1:C:2871:GLU:OE1	1:C:2875:MET:HE1	2.15	0.47
1:D:165:ARG:N	1:D:168:ASP:OD2	2.48	0.47
1:D:2640:MET:HB3	1:D:2641:PRO:HD3	1.96	0.47
1:D:3212:ASN:HD22	1:D:3237:VAL:HG21	1.78	0.47
1:B:2224:ILE:HD11	1:B:2268:MET:SD	2.54	0.47
7:D:5101:PCW:H232	7:D:5101:PCW:H20	1.72	0.47
1:A:2755:PHE:HD2	1:A:2814:LEU:HD11	1.80	0.47
1:B:1066:SER:OG	1:B:1067:GLN:NE2	2.48	0.47
1:B:2640:MET:HB3	1:B:2641:PRO:HD3	1.96	0.47
1:C:2213:VAL:HG11	1:C:2257:TYR:CE2	2.42	0.47
1:D:1042:GLN:O	1:D:1046:THR:HG23	2.15	0.47
1:D:1066:SER:OG	1:D:1067:GLN:NE2	2.48	0.47
1:D:2224:ILE:HD11	1:D:2268:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3413:LEU:HD11	1:A:3435:LEU:HD21	1.96	0.47
2:G:26:HIS:CE1	2:G:105:LEU:HD11	2.50	0.47
1:B:3413:LEU:HD11	1:B:3435:LEU:HD21	1.96	0.47
1:D:1424:ASP:O	1:D:1428:ILE:HG22	2.13	0.47
1:A:1042:GLN:O	1:A:1046:THR:HG23	2.15	0.46
1:A:4803:ASN:ND2	7:A:8007:PCW:O3P	2.48	0.46
1:B:3828:GLU:OE1	1:B:3828:GLU:N	2.38	0.46
1:C:2224:ILE:HD11	1:C:2268:MET:SD	2.54	0.46
1:C:4803:ASN:ND2	7:C:8007:PCW:O3P	2.48	0.46
1:A:1066:SER:OG	1:A:1067:GLN:NE2	2.48	0.46
1:C:1042:GLN:O	1:C:1046:THR:HG23	2.15	0.46
1:C:1555:VAL:HG21	1:C:1562:VAL:CG1	2.46	0.46
1:B:3591:GLU:O	1:B:3595:ARG:HG2	2.15	0.46
1:C:3413:LEU:HD11	1:C:3435:LEU:HD21	1.96	0.46
1:C:3789:CYS:SG	1:C:3834:SER:OG	2.73	0.46
1:D:3366:LEU:HD13	1:D:3406:LEU:HD23	1.96	0.46
1:D:3820:LEU:HD13	1:D:3902:PHE:CD1	2.50	0.46
1:A:878:ASN:HD22	1:A:1046:THR:HG21	1.80	0.46
1:A:2695:GLU:OE1	1:A:2698:ARG:NH2	2.49	0.46
1:D:2432:ASP:O	1:D:2436:ARG:HG2	2.16	0.46
1:A:2631:VAL:HG22	1:A:2641:PRO:HB2	1.98	0.46
1:B:3458:ASN:O	1:B:3462:GLN:OE1	2.34	0.46
1:C:165:ARG:N	1:C:168:ASP:OD2	2.48	0.46
1:C:878:ASN:HD22	1:C:1046:THR:HG21	1.80	0.46
1:D:308:ALA:HB1	1:D:313:THR:HG21	1.98	0.46
1:D:2103:VAL:HG13	1:D:2121:MET:HB2	1.97	0.46
1:D:3789:CYS:SG	1:D:3834:SER:OG	2.73	0.46
1:A:70:LEU:HD21	1:A:203:MET:HE1	1.98	0.46
1:A:308:ALA:HB1	1:A:313:THR:HG21	1.98	0.46
1:A:3771:SER:HA	1:A:3774:HIS:CE1	2.51	0.46
1:B:1042:GLN:O	1:B:1046:THR:HG23	2.15	0.46
1:B:3683:GLU:O	1:B:3686:GLU:N	2.49	0.46
1:A:3366:LEU:HD13	1:A:3406:LEU:HD23	1.96	0.46
1:A:3591:GLU:O	1:A:3595:ARG:HG2	2.15	0.46
1:C:973:LEU:HD11	1:C:1046:THR:HG22	1.98	0.46
1:C:1066:SER:OG	1:C:1067:GLN:NE2	2.48	0.46
1:C:2314:LEU:HD11	1:C:2417:VAL:HG22	1.98	0.46
1:C:2482:LYS:HD2	1:C:2483:ASP:N	2.28	0.46
1:C:3460:VAL:HG23	1:C:3465:ILE:HB	1.98	0.46
1:C:3820:LEU:HD13	1:C:3902:PHE:CD1	2.50	0.46
7:C:8007:PCW:H232	7:C:8007:PCW:H20	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1555:VAL:HG21	1:D:1562:VAL:CG1	2.46	0.46
1:A:3683:GLU:O	1:A:3686:GLU:N	2.49	0.46
1:B:308:ALA:HB1	1:B:313:THR:HG21	1.98	0.46
1:B:3771:SER:HA	1:B:3774:HIS:CE1	2.51	0.46
1:B:3820:LEU:HD13	1:B:3902:PHE:CD1	2.51	0.46
1:C:2755:PHE:HD2	1:C:2814:LEU:HD11	1.80	0.46
1:D:878:ASN:HD22	1:D:1046:THR:HG21	1.80	0.46
1:D:3460:VAL:HG23	1:D:3465:ILE:HB	1.98	0.46
1:D:3683:GLU:O	1:D:3686:GLU:N	2.49	0.46
2:G:91:ILE:N	2:G:91:ILE:HD12	2.31	0.46
1:B:1304:CYS:O	1:B:1305:THR:OG1	2.29	0.46
1:B:2746:VAL:HG21	1:B:2818:ILE:HG22	1.98	0.46
1:C:2746:VAL:HG21	1:C:2818:ILE:HG22	1.98	0.46
1:C:3683:GLU:O	1:C:3686:GLU:N	2.49	0.46
1:D:2314:LEU:HD11	1:D:2417:VAL:HG22	1.98	0.46
1:A:1144:TRP:HB2	1:A:1148:ASP:HB2	1.98	0.46
1:B:1555:VAL:HG21	1:B:1562:VAL:CG1	2.46	0.46
1:B:2103:VAL:HG13	1:B:2121:MET:HB2	1.97	0.46
1:B:2432:ASP:O	1:B:2436:ARG:HG2	2.16	0.46
7:B:8007:PCW:H232	7:B:8007:PCW:H20	1.72	0.46
1:C:308:ALA:HB1	1:C:313:THR:HG21	1.98	0.46
1:C:2432:ASP:O	1:C:2436:ARG:HG2	2.16	0.46
1:D:2695:GLU:OE1	1:D:2698:ARG:NH2	2.49	0.46
1:A:3820:LEU:HD13	1:A:3902:PHE:CD1	2.50	0.45
1:B:4803:ASN:ND2	7:B:8007:PCW:O3P	2.48	0.45
1:C:3458:ASN:O	1:C:3462:GLN:OE1	2.34	0.45
1:D:1423:ASP:OD2	1:D:1569:LYS:NZ	2.33	0.45
1:D:3082:MET:HE2	1:D:3093:LEU:HD23	1.97	0.45
1:D:3458:ASN:O	1:D:3462:GLN:OE1	2.34	0.45
1:A:165:ARG:N	1:A:168:ASP:OD2	2.48	0.45
1:A:2103:VAL:HG13	1:A:2121:MET:HB2	1.97	0.45
2:F:91:ILE:HD12	2:F:91:ILE:N	2.31	0.45
2:G:41:ARG:NH2	2:G:103:GLU:OE1	2.47	0.45
1:B:3004:LEU:HB2	1:B:3005:PRO:HD3	1.99	0.45
1:B:3974:GLY:N	1:B:3975:PRO:HA	2.32	0.45
1:D:552:LEU:HD22	1:D:590:LEU:HD11	1.99	0.45
1:D:3248:GLU:OE1	1:D:3249:ARG:NH2	2.50	0.45
1:D:3413:LEU:HD11	1:D:3435:LEU:HD21	1.96	0.45
1:A:1761:ARG:NH2	1:A:2093:GLN:O	2.41	0.45
1:B:3369:ARG:NH2	1:B:3405:ASP:OD2	2.41	0.45
1:C:2631:VAL:HG22	1:C:2641:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3004:LEU:HB2	1:C:3005:PRO:HD3	1.99	0.45
1:C:3248:GLU:OE1	1:C:3249:ARG:NH2	2.50	0.45
1:D:973:LEU:HD11	1:D:1046:THR:HG22	1.98	0.45
1:A:2910:ASP:OD1	1:A:2911:THR:N	2.50	0.45
1:B:973:LEU:HD11	1:B:1046:THR:HG22	1.98	0.45
1:B:2314:LEU:HD11	1:B:2417:VAL:HG22	1.98	0.45
1:B:4637:MET:O	1:B:4641:LEU:N	2.41	0.45
1:C:690:SER:N	1:C:777:LEU:O	2.49	0.45
1:C:2695:GLU:OE1	1:C:2698:ARG:NH2	2.49	0.45
1:C:3771:SER:HA	1:C:3774:HIS:CE1	2.51	0.45
1:D:2482:LYS:HD2	1:D:2483:ASP:N	2.28	0.45
1:D:3004:LEU:HB2	1:D:3005:PRO:HD3	1.99	0.45
1:A:1555:VAL:HG21	1:A:1562:VAL:CG1	2.46	0.45
1:B:2755:PHE:HD2	1:B:2814:LEU:HD11	1.80	0.45
1:B:3248:GLU:OE1	1:B:3249:ARG:NH2	2.50	0.45
1:C:552:LEU:HD22	1:C:590:LEU:HD11	1.99	0.45
1:D:2124:LEU:O	1:D:2128:GLN:HG2	2.17	0.45
1:A:2432:ASP:O	1:A:2436:ARG:HG2	2.16	0.45
1:A:2482:LYS:HD2	1:A:2483:ASP:N	2.28	0.45
2:E:36:LYS:NZ	2:E:42:ASP:OD1	2.40	0.45
1:B:1737:VAL:HG11	1:B:1960:ALA:CB	2.47	0.45
1:B:2124:LEU:O	1:B:2128:GLN:HG2	2.17	0.45
1:B:3789:CYS:SG	1:B:3834:SER:OG	2.73	0.45
7:C:8006:PCW:H172	7:C:8006:PCW:H20	1.91	0.45
1:D:3591:GLU:O	1:D:3595:ARG:HG2	2.15	0.45
1:D:3771:SER:HA	1:D:3774:HIS:CE1	2.51	0.45
1:A:552:LEU:HD22	1:A:590:LEU:HD11	1.99	0.45
1:A:3004:LEU:HB2	1:A:3005:PRO:HD3	1.99	0.45
1:B:3460:VAL:HG23	1:B:3465:ILE:HB	1.98	0.45
1:C:554:ARG:NE	1:C:556:GLU:OE2	2.40	0.45
1:C:3591:GLU:O	1:C:3595:ARG:HG2	2.15	0.45
2:H:91:ILE:N	2:H:91:ILE:HD12	2.31	0.45
1:B:1144:TRP:HB2	1:B:1148:ASP:HB2	1.98	0.45
1:C:1144:TRP:HB2	1:C:1148:ASP:HB2	1.98	0.45
1:C:1807:GLU:O	1:C:1810:ARG:HG2	2.17	0.45
1:C:2910:ASP:OD1	1:C:2911:THR:N	2.50	0.45
1:C:3974:GLY:N	1:C:3975:PRO:HA	2.32	0.45
1:D:2746:VAL:HG21	1:D:2818:ILE:HG22	1.98	0.45
1:A:973:LEU:HD11	1:A:1046:THR:HG22	1.98	0.45
1:A:1737:VAL:HG11	1:A:1960:ALA:CB	2.47	0.45
1:A:2746:VAL:HG21	1:A:2818:ILE:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3458:ASN:O	1:A:3462:GLN:OE1	2.34	0.45
1:B:2695:GLU:OE1	1:B:2698:ARG:NH2	2.49	0.45
1:B:2942:LEU:HB2	1:B:2945:MET:CE	2.47	0.45
1:A:3974:GLY:N	1:A:3975:PRO:HA	2.32	0.45
1:A:4638:GLU:HB3	1:A:4639:PRO:HD3	1.99	0.45
1:C:552:LEU:HD11	1:C:565:LEU:HD22	1.99	0.45
1:C:2942:LEU:HB2	1:C:2945:MET:CE	2.47	0.45
1:C:3076:LEU:O	1:C:3147:HIS:NE2	2.50	0.45
1:D:552:LEU:HD11	1:D:565:LEU:HD22	1.99	0.45
1:A:2213:VAL:HG11	1:A:2257:TYR:CE2	2.42	0.44
1:A:2314:LEU:HD11	1:A:2417:VAL:HG22	1.98	0.44
1:D:1737:VAL:HG11	1:D:1960:ALA:CB	2.47	0.44
1:D:2868:LEU:HD21	1:D:2929:LYS:HG3	1.99	0.44
1:A:1807:GLU:O	1:A:1810:ARG:HG2	2.17	0.44
1:A:3248:GLU:OE1	1:A:3249:ARG:NH2	2.50	0.44
2:E:91:ILE:N	2:E:91:ILE:HD12	2.32	0.44
2:H:41:ARG:NH2	2:H:103:GLU:OE1	2.46	0.44
1:B:2822:TRP:CE2	1:B:2940:ARG:HD3	2.53	0.44
1:B:2910:ASP:OD1	1:B:2911:THR:N	2.50	0.44
1:A:2782:ILE:HG23	1:A:2790:PRO:HD3	2.00	0.44
1:B:552:LEU:HD22	1:B:590:LEU:HD11	1.99	0.44
1:B:1807:GLU:O	1:B:1810:ARG:HG2	2.17	0.44
1:C:2124:LEU:O	1:C:2128:GLN:HG2	2.17	0.44
1:C:2814:LEU:HA	1:C:2817:MET:HE2	2.00	0.44
1:A:2486:LEU:HD11	1:A:2542:PHE:CE1	2.53	0.44
1:A:2942:LEU:HB2	1:A:2945:MET:CE	2.47	0.44
1:B:1423:ASP:OD2	1:B:1569:LYS:NZ	2.33	0.44
1:B:2631:VAL:HG22	1:B:2641:PRO:HB2	1.98	0.44
1:D:575:VAL:O	1:D:579:ILE:HG12	2.18	0.44
1:D:2631:VAL:HG22	1:D:2641:PRO:HB2	1.98	0.44
1:D:2782:ILE:HG23	1:D:2790:PRO:HD3	2.00	0.44
1:A:552:LEU:HD11	1:A:565:LEU:HD22	1.99	0.44
1:A:690:SER:N	1:A:777:LEU:O	2.49	0.44
1:C:575:VAL:O	1:C:579:ILE:HG12	2.18	0.44
1:A:2124:LEU:O	1:A:2128:GLN:HG2	2.17	0.44
1:A:3104:ILE:CD1	1:A:3169:THR:HG23	2.48	0.44
1:A:3460:VAL:HG23	1:A:3465:ILE:HB	1.98	0.44
1:A:3536:LEU:HD11	1:A:3560:LEU:HD22	1.99	0.44
1:B:2486:LEU:HD11	1:B:2542:PHE:CE1	2.53	0.44
1:B:2883:TYR:HB2	1:B:2920:ASP:OD2	2.18	0.44
1:B:3458:ASN:O	1:B:3459:PHE:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2782:ILE:HG23	1:C:2790:PRO:HD3	2.00	0.44
1:C:2822:TRP:CE2	1:C:2940:ARG:HD3	2.52	0.44
1:C:2868:LEU:HD21	1:C:2929:LYS:HG3	1.99	0.44
1:D:1807:GLU:O	1:D:1810:ARG:HG2	2.17	0.44
1:B:908:LEU:HD13	1:B:962:MET:HE1	2.00	0.44
1:B:2782:ILE:HG23	1:B:2790:PRO:HD3	2.00	0.44
1:B:3536:LEU:HD11	1:B:3560:LEU:HD13	2.00	0.44
1:C:2883:TYR:HB2	1:C:2920:ASP:OD2	2.17	0.44
1:D:1144:TRP:HB2	1:D:1148:ASP:HB2	1.98	0.44
1:D:2942:LEU:HB2	1:D:2945:MET:CE	2.47	0.44
1:D:3104:ILE:CD1	1:D:3169:THR:HG23	2.48	0.44
1:D:3974:GLY:N	1:D:3975:PRO:HA	2.32	0.44
1:A:1423:ASP:OD2	1:A:1569:LYS:NZ	2.33	0.44
1:A:1930:MET:HE3	1:A:1932:LEU:HD21	1.96	0.44
1:B:2868:LEU:HD21	1:B:2929:LYS:HG3	1.99	0.44
1:B:3104:ILE:CD1	1:B:3169:THR:HG23	2.48	0.44
1:C:4638:GLU:HB3	1:C:4639:PRO:HD3	1.99	0.44
1:D:690:SER:N	1:D:777:LEU:O	2.49	0.44
1:D:2486:LEU:HD11	1:D:2542:PHE:CE1	2.53	0.44
1:D:2822:TRP:CE2	1:D:2940:ARG:HD3	2.52	0.44
1:A:31:LYS:HG3	1:A:31:LYS:O	2.18	0.44
1:A:914:LEU:HD23	1:A:919:ARG:HA	2.00	0.44
1:A:1699:LEU:HD22	1:A:1713:TYR:CE1	2.53	0.44
1:A:2578:ILE:HD12	1:A:2578:ILE:H	1.83	0.44
1:A:2868:LEU:HD21	1:A:2929:LYS:HG3	1.99	0.43
1:B:2213:VAL:HG11	1:B:2257:TYR:CE2	2.42	0.43
1:B:2769:PHE:O	1:B:2772:ILE:HG22	2.18	0.43
1:B:3362:THR:CG2	1:B:3409:LEU:HD13	2.48	0.43
1:C:576:LEU:HD22	1:C:610:CYS:HB2	2.00	0.43
1:C:2212:MET:O	1:C:2215:VAL:HG22	2.18	0.43
1:C:3293:PRO:O	1:C:3295:PRO:CD	2.66	0.43
1:A:3246:VAL:HG12	1:A:3247:LEU:N	2.34	0.43
1:B:575:VAL:O	1:B:579:ILE:HG12	2.18	0.43
1:B:981:ALA:O	1:B:984:THR:OG1	2.33	0.43
1:B:2871:GLU:OE1	1:B:2875:MET:HE1	2.18	0.43
1:B:3293:PRO:O	1:B:3295:PRO:CD	2.66	0.43
1:C:914:LEU:HD23	1:C:919:ARG:HA	2.00	0.43
1:C:1737:VAL:HG11	1:C:1960:ALA:CB	2.47	0.43
1:D:31:LYS:O	1:D:31:LYS:HG3	2.18	0.43
1:D:576:LEU:HD22	1:D:610:CYS:HB2	2.00	0.43
1:D:2212:MET:O	1:D:2215:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2883:TYR:HB2	1:D:2920:ASP:OD2	2.18	0.43
1:D:3536:LEU:HD11	1:D:3560:LEU:HD22	1.99	0.43
1:A:2871:GLU:OE1	1:A:2875:MET:HE1	2.18	0.43
1:C:2701:MET:HB3	1:C:2702:PRO:HD3	2.01	0.43
1:C:2863:LEU:HD11	1:C:2930:PHE:HB2	2.01	0.43
1:D:2578:ILE:HD12	1:D:2578:ILE:H	1.83	0.43
1:D:3410:TYR:N	1:D:3411:PRO:HD2	2.33	0.43
1:A:2883:TYR:HB2	1:A:2920:ASP:OD2	2.17	0.43
1:A:3362:THR:CG2	1:A:3409:LEU:HD13	2.48	0.43
1:A:3536:LEU:HD11	1:A:3560:LEU:HD13	2.00	0.43
1:B:31:LYS:O	1:B:31:LYS:HG3	2.18	0.43
1:B:3536:LEU:HD11	1:B:3560:LEU:HD22	1.99	0.43
1:B:4638:GLU:HB3	1:B:4639:PRO:HD3	1.99	0.43
1:C:1699:LEU:HD22	1:C:1713:TYR:CE1	2.53	0.43
1:C:3458:ASN:O	1:C:3459:PHE:C	2.56	0.43
1:D:1699:LEU:HD22	1:D:1713:TYR:CE1	2.53	0.43
1:D:1929:GLN:CG	1:D:1929:GLN:O	2.67	0.43
1:A:1793:ALA:O	1:A:1794:THR:OG1	2.24	0.43
1:A:2822:TRP:CE2	1:A:2940:ARG:HD3	2.52	0.43
1:A:2863:LEU:HD11	1:A:2930:PHE:HB2	2.01	0.43
1:A:3293:PRO:O	1:A:3295:PRO:CD	2.66	0.43
1:B:614:ALA:HB2	1:B:1677:LEU:HD12	2.01	0.43
1:B:1929:GLN:CG	1:B:1929:GLN:O	2.67	0.43
1:B:2768:ALA:HA	1:B:2771:LYS:HE2	2.01	0.43
1:B:2863:LEU:HD11	1:B:2930:PHE:HB2	2.01	0.43
1:B:3088:ILE:HD12	1:B:3088:ILE:H	1.84	0.43
1:C:1297:GLN:NE2	1:C:1546:ASN:OD1	2.46	0.43
1:C:1929:GLN:CG	1:C:1929:GLN:O	2.67	0.43
1:C:3246:VAL:HG12	1:C:3247:LEU:N	2.34	0.43
1:D:569:LEU:HD12	1:D:603:VAL:HG13	2.01	0.43
1:D:2768:ALA:HA	1:D:2771:LYS:HE2	2.01	0.43
1:D:2769:PHE:O	1:D:2772:ILE:HG22	2.19	0.43
1:D:4638:GLU:HB3	1:D:4639:PRO:HD3	1.99	0.43
1:A:1959:LEU:HD23	1:A:2139:LEU:HD21	2.01	0.43
1:A:2701:MET:HB3	1:A:2702:PRO:HD3	2.01	0.43
1:B:1959:LEU:HD23	1:B:2139:LEU:HD21	2.01	0.43
1:B:2482:LYS:HD2	1:B:2483:ASP:N	2.28	0.43
1:C:4876:ASP:OD2	1:C:4879:THR:OG1	2.29	0.43
1:D:2701:MET:HB3	1:D:2702:PRO:HD3	2.01	0.43
1:D:2794:PRO:O	1:D:2798:PHE:N	2.51	0.43
1:D:2910:ASP:OD1	1:D:2911:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1699:LEU:HD22	1:B:1713:TYR:CE1	2.53	0.43
1:B:2212:MET:O	1:B:2215:VAL:HG22	2.18	0.43
1:B:3369:ARG:O	1:B:3373:VAL:HG23	2.19	0.43
1:C:2486:LEU:HD11	1:C:2542:PHE:CE1	2.53	0.43
1:C:3536:LEU:HD11	1:C:3560:LEU:HD22	1.99	0.43
1:D:731:VAL:HG21	1:D:765:VAL:HG12	2.01	0.43
1:D:1080:LYS:HA	1:D:1190:LEU:HD11	2.01	0.43
1:D:3246:VAL:HG12	1:D:3247:LEU:N	2.34	0.43
1:D:3293:PRO:O	1:D:3295:PRO:CD	2.66	0.43
1:A:575:VAL:O	1:A:579:ILE:HG12	2.18	0.43
1:A:2814:LEU:HA	1:A:2817:MET:HE2	2.01	0.43
1:B:552:LEU:HD11	1:B:565:LEU:HD22	1.99	0.43
1:C:971:LEU:HD12	1:C:973:LEU:HG	2.01	0.43
1:C:3104:ILE:CD1	1:C:3169:THR:HG23	2.48	0.43
1:C:3362:THR:CG2	1:C:3409:LEU:HD13	2.49	0.43
1:D:3088:ILE:HD12	1:D:3088:ILE:H	1.84	0.43
1:A:576:LEU:HD22	1:A:610:CYS:HB2	2.00	0.43
1:A:2212:MET:O	1:A:2215:VAL:HG22	2.18	0.43
1:A:2768:ALA:HA	1:A:2771:LYS:HE2	2.01	0.43
1:A:2769:PHE:O	1:A:2772:ILE:HG22	2.19	0.43
1:B:576:LEU:HD22	1:B:610:CYS:HB2	2.01	0.43
1:B:690:SER:N	1:B:777:LEU:O	2.49	0.43
1:B:971:LEU:HD12	1:B:973:LEU:HG	2.01	0.43
1:B:2701:MET:HB3	1:B:2702:PRO:HD3	2.01	0.43
1:B:3076:LEU:O	1:B:3147:HIS:NE2	2.50	0.43
1:C:31:LYS:HG3	1:C:31:LYS:O	2.18	0.43
1:C:579:ILE:HG13	1:C:607:LEU:HD22	2.01	0.43
1:C:1850:LEU:HD22	1:C:1855:VAL:HG21	2.01	0.43
1:C:1959:LEU:HD23	1:C:2139:LEU:HD21	2.01	0.43
1:C:3088:ILE:HD12	1:C:3088:ILE:H	1.84	0.43
1:C:3536:LEU:HD11	1:C:3560:LEU:HD13	2.00	0.43
1:C:4993:LEU:HD23	1:C:4993:LEU:HA	1.83	0.43
1:D:914:LEU:HD23	1:D:919:ARG:HA	2.00	0.43
1:A:569:LEU:HD12	1:A:603:VAL:HG13	2.01	0.43
1:A:971:LEU:HD12	1:A:973:LEU:HG	2.01	0.43
1:A:1080:LYS:HA	1:A:1190:LEU:HD11	2.01	0.43
1:A:2564:THR:HG22	1:A:2607:CYS:CA	2.46	0.43
1:A:3369:ARG:NH2	1:A:3405:ASP:OD2	2.41	0.43
1:A:3410:TYR:N	1:A:3411:PRO:HD2	2.33	0.43
1:B:579:ILE:HG13	1:B:607:LEU:HD22	2.01	0.43
1:D:1959:LEU:HD23	1:D:2139:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3362:THR:CG2	1:D:3409:LEU:HD13	2.48	0.43
1:B:576:LEU:HA	1:B:579:ILE:HG12	2.01	0.42
1:B:2578:ILE:HD12	1:B:2578:ILE:H	1.83	0.42
1:B:3410:TYR:N	1:B:3411:PRO:HD2	2.33	0.42
1:B:3994:GLY:O	1:B:3998:VAL:HG23	2.19	0.42
7:B:8006:PCW:H172	7:B:8006:PCW:H20	1.90	0.42
1:C:614:ALA:HB2	1:C:1677:LEU:HD12	2.01	0.42
1:C:3051:VAL:HG22	1:C:3065:VAL:HG11	2.01	0.42
1:D:2863:LEU:HD11	1:D:2930:PHE:HB2	2.01	0.42
1:D:3536:LEU:HD11	1:D:3560:LEU:HD13	2.00	0.42
1:D:3820:LEU:HB2	1:D:3902:PHE:CE1	2.54	0.42
1:A:464:GLU:OE2	1:A:468:LYS:NZ	2.53	0.42
2:E:24:VAL:HG12	2:E:105:LEU:HD12	2.00	0.42
1:B:464:GLU:OE2	1:B:468:LYS:NZ	2.53	0.42
1:B:1080:LYS:HA	1:B:1190:LEU:HD11	2.01	0.42
1:B:3246:VAL:HG12	1:B:3247:LEU:N	2.33	0.42
1:B:3457:GLN:O	1:B:3460:VAL:HG12	2.19	0.42
1:C:673:ALA:O	1:C:681:THR:OG1	2.30	0.42
1:C:1023:VAL:HG22	1:C:1024:PRO:HD2	2.01	0.42
1:C:2578:ILE:HD12	1:C:2578:ILE:H	1.83	0.42
1:B:914:LEU:HD23	1:B:919:ARG:HA	2.00	0.42
1:C:576:LEU:HA	1:C:579:ILE:HG12	2.01	0.42
1:C:731:VAL:HG21	1:C:765:VAL:HG12	2.01	0.42
1:D:1023:VAL:HG22	1:D:1024:PRO:HD2	2.01	0.42
1:D:3051:VAL:HG22	1:D:3065:VAL:HG11	2.01	0.42
1:A:1929:GLN:CG	1:A:1929:GLN:O	2.67	0.42
1:A:3443:PHE:CG	1:A:3515:LEU:HD13	2.54	0.42
1:A:3789:CYS:SG	1:A:3834:SER:OG	2.73	0.42
1:B:74:LEU:HD11	1:B:82:MET:HE3	2.01	0.42
1:B:3417:VAL:O	1:B:3421:ARG:N	2.53	0.42
1:C:1080:LYS:HA	1:C:1190:LEU:HD11	2.01	0.42
1:C:3360:ILE:HB	1:C:3361:PRO:HD3	2.02	0.42
1:C:3457:GLN:O	1:C:3460:VAL:HG12	2.20	0.42
1:D:3443:PHE:CG	1:D:3515:LEU:HD13	2.54	0.42
1:A:731:VAL:HG21	1:A:765:VAL:HG12	2.01	0.42
1:A:2794:PRO:O	1:A:2798:PHE:N	2.51	0.42
1:A:3360:ILE:HB	1:A:3361:PRO:HD3	2.02	0.42
1:B:3360:ILE:HB	1:B:3361:PRO:HD3	2.02	0.42
1:B:3443:PHE:CG	1:B:3515:LEU:HD13	2.54	0.42
1:C:3410:TYR:N	1:C:3411:PRO:HD2	2.33	0.42
1:C:3443:PHE:CG	1:C:3515:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:LEU:HD13	1:D:1667:THR:HG23	2.02	0.42
1:D:1850:LEU:HD22	1:D:1855:VAL:HG21	2.01	0.42
1:D:3369:ARG:O	1:D:3373:VAL:HG23	2.19	0.42
1:D:3768:TYR:HH	1:D:4751:HIS:CE1	2.38	0.42
1:A:2799:SER:O	1:A:2803:LYS:HG3	2.20	0.42
1:B:1850:LEU:HD22	1:B:1855:VAL:HG21	2.01	0.42
1:C:47:LEU:CD2	1:C:126:ARG:HE	2.33	0.42
1:C:973:LEU:HD13	1:C:1045:ARG:HB3	2.01	0.42
1:C:1930:MET:O	1:C:1930:MET:HG2	2.20	0.42
1:C:2768:ALA:HA	1:C:2771:LYS:HE2	2.01	0.42
1:C:2769:PHE:O	1:C:2772:ILE:HG22	2.18	0.42
1:C:3369:ARG:O	1:C:3373:VAL:HG23	2.19	0.42
1:C:3820:LEU:HB2	1:C:3902:PHE:CE1	2.54	0.42
1:A:614:ALA:HB2	1:A:1677:LEU:HD12	2.01	0.42
1:A:633:LEU:HD13	1:A:1667:THR:HG23	2.02	0.42
1:A:1229:ILE:HG23	1:A:1230:ASN:N	2.35	0.42
1:A:3820:LEU:HB2	1:A:3902:PHE:CE1	2.54	0.42
1:A:3994:GLY:O	1:A:3998:VAL:HG23	2.19	0.42
2:F:60:TRP:CZ2	1:B:1785:VAL:HG11	2.54	0.42
1:B:569:LEU:HD12	1:B:603:VAL:HG13	2.01	0.42
1:B:1052:TYR:O	1:B:1054:ILE:HD12	2.20	0.42
1:B:3522:GLY:HA2	1:B:3525:MET:HE2	2.00	0.42
1:B:3820:LEU:HB2	1:B:3902:PHE:CE1	2.55	0.42
1:C:464:GLU:OE2	1:C:468:LYS:NZ	2.53	0.42
1:C:2215:VAL:HG21	1:C:2229:MET:HE3	2.02	0.42
1:C:3768:TYR:HH	1:C:4751:HIS:CE1	2.38	0.42
1:D:973:LEU:HD13	1:D:1045:ARG:HB3	2.01	0.42
1:D:3360:ILE:HB	1:D:3361:PRO:HD3	2.02	0.42
1:A:579:ILE:HG13	1:A:607:LEU:HD22	2.01	0.42
1:A:1930:MET:O	1:A:1930:MET:HG2	2.20	0.42
1:A:3088:ILE:H	1:A:3088:ILE:HD12	1.84	0.42
2:G:60:TRP:CZ2	1:C:1785:VAL:HG11	2.55	0.42
1:C:569:LEU:HD12	1:C:603:VAL:HG13	2.01	0.42
1:C:1282:ASN:OD1	1:C:1282:ASN:C	2.58	0.42
1:D:1930:MET:O	1:D:1930:MET:HG2	2.20	0.42
1:D:3994:GLY:O	1:D:3998:VAL:HG23	2.19	0.42
1:A:1282:ASN:C	1:A:1282:ASN:OD1	2.58	0.42
1:A:3106:LYS:O	1:A:3109:GLU:HG3	2.20	0.42
1:B:1229:ILE:HG23	1:B:1230:ASN:N	2.35	0.42
1:C:3106:LYS:O	1:C:3109:GLU:HG3	2.20	0.42
1:D:464:GLU:OE2	1:D:468:LYS:NZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:LEU:HD12	1:D:973:LEU:HG	2.01	0.42
1:D:1521:VAL:HG12	1:D:1528:MET:HG2	2.02	0.42
1:D:2822:TRP:CZ3	1:D:2875:MET:CG	3.03	0.42
1:D:2942:LEU:HB2	1:D:2945:MET:SD	2.60	0.42
1:D:3106:LYS:O	1:D:3109:GLU:HG3	2.20	0.42
1:D:3550:VAL:O	1:D:3554:LEU:HD13	2.20	0.42
1:D:4664:VAL:N	1:D:4665:PRO:CD	2.83	0.42
1:A:591:LEU:HG	1:A:600:VAL:HG11	2.02	0.42
1:A:596:ARG:NH2	1:A:1644:GLU:OE1	2.53	0.42
1:A:3369:ARG:O	1:A:3373:VAL:HG23	2.19	0.42
1:B:2799:SER:O	1:B:2803:LYS:HG3	2.20	0.42
1:B:3768:TYR:HH	1:B:4751:HIS:CE1	2.38	0.42
1:C:591:LEU:HG	1:C:600:VAL:HG11	2.02	0.42
1:C:2822:TRP:CZ3	1:C:2875:MET:CG	3.03	0.42
1:C:3994:GLY:O	1:C:3998:VAL:HG23	2.19	0.42
1:C:4239:SER:OG	1:C:4673:LYS:NZ	2.53	0.42
1:A:141:ASP:OD1	1:A:143:THR:OG1	2.10	0.41
1:A:3458:ASN:O	1:A:3459:PHE:C	2.56	0.41
1:B:1531:THR:HG22	1:B:1536:GLU:HA	2.02	0.41
1:B:3051:VAL:HG22	1:B:3065:VAL:HG11	2.01	0.41
1:B:3106:LYS:O	1:B:3109:GLU:HG3	2.20	0.41
1:B:3167:TYR:CD2	1:B:3240:MET:HG2	2.55	0.41
1:B:3940:TYR:OH	1:B:3947:GLU:OE2	2.37	0.41
1:C:633:LEU:HD13	1:C:1667:THR:HG23	2.02	0.41
1:C:760:ILE:HG23	1:C:760:ILE:O	2.20	0.41
1:C:1521:VAL:HG12	1:C:1528:MET:HG2	2.02	0.41
1:D:1052:TYR:O	1:D:1054:ILE:HD12	2.20	0.41
1:D:2215:VAL:HG21	1:D:2229:MET:HE3	2.02	0.41
1:D:3167:TYR:CD2	1:D:3240:MET:HG2	2.55	0.41
1:A:878:ASN:ND2	1:A:1046:THR:HG21	2.35	0.41
1:A:2942:LEU:HB2	1:A:2945:MET:SD	2.60	0.41
1:B:633:LEU:HD13	1:B:1667:THR:HG23	2.02	0.41
1:B:731:VAL:HG21	1:B:765:VAL:HG12	2.01	0.41
1:B:1023:VAL:HG22	1:B:1024:PRO:HD2	2.01	0.41
1:C:2596:LEU:HD21	1:C:2604:ILE:CD1	2.45	0.41
1:C:3417:VAL:O	1:C:3421:ARG:N	2.53	0.41
1:C:4148:VAL:HG22	1:C:4181:LEU:HD13	2.02	0.41
1:D:579:ILE:HG13	1:D:607:LEU:HD22	2.01	0.41
1:D:1967:VAL:CG2	1:D:3650:ALA:HB1	2.49	0.41
1:D:2799:SER:O	1:D:2803:LYS:HG3	2.20	0.41
1:D:3417:VAL:O	1:D:3421:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3954:PHE:O	1:D:3958:MET:HG3	2.20	0.41
1:A:973:LEU:HD13	1:A:1045:ARG:HB3	2.01	0.41
1:A:2523:LEU:HD23	1:A:2579:MET:SD	2.61	0.41
1:A:2822:TRP:CZ3	1:A:2875:MET:CG	3.03	0.41
1:A:3167:TYR:CD2	1:A:3240:MET:HG2	2.55	0.41
1:B:591:LEU:HG	1:B:600:VAL:HG11	2.02	0.41
1:B:1930:MET:HG2	1:B:1930:MET:O	2.20	0.41
1:B:3004:LEU:HD11	1:B:3065:VAL:HG22	2.02	0.41
1:C:1052:TYR:O	1:C:1054:ILE:HD12	2.20	0.41
1:C:1718:SER:HA	1:C:1722:GLU:HB2	2.02	0.41
1:C:2794:PRO:O	1:C:2798:PHE:N	2.51	0.41
1:C:2799:SER:O	1:C:2803:LYS:HG3	2.20	0.41
1:D:591:LEU:HG	1:D:600:VAL:HG11	2.02	0.41
1:D:614:ALA:HB2	1:D:1677:LEU:HD12	2.01	0.41
1:D:760:ILE:O	1:D:760:ILE:HG23	2.20	0.41
1:D:1930:MET:HE3	1:D:1932:LEU:HD21	1.99	0.41
1:D:3004:LEU:HD11	1:D:3065:VAL:HG22	2.03	0.41
1:D:3458:ASN:O	1:D:3459:PHE:C	2.56	0.41
1:A:47:LEU:CD2	1:A:126:ARG:HE	2.33	0.41
1:A:760:ILE:HG23	1:A:760:ILE:O	2.20	0.41
1:A:1052:TYR:O	1:A:1054:ILE:HD12	2.20	0.41
1:A:1718:SER:HA	1:A:1722:GLU:HB2	2.02	0.41
1:A:1850:LEU:HD22	1:A:1855:VAL:HG21	2.01	0.41
1:A:4664:VAL:N	1:A:4665:PRO:CD	2.83	0.41
1:B:2624:LEU:O	1:B:2628:VAL:HG23	2.21	0.41
1:B:2794:PRO:O	1:B:2798:PHE:N	2.51	0.41
1:B:4664:VAL:N	1:B:4665:PRO:CD	2.83	0.41
1:B:4876:ASP:OD2	1:B:4879:THR:OG1	2.29	0.41
1:C:1229:ILE:HG23	1:C:1230:ASN:N	2.35	0.41
1:C:3940:TYR:OH	1:C:3947:GLU:OE2	2.37	0.41
1:D:47:LEU:HD21	1:D:126:ARG:HE	1.85	0.41
1:D:2539:THR:HG21	1:D:2900:GLY:HA3	2.02	0.41
1:D:3076:LEU:O	1:D:3147:HIS:NE2	2.50	0.41
7:D:5107:PCW:H172	7:D:5107:PCW:H20	1.91	0.41
1:A:1521:VAL:HG12	1:A:1528:MET:HG2	2.02	0.41
1:A:2539:THR:HG21	1:A:2900:GLY:HA3	2.02	0.41
1:A:3076:LEU:O	1:A:3147:HIS:NE2	2.50	0.41
1:B:47:LEU:CD2	1:B:126:ARG:HE	2.33	0.41
1:B:70:LEU:HD21	1:B:203:MET:HE3	2.03	0.41
1:B:1282:ASN:OD1	1:B:1282:ASN:C	2.58	0.41
1:B:2523:LEU:HD23	1:B:2579:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2539:THR:HG21	1:B:2900:GLY:HA3	2.02	0.41
1:B:4148:VAL:HG22	1:B:4181:LEU:HD13	2.02	0.41
1:B:4723:LEU:HA	1:B:4735:ILE:HG21	2.03	0.41
1:C:596:ARG:NH2	1:C:1644:GLU:OE1	2.53	0.41
1:C:2624:LEU:O	1:C:2628:VAL:HG23	2.21	0.41
1:C:3334:SER:O	1:C:3337:LYS:NZ	2.47	0.41
1:D:576:LEU:HA	1:D:579:ILE:HG12	2.01	0.41
1:D:596:ARG:NH2	1:D:1644:GLU:OE1	2.53	0.41
1:D:2624:LEU:O	1:D:2628:VAL:HG23	2.21	0.41
1:A:3051:VAL:HG22	1:A:3065:VAL:HG11	2.01	0.41
1:A:3768:TYR:HH	1:A:4751:HIS:CE1	2.38	0.41
1:B:973:LEU:HD13	1:B:1045:ARG:HB3	2.01	0.41
1:B:1822:ARG:O	1:B:1826:GLN:HG2	2.21	0.41
1:B:1967:VAL:CG2	1:B:3650:ALA:HB1	2.49	0.41
1:B:3550:VAL:O	1:B:3554:LEU:HD13	2.20	0.41
1:C:877:GLU:O	1:C:881:GLU:HG2	2.21	0.41
1:C:3550:VAL:O	1:C:3554:LEU:HD13	2.20	0.41
1:C:3954:PHE:O	1:C:3958:MET:HG3	2.20	0.41
1:D:4723:LEU:HA	1:D:4735:ILE:HG21	2.03	0.41
1:A:1023:VAL:HG22	1:A:1024:PRO:HD2	2.01	0.41
1:A:3230:ILE:H	1:A:3230:ILE:HD12	1.86	0.41
1:A:3550:VAL:O	1:A:3554:LEU:HD13	2.20	0.41
1:B:1154:ILE:O	1:B:1154:ILE:HG23	2.21	0.41
1:B:1973:ASN:OD1	1:B:2025:PRO:HD3	2.21	0.41
1:B:4153:LEU:HB3	1:B:4163:LEU:HD21	2.03	0.41
1:C:1967:VAL:CG2	1:C:3650:ALA:HB1	2.49	0.41
1:C:2539:THR:HG21	1:C:2900:GLY:HA3	2.02	0.41
1:C:3167:TYR:CD2	1:C:3240:MET:HG2	2.55	0.41
1:C:3369:ARG:NH2	1:C:3405:ASP:OD2	2.41	0.41
1:C:3894:LEU:O	1:C:3902:PHE:HD2	2.04	0.41
1:C:4723:LEU:HA	1:C:4735:ILE:HG21	2.03	0.41
1:D:258:ARG:O	1:D:285:HIS:NE2	2.43	0.41
1:D:1718:SER:HA	1:D:1722:GLU:HB2	2.02	0.41
1:D:1740:THR:HG22	1:D:2147:VAL:HG22	2.03	0.41
1:A:74:LEU:HD11	1:A:82:MET:HE3	2.01	0.41
1:A:877:GLU:O	1:A:881:GLU:HG2	2.21	0.41
1:A:1740:THR:HG22	1:A:2147:VAL:HG22	2.03	0.41
1:A:2820:TRP:CE3	1:A:2822:TRP:CH2	3.09	0.41
1:A:3417:VAL:O	1:A:3421:ARG:N	2.53	0.41
2:H:60:TRP:CZ2	1:D:1785:VAL:HG11	2.56	0.41
1:B:2215:VAL:HG21	1:B:2229:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2822:TRP:CZ3	1:B:2875:MET:CG	3.03	0.41
1:B:2871:GLU:OE1	1:B:2875:MET:CE	2.69	0.41
1:C:878:ASN:ND2	1:C:1046:THR:HG21	2.35	0.41
1:C:3004:LEU:HD11	1:C:3065:VAL:HG22	2.03	0.41
1:D:1229:ILE:HG23	1:D:1230:ASN:N	2.35	0.41
1:D:1531:THR:HG22	1:D:1536:GLU:HA	2.01	0.41
1:D:2820:TRP:CE3	1:D:2822:TRP:CH2	3.09	0.41
1:A:258:ARG:O	1:A:285:HIS:NE2	2.43	0.41
1:A:1043:ALA:O	1:A:1047:LEU:HD23	2.21	0.41
1:A:1785:VAL:HG11	2:E:60:TRP:CZ2	2.56	0.41
1:A:1964:GLU:HA	1:A:3651:CYS:SG	2.61	0.41
1:A:1967:VAL:CG2	1:A:3650:ALA:HB1	2.49	0.41
1:A:1973:ASN:OD1	1:A:2025:PRO:HD3	2.21	0.41
1:A:2624:LEU:O	1:A:2628:VAL:HG23	2.21	0.41
1:A:3004:LEU:HD11	1:A:3065:VAL:HG22	2.03	0.41
1:A:3061:ASP:O	1:A:3065:VAL:HG23	2.21	0.41
1:A:3457:GLN:O	1:A:3460:VAL:HG12	2.20	0.41
1:A:4239:SER:OG	1:A:4673:LYS:NZ	2.53	0.41
1:A:4723:LEU:HA	1:A:4735:ILE:HG21	2.03	0.41
1:B:760:ILE:O	1:B:760:ILE:HG23	2.20	0.41
1:B:1014:ILE:H	1:B:1014:ILE:HD12	1.86	0.41
1:B:3447:SER:O	1:B:3453:LYS:NZ	2.53	0.41
1:B:3537:ALA:HB3	1:B:3601:SER:CB	2.51	0.41
1:B:4993:LEU:HD23	1:B:4993:LEU:HA	1.82	0.41
1:C:47:LEU:HD21	1:C:126:ARG:HE	1.85	0.41
1:C:1014:ILE:H	1:C:1014:ILE:HD12	1.86	0.41
1:C:1053:ASN:OD1	1:C:1053:ASN:O	2.39	0.41
1:C:1973:ASN:OD1	1:C:2025:PRO:HD3	2.21	0.41
1:C:2215:VAL:HG21	1:C:2229:MET:CE	2.51	0.41
1:C:2306:CYS:O	1:C:2325:ASN:N	2.50	0.41
1:C:2523:LEU:HD23	1:C:2579:MET:SD	2.61	0.41
1:C:2871:GLU:OE1	1:C:2875:MET:CE	2.69	0.41
1:C:4153:LEU:HB3	1:C:4163:LEU:HD21	2.03	0.41
1:C:4664:VAL:N	1:C:4665:PRO:CD	2.83	0.41
1:D:47:LEU:CD2	1:D:126:ARG:HE	2.33	0.41
1:D:1014:ILE:H	1:D:1014:ILE:HD12	1.86	0.41
1:D:1964:GLU:HA	1:D:3651:CYS:SG	2.61	0.41
1:D:3457:GLN:O	1:D:3460:VAL:HG12	2.20	0.41
1:D:3894:LEU:O	1:D:3902:PHE:HD2	2.04	0.41
1:D:5011:MET:HE1	1:D:5018:ASP:HB2	2.02	0.41
1:A:369:ARG:HH21	1:A:2309:GLN:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1822:ARG:O	1:A:1826:GLN:HG2	2.21	0.41
1:A:3037:LYS:O	1:A:3040:ILE:HG22	2.21	0.41
1:A:3515:LEU:O	1:A:3516:LYS:C	2.60	0.41
1:A:3537:ALA:HB3	1:A:3601:SER:CB	2.51	0.41
1:A:3908:THR:HG23	1:A:3908:THR:O	2.21	0.41
2:F:24:VAL:HG12	2:F:105:LEU:HD12	2.03	0.41
1:B:369:ARG:HH21	1:B:2309:GLN:CB	2.34	0.41
1:B:596:ARG:NH2	1:B:1644:GLU:OE1	2.53	0.41
1:B:1740:THR:HG22	1:B:2147:VAL:HG22	2.03	0.41
1:B:2564:THR:HG22	1:B:2607:CYS:CA	2.46	0.41
1:B:3316:LEU:HD23	1:B:3346:ILE:HD13	2.03	0.41
1:B:3954:PHE:O	1:B:3958:MET:HG3	2.20	0.41
1:B:4239:SER:OG	1:B:4673:LYS:NZ	2.53	0.41
1:C:369:ARG:HH21	1:C:2309:GLN:CB	2.34	0.41
1:C:782:VAL:O	1:C:782:VAL:HG13	2.21	0.41
1:C:1043:ALA:O	1:C:1047:LEU:HD23	2.21	0.41
1:C:1531:THR:HG22	1:C:1536:GLU:HA	2.02	0.41
1:C:1740:THR:HG22	1:C:2147:VAL:HG22	2.03	0.41
1:C:3230:ILE:HD12	1:C:3230:ILE:H	1.86	0.41
1:C:3908:THR:O	1:C:3908:THR:HG23	2.21	0.41
1:D:877:GLU:O	1:D:881:GLU:HG2	2.21	0.41
1:D:1154:ILE:O	1:D:1154:ILE:HG23	2.21	0.41
1:D:1822:ARG:O	1:D:1826:GLN:HG2	2.21	0.41
1:D:3515:LEU:O	1:D:3516:LYS:C	2.60	0.41
1:D:3908:THR:HG23	1:D:3908:THR:O	2.21	0.41
1:D:3940:TYR:OH	1:D:3947:GLU:OE2	2.37	0.41
1:D:4148:VAL:HG22	1:D:4181:LEU:HD13	2.02	0.41
1:A:2215:VAL:HG21	1:A:2229:MET:CE	2.51	0.40
1:A:2507:LEU:C	1:A:2507:LEU:HD23	2.41	0.40
1:A:2746:VAL:HG21	1:A:2818:ILE:CG2	2.52	0.40
7:A:8006:PCW:H41	7:A:8006:PCW:H63	1.88	0.40
2:E:27:TYR:HB2	2:E:60:TRP:HH2	1.86	0.40
2:H:27:TYR:HB2	2:H:60:TRP:HH2	1.86	0.40
1:B:47:LEU:HD21	1:B:126:ARG:HE	1.85	0.40
1:B:1521:VAL:HG12	1:B:1528:MET:HG2	2.02	0.40
1:B:1675:CYS:HB3	1:B:1686:LEU:HD12	2.03	0.40
1:B:3037:LYS:O	1:B:3040:ILE:HG22	2.21	0.40
1:B:3820:LEU:HD13	1:B:3902:PHE:CE1	2.56	0.40
1:C:627:LEU:N	1:C:628:PRO:HD2	2.36	0.40
1:C:3591:GLU:HA	1:C:3594:VAL:HG22	2.04	0.40
1:D:369:ARG:HH21	1:D:2309:GLN:CB	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:782:VAL:O	1:D:782:VAL:HG13	2.21	0.40
1:D:1675:CYS:HB3	1:D:1686:LEU:HD12	2.03	0.40
1:D:2215:VAL:HG21	1:D:2229:MET:CE	2.51	0.40
1:D:2523:LEU:HD23	1:D:2579:MET:SD	2.60	0.40
1:D:3037:LYS:O	1:D:3040:ILE:HG22	2.21	0.40
1:D:3253:GLU:O	1:D:3257:LEU:HD23	2.21	0.40
1:D:3820:LEU:HD11	1:D:3824:LYS:HE3	2.03	0.40
1:A:47:LEU:HD21	1:A:126:ARG:HE	1.85	0.40
1:A:576:LEU:HA	1:A:579:ILE:HG12	2.01	0.40
1:A:3316:LEU:HD23	1:A:3346:ILE:HD13	2.03	0.40
1:A:3820:LEU:HD13	1:A:3902:PHE:CE1	2.56	0.40
1:A:3954:PHE:O	1:A:3958:MET:HG3	2.20	0.40
1:B:2096:GLN:HA	1:B:2128:GLN:NE2	2.36	0.40
1:B:3230:ILE:H	1:B:3230:ILE:HD12	1.86	0.40
1:B:3253:GLU:O	1:B:3257:LEU:HD23	2.21	0.40
1:B:3591:GLU:HA	1:B:3594:VAL:HG22	2.03	0.40
1:B:3894:LEU:O	1:B:3902:PHE:HD2	2.04	0.40
1:C:2507:LEU:C	1:C:2507:LEU:HD23	2.41	0.40
1:C:2942:LEU:HB2	1:C:2945:MET:SD	2.60	0.40
1:C:3820:LEU:HD13	1:C:3902:PHE:CE1	2.56	0.40
1:D:878:ASN:ND2	1:D:1046:THR:HG21	2.35	0.40
1:D:2096:GLN:HA	1:D:2128:GLN:NE2	2.36	0.40
1:D:3061:ASP:O	1:D:3065:VAL:HG23	2.21	0.40
1:D:3820:LEU:HD13	1:D:3902:PHE:CE1	2.56	0.40
1:A:1014:ILE:HD12	1:A:1014:ILE:H	1.86	0.40
1:A:1154:ILE:HG23	1:A:1154:ILE:O	2.21	0.40
1:A:2908:PRO:O	1:A:2911:THR:OG1	2.33	0.40
1:A:3166:CYS:HB3	1:A:3202:MET:SD	2.62	0.40
1:A:4148:VAL:HG22	1:A:4181:LEU:HD13	2.02	0.40
1:B:878:ASN:ND2	1:B:1046:THR:HG21	2.35	0.40
1:B:2507:LEU:HD23	1:B:2507:LEU:C	2.41	0.40
1:B:2820:TRP:CE3	1:B:2822:TRP:CH2	3.09	0.40
1:B:2942:LEU:HB2	1:B:2945:MET:SD	2.60	0.40
1:C:369:ARG:NH2	1:C:2305:GLY:O	2.55	0.40
1:C:3533:LEU:HB3	1:C:3597:VAL:HG11	2.04	0.40
1:D:2564:THR:HG22	1:D:2607:CYS:CA	2.46	0.40
1:D:3537:ALA:HB3	1:D:3601:SER:CB	2.51	0.40
1:A:627:LEU:N	1:A:628:PRO:HD2	2.36	0.40
1:A:1531:THR:HG22	1:A:1536:GLU:HA	2.02	0.40
1:B:3061:ASP:O	1:B:3065:VAL:HG23	2.21	0.40
1:C:1822:ARG:O	1:C:1826:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2820:TRP:CE3	1:C:2822:TRP:CH2	3.09	0.40
1:C:3537:ALA:HB3	1:C:3601:SER:CB	2.52	0.40
1:D:4993:LEU:HD23	1:D:4993:LEU:HA	1.83	0.40
1:A:782:VAL:O	1:A:782:VAL:HG13	2.21	0.40
1:A:1053:ASN:OD1	1:A:1053:ASN:O	2.39	0.40
1:A:1297:GLN:NE2	1:A:1546:ASN:OD1	2.46	0.40
1:A:2871:GLU:OE1	1:A:2875:MET:CE	2.69	0.40
1:A:3894:LEU:O	1:A:3902:PHE:HD2	2.04	0.40
1:A:4153:LEU:HB3	1:A:4163:LEU:HD21	2.03	0.40
1:B:877:GLU:O	1:B:881:GLU:HG2	2.21	0.40
1:B:1043:ALA:O	1:B:1047:LEU:HD23	2.20	0.40
1:C:1124:VAL:HG23	1:C:1133:TRP:HB2	2.04	0.40
1:C:1821:VAL:HG22	1:C:1927:LEU:HD21	2.04	0.40
1:C:3061:ASP:O	1:C:3065:VAL:HG23	2.21	0.40
1:D:74:LEU:HD11	1:D:82:MET:HE3	2.03	0.40
1:D:1053:ASN:OD1	1:D:1053:ASN:O	2.39	0.40
1:D:1127:GLY:O	1:D:1143:PRO:HA	2.22	0.40
1:D:1282:ASN:OD1	1:D:1282:ASN:C	2.58	0.40
1:D:3316:LEU:HD23	1:D:3346:ILE:HD13	2.03	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	4345/5035 (86%)	4264 (98%)	81 (2%)	0	100	100
1	B	4345/5035 (86%)	4264 (98%)	81 (2%)	0	100	100
1	C	4345/5035 (86%)	4265 (98%)	80 (2%)	0	100	100
1	D	4345/5035 (86%)	4264 (98%)	81 (2%)	0	100	100
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
All	All	17800/20572 (86%)	17465 (98%)	335 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	3806/4296 (89%)	3802 (100%)	4 (0%)	93	98
1	B	3806/4296 (89%)	3802 (100%)	4 (0%)	93	98
1	C	3806/4296 (89%)	3802 (100%)	4 (0%)	93	98
1	D	3806/4296 (89%)	3802 (100%)	4 (0%)	93	98
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
All	All	15580/17544 (89%)	15564 (100%)	16 (0%)	93	98

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	953	LYS
1	A	992	ASN
1	A	1421	ASN
1	A	5010	LYS
1	B	953	LYS
1	B	992	ASN
1	B	1421	ASN
1	B	5010	LYS

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Mol	Chain	Res	Type
1	C	953	LYS
1	C	992	ASN
1	C	1421	ASN
1	C	5010	LYS
1	D	953	LYS
1	D	992	ASN
1	D	1421	ASN
1	D	5010	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	152	HIS
1	A	1275	HIS
1	A	2689	HIS
1	A	2764	HIS
1	A	2992	HIS
1	A	3070	HIS
1	A	3898	HIS
1	B	72	GLN
1	B	152	HIS
1	B	1275	HIS
1	B	2689	HIS
1	B	2764	HIS
1	B	2992	HIS
1	B	3070	HIS
1	B	3898	HIS
1	C	72	GLN
1	C	152	HIS
1	C	1275	HIS
1	C	2689	HIS
1	C	2764	HIS
1	C	2992	HIS
1	C	3070	HIS
1	C	3898	HIS
1	D	152	HIS
1	D	1275	HIS
1	D	2689	HIS
1	D	2764	HIS
1	D	2992	HIS
1	D	3070	HIS

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Mol	Chain	Res	Type
1	D	3898	HIS

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 28 ligands modelled in this entry, 8 are monoatomic - leaving 20 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	$\#\|Z\| > 2$
7	PCW	D	5107	-	53,53,53	1.17	5 (9%)	59,61,61	2.38	9 (15%)
5	ATP	A	8005	-	26,33,33	0.60	0	31,52,52	1.04	2 (6%)
5	ATP	A	8003	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
4	CFF	B	8002	-	8,15,15	0.92	0	8,23,23	2.82	2 (25%)
4	CFF	A	8002	-	8,15,15	0.91	0	8,23,23	2.82	2 (25%)
7	PCW	A	8007	-	53,53,53	1.16	4 (7%)	59,61,61	2.29	9 (15%)
5	ATP	C	8005	-	26,33,33	0.60	0	31,52,52	1.05	2 (6%)
4	CFF	D	5103	-	8,15,15	0.90	0	8,23,23	2.82	2 (25%)
5	ATP	B	8003	-	26,33,33	0.67	0	31,52,52	0.72	1 (3%)
4	CFF	C	8002	-	8,15,15	0.90	0	8,23,23	2.83	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	PCW	D	5101	-	53,53,53	1.16	4 (7%)	59,61,61	2.29	9 (15%)
7	PCW	B	8006	-	53,53,53	1.17	5 (9%)	59,61,61	2.38	9 (15%)
7	PCW	C	8007	-	53,53,53	1.16	4 (7%)	59,61,61	2.29	9 (15%)
5	ATP	C	8003	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
5	ATP	D	5104	-	26,33,33	0.68	0	31,52,52	0.72	1 (3%)
7	PCW	C	8006	-	53,53,53	1.17	5 (9%)	59,61,61	2.38	9 (15%)
7	PCW	B	8007	-	53,53,53	1.16	4 (7%)	59,61,61	2.29	9 (15%)
5	ATP	D	5106	-	26,33,33	0.60	0	31,52,52	1.04	2 (6%)
5	ATP	B	8005	-	26,33,33	0.60	0	31,52,52	1.04	2 (6%)
7	PCW	A	8006	-	53,53,53	1.17	5 (9%)	59,61,61	2.38	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
7	PCW	D	5107	-	-	25/57/57/57	-
5	ATP	A	8005	-	-	7/18/38/38	0/3/3/3
5	ATP	A	8003	-	-	6/18/38/38	0/3/3/3
4	CFF	B	8002	-	-	-	0/2/2/2
4	CFF	A	8002	-	-	-	0/2/2/2
7	PCW	A	8007	-	-	15/57/57/57	-
5	ATP	C	8005	-	-	7/18/38/38	0/3/3/3
4	CFF	D	5103	-	-	-	0/2/2/2
5	ATP	B	8003	-	-	6/18/38/38	0/3/3/3
7	PCW	D	5101	-	-	15/57/57/57	-
4	CFF	C	8002	-	-	-	0/2/2/2
7	PCW	B	8006	-	-	25/57/57/57	-
7	PCW	C	8007	-	-	15/57/57/57	-
5	ATP	C	8003	-	-	6/18/38/38	0/3/3/3
5	ATP	D	5104	-	-	6/18/38/38	0/3/3/3
7	PCW	C	8006	-	-	25/57/57/57	-
7	PCW	B	8007	-	-	15/57/57/57	-
5	ATP	D	5106	-	-	7/18/38/38	0/3/3/3
5	ATP	B	8005	-	-	7/18/38/38	0/3/3/3
7	PCW	A	8006	-	-	25/57/57/57	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	8006	PCW	O3-C11	3.18	1.42	1.33
7	A	8006	PCW	O3-C11	3.17	1.42	1.33
7	C	8006	PCW	O3-C11	3.17	1.42	1.33
7	D	5107	PCW	O3-C11	3.17	1.42	1.33
7	A	8007	PCW	O3-C11	3.03	1.42	1.33
7	B	8007	PCW	O3-C11	3.03	1.42	1.33
7	C	8007	PCW	O3-C11	3.03	1.42	1.33
7	D	5101	PCW	O3-C11	3.03	1.42	1.33
7	A	8007	PCW	O2-C31	2.99	1.42	1.34
7	B	8007	PCW	O2-C31	2.97	1.42	1.34
7	D	5101	PCW	O2-C31	2.97	1.42	1.34
7	C	8007	PCW	O2-C31	2.94	1.42	1.34
7	B	8006	PCW	O2-C31	2.87	1.42	1.34
7	A	8006	PCW	O2-C31	2.85	1.42	1.34
7	C	8006	PCW	O2-C31	2.85	1.42	1.34
7	D	5107	PCW	O2-C31	2.82	1.42	1.34
7	B	8006	PCW	O2-C2	-2.51	1.40	1.46
7	D	5107	PCW	O2-C2	-2.51	1.40	1.46
7	A	8006	PCW	O2-C2	-2.51	1.40	1.46
7	C	8006	PCW	O2-C2	-2.51	1.40	1.46
7	A	8007	PCW	O2-C2	-2.41	1.40	1.46
7	D	5101	PCW	O2-C2	-2.40	1.40	1.46
7	C	8007	PCW	O2-C2	-2.38	1.40	1.46
7	B	8007	PCW	O2-C2	-2.37	1.40	1.46
7	A	8006	PCW	C5-C4	2.19	1.58	1.51
7	C	8006	PCW	C5-C4	2.19	1.58	1.51
7	D	5107	PCW	C5-C4	2.19	1.58	1.51
7	B	8006	PCW	C5-C4	2.19	1.58	1.51
7	B	8006	PCW	P-O4P	2.11	1.67	1.59
7	A	8006	PCW	P-O4P	2.09	1.67	1.59
7	C	8006	PCW	P-O4P	2.09	1.67	1.59
7	D	5107	PCW	P-O4P	2.09	1.67	1.59
7	B	8007	PCW	P-O4P	2.08	1.67	1.59
7	C	8007	PCW	P-O4P	2.06	1.67	1.59
7	D	5101	PCW	P-O4P	2.06	1.67	1.59
7	A	8007	PCW	P-O4P	2.06	1.67	1.59

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	8006	PCW	C8-N-C6	12.51	141.14	108.97
7	A	8006	PCW	C8-N-C6	12.50	141.12	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	8006	PCW	C8-N-C6	12.50	141.12	108.97
7	D	5107	PCW	C8-N-C6	12.50	141.12	108.97
7	A	8007	PCW	C8-N-C6	11.23	137.85	108.97
7	B	8007	PCW	C8-N-C6	11.23	137.85	108.97
7	C	8007	PCW	C8-N-C6	11.23	137.85	108.97
7	D	5101	PCW	C8-N-C6	11.23	137.85	108.97
7	C	8007	PCW	C7-N-C5	7.44	140.35	109.92
7	A	8007	PCW	C7-N-C5	7.43	140.33	109.92
7	D	5101	PCW	C7-N-C5	7.43	140.32	109.92
7	B	8007	PCW	C7-N-C5	7.42	140.29	109.92
7	D	5107	PCW	C7-N-C5	6.70	137.34	109.92
7	A	8006	PCW	C7-N-C5	6.69	137.31	109.92
7	C	8006	PCW	C7-N-C5	6.69	137.31	109.92
7	B	8006	PCW	C7-N-C5	6.68	137.25	109.92
4	B	8002	CFF	C5-C6-N1	-6.01	111.80	118.20
4	A	8002	CFF	C5-C6-N1	-5.99	111.81	118.20
4	C	8002	CFF	C5-C6-N1	-5.99	111.81	118.20
4	D	5103	CFF	C5-C6-N1	-5.99	111.81	118.20
7	A	8006	PCW	C8-N-C7	-5.86	93.92	108.97
7	C	8006	PCW	C8-N-C7	-5.86	93.92	108.97
7	D	5107	PCW	C8-N-C7	-5.86	93.92	108.97
7	B	8006	PCW	C8-N-C7	-5.86	93.92	108.97
7	A	8007	PCW	C7-N-C6	-5.28	95.40	108.97
7	C	8007	PCW	C7-N-C6	-5.27	95.41	108.97
7	D	5101	PCW	C7-N-C6	-5.27	95.41	108.97
7	B	8007	PCW	C7-N-C6	-5.27	95.43	108.97
7	C	8007	PCW	C8-N-C7	-5.21	95.58	108.97
7	D	5101	PCW	C8-N-C7	-5.21	95.58	108.97
7	B	8007	PCW	C8-N-C7	-5.21	95.59	108.97
7	A	8007	PCW	C8-N-C7	-5.20	95.61	108.97
7	B	8006	PCW	C7-N-C6	-5.05	95.99	108.97
7	A	8006	PCW	C7-N-C6	-5.05	95.99	108.97
7	C	8006	PCW	C7-N-C6	-5.05	95.99	108.97
7	D	5107	PCW	C7-N-C6	-5.05	95.99	108.97
4	C	8002	CFF	C4-C5-C6	4.68	122.97	119.96
4	D	5103	CFF	C4-C5-C6	4.68	122.97	119.96
4	A	8002	CFF	C4-C5-C6	4.66	122.95	119.96
4	B	8002	CFF	C4-C5-C6	4.64	122.94	119.96
7	B	8007	PCW	C21-C20-C19	3.80	153.88	124.73
7	D	5101	PCW	C21-C20-C19	3.80	153.88	124.73
7	C	8007	PCW	C21-C20-C19	3.80	153.87	124.73
7	A	8007	PCW	C21-C20-C19	3.80	153.85	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	8006	PCW	C21-C20-C19	3.76	153.59	124.73
7	A	8006	PCW	C21-C20-C19	3.76	153.58	124.73
7	D	5107	PCW	C21-C20-C19	3.76	153.58	124.73
7	B	8006	PCW	C21-C20-C19	3.76	153.57	124.73
7	D	5107	PCW	O2-C31-C32	3.55	119.15	111.50
7	A	8006	PCW	O2-C31-C32	3.55	119.14	111.50
7	C	8006	PCW	O2-C31-C32	3.55	119.14	111.50
7	B	8006	PCW	O2-C31-C32	3.54	119.14	111.50
7	C	8007	PCW	O2-C31-C32	3.28	118.57	111.50
7	B	8007	PCW	O2-C31-C32	3.28	118.56	111.50
7	D	5101	PCW	O2-C31-C32	3.28	118.56	111.50
7	A	8007	PCW	O2-C31-C32	3.27	118.55	111.50
7	A	8007	PCW	C8-N-C5	-3.21	96.79	109.92
7	C	8007	PCW	C8-N-C5	-3.21	96.79	109.92
7	B	8007	PCW	C8-N-C5	-3.21	96.80	109.92
7	D	5101	PCW	C8-N-C5	-3.21	96.80	109.92
7	D	5107	PCW	C8-N-C5	-2.71	98.82	109.92
7	A	8006	PCW	C8-N-C5	-2.71	98.82	109.92
7	B	8006	PCW	C8-N-C5	-2.71	98.82	109.92
7	C	8006	PCW	C8-N-C5	-2.71	98.82	109.92
7	D	5107	PCW	C6-N-C5	-2.69	98.93	109.92
7	A	8006	PCW	C6-N-C5	-2.68	98.95	109.92
7	C	8006	PCW	C6-N-C5	-2.68	98.95	109.92
7	B	8006	PCW	C6-N-C5	-2.68	98.96	109.92
7	A	8007	PCW	C6-N-C5	-2.39	100.14	109.92
7	C	8007	PCW	C6-N-C5	-2.39	100.14	109.92
7	B	8007	PCW	C6-N-C5	-2.38	100.16	109.92
7	D	5101	PCW	C6-N-C5	-2.38	100.16	109.92
7	B	8006	PCW	O3-C11-C12	2.33	119.23	111.91
7	A	8006	PCW	O3-C11-C12	2.33	119.21	111.91
7	D	5107	PCW	O3-C11-C12	2.33	119.21	111.91
7	C	8006	PCW	O3-C11-C12	2.32	119.20	111.91
7	A	8007	PCW	O3-C11-C12	2.32	119.18	111.91
7	B	8007	PCW	O3-C11-C12	2.32	119.18	111.91
7	C	8007	PCW	O3-C11-C12	2.32	119.18	111.91
7	D	5101	PCW	O3-C11-C12	2.32	119.18	111.91
5	C	8005	ATP	C5-C6-N6	2.29	123.83	120.35
5	B	8005	ATP	C5-C6-N6	2.28	123.82	120.35
5	A	8005	ATP	C5-C6-N6	2.27	123.80	120.35
5	D	5106	ATP	C5-C6-N6	2.27	123.80	120.35
5	C	8003	ATP	C5-C6-N6	2.18	123.66	120.35
5	A	8003	ATP	C5-C6-N6	2.18	123.66	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	8003	ATP	C5-C6-N6	2.18	123.66	120.35
5	D	5104	ATP	C5-C6-N6	2.16	123.63	120.35
5	B	8005	ATP	PB-O3B-PG	2.04	139.83	132.83
5	A	8005	ATP	PB-O3B-PG	2.04	139.82	132.83
5	C	8005	ATP	PB-O3B-PG	2.04	139.82	132.83
5	D	5106	ATP	PB-O3B-PG	2.04	139.82	132.83

There are no chirality outliers.

All (212) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	8003	ATP	C5'-O5'-PA-O1A
5	A	8005	ATP	PB-O3B-PG-O2G
5	A	8005	ATP	C5'-O5'-PA-O3A
5	A	8005	ATP	C3'-C4'-C5'-O5'
5	B	8003	ATP	C5'-O5'-PA-O1A
5	B	8005	ATP	PB-O3B-PG-O2G
5	B	8005	ATP	C5'-O5'-PA-O3A
5	B	8005	ATP	C3'-C4'-C5'-O5'
5	C	8003	ATP	C5'-O5'-PA-O1A
5	C	8005	ATP	PB-O3B-PG-O2G
5	C	8005	ATP	C5'-O5'-PA-O3A
5	C	8005	ATP	C3'-C4'-C5'-O5'
5	D	5104	ATP	C5'-O5'-PA-O1A
5	D	5106	ATP	PB-O3B-PG-O2G
5	D	5106	ATP	C5'-O5'-PA-O3A
5	D	5106	ATP	C3'-C4'-C5'-O5'
5	A	8005	ATP	O4'-C4'-C5'-O5'
5	B	8005	ATP	O4'-C4'-C5'-O5'
5	C	8005	ATP	O4'-C4'-C5'-O5'
5	D	5106	ATP	O4'-C4'-C5'-O5'
7	A	8006	PCW	C24-C25-C26-C27
7	B	8006	PCW	C24-C25-C26-C27
7	C	8006	PCW	C24-C25-C26-C27
7	D	5107	PCW	C24-C25-C26-C27
7	A	8006	PCW	C1-O3P-P-O4P
7	A	8006	PCW	C4-O4P-P-O3P
7	B	8006	PCW	C1-O3P-P-O4P
7	B	8006	PCW	C4-O4P-P-O3P
7	C	8006	PCW	C1-O3P-P-O4P
7	C	8006	PCW	C4-O4P-P-O3P
7	D	5107	PCW	C1-O3P-P-O4P

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Mol	Chain	Res	Type	Atoms
7	D	5107	PCW	C4-O4P-P-O3P
7	D	5107	PCW	C14-C15-C16-C17
7	A	8006	PCW	C14-C15-C16-C17
7	A	8006	PCW	C15-C16-C17-C18
7	B	8006	PCW	C14-C15-C16-C17
7	B	8006	PCW	C15-C16-C17-C18
7	C	8006	PCW	C14-C15-C16-C17
7	C	8006	PCW	C15-C16-C17-C18
7	D	5107	PCW	C15-C16-C17-C18
7	A	8007	PCW	C44-C45-C46-C47
7	B	8007	PCW	C44-C45-C46-C47
7	C	8007	PCW	C44-C45-C46-C47
7	D	5101	PCW	C44-C45-C46-C47
7	A	8007	PCW	C24-C25-C26-C27
7	B	8007	PCW	C24-C25-C26-C27
7	C	8007	PCW	C24-C25-C26-C27
7	D	5101	PCW	C24-C25-C26-C27
7	A	8006	PCW	C35-C36-C37-C38
7	B	8006	PCW	C35-C36-C37-C38
7	C	8006	PCW	C35-C36-C37-C38
7	D	5107	PCW	C35-C36-C37-C38
7	B	8006	PCW	C43-C44-C45-C46
7	A	8006	PCW	C43-C44-C45-C46
7	C	8006	PCW	C43-C44-C45-C46
7	D	5107	PCW	C43-C44-C45-C46
7	A	8007	PCW	C4-C5-N-C8
7	B	8007	PCW	C4-C5-N-C8
7	C	8007	PCW	C4-C5-N-C8
7	D	5101	PCW	C4-C5-N-C8
7	B	8007	PCW	C14-C15-C16-C17
7	C	8007	PCW	C14-C15-C16-C17
7	A	8007	PCW	C14-C15-C16-C17
7	D	5101	PCW	C14-C15-C16-C17
7	A	8006	PCW	C44-C45-C46-C47
7	B	8006	PCW	C44-C45-C46-C47
7	C	8006	PCW	C44-C45-C46-C47
7	D	5107	PCW	C44-C45-C46-C47
7	A	8006	PCW	C32-C31-O2-C2
7	B	8006	PCW	C32-C31-O2-C2
7	C	8006	PCW	C32-C31-O2-C2
7	D	5107	PCW	C32-C31-O2-C2
7	A	8006	PCW	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	B	8006	PCW	C1-C2-C3-O3
7	C	8006	PCW	C1-C2-C3-O3
7	D	5107	PCW	C1-C2-C3-O3
7	A	8006	PCW	C17-C18-C19-C20
7	B	8006	PCW	C17-C18-C19-C20
7	C	8006	PCW	C17-C18-C19-C20
7	D	5107	PCW	C17-C18-C19-C20
5	A	8003	ATP	PG-O3B-PB-O1B
5	B	8003	ATP	PG-O3B-PB-O1B
5	C	8003	ATP	PG-O3B-PB-O1B
5	D	5104	ATP	PG-O3B-PB-O1B
7	A	8007	PCW	O3P-C1-C2-C3
7	B	8007	PCW	O3P-C1-C2-C3
7	C	8007	PCW	O3P-C1-C2-C3
7	D	5101	PCW	O3P-C1-C2-C3
7	A	8007	PCW	C2-C1-O3P-P
7	B	8007	PCW	C2-C1-O3P-P
7	C	8007	PCW	C2-C1-O3P-P
7	D	5101	PCW	C2-C1-O3P-P
7	A	8006	PCW	C40-C41-C42-C43
7	B	8006	PCW	C40-C41-C42-C43
7	C	8006	PCW	C40-C41-C42-C43
7	D	5107	PCW	C40-C41-C42-C43
7	B	8006	PCW	C13-C14-C15-C16
7	A	8006	PCW	C13-C14-C15-C16
7	D	5107	PCW	C13-C14-C15-C16
7	C	8006	PCW	C13-C14-C15-C16
7	A	8006	PCW	O31-C31-O2-C2
7	B	8006	PCW	O31-C31-O2-C2
7	C	8006	PCW	O31-C31-O2-C2
7	D	5107	PCW	O31-C31-O2-C2
7	B	8007	PCW	C23-C24-C25-C26
7	A	8007	PCW	C23-C24-C25-C26
7	C	8007	PCW	C23-C24-C25-C26
7	D	5101	PCW	C23-C24-C25-C26
5	A	8003	ATP	C5'-O5'-PA-O3A
5	B	8003	ATP	C5'-O5'-PA-O3A
5	C	8003	ATP	C5'-O5'-PA-O3A
5	D	5104	ATP	C5'-O5'-PA-O3A
5	A	8003	ATP	C5'-O5'-PA-O2A
5	A	8005	ATP	C5'-O5'-PA-O1A
5	A	8005	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	B	8003	ATP	C5'-O5'-PA-O2A
5	B	8005	ATP	C5'-O5'-PA-O1A
5	B	8005	ATP	C5'-O5'-PA-O2A
5	C	8003	ATP	C5'-O5'-PA-O2A
5	C	8005	ATP	C5'-O5'-PA-O1A
5	C	8005	ATP	C5'-O5'-PA-O2A
5	D	5104	ATP	C5'-O5'-PA-O2A
5	D	5106	ATP	C5'-O5'-PA-O1A
5	D	5106	ATP	C5'-O5'-PA-O2A
7	A	8006	PCW	C1-O3P-P-O2P
7	A	8006	PCW	C4-O4P-P-O1P
7	A	8006	PCW	C4-O4P-P-O2P
7	B	8006	PCW	C1-O3P-P-O2P
7	B	8006	PCW	C4-O4P-P-O1P
7	B	8006	PCW	C4-O4P-P-O2P
7	C	8006	PCW	C1-O3P-P-O2P
7	C	8006	PCW	C4-O4P-P-O1P
7	C	8006	PCW	C4-O4P-P-O2P
7	D	5107	PCW	C1-O3P-P-O2P
7	D	5107	PCW	C4-O4P-P-O1P
7	D	5107	PCW	C4-O4P-P-O2P
7	A	8007	PCW	C35-C36-C37-C38
7	B	8007	PCW	C35-C36-C37-C38
7	C	8007	PCW	C35-C36-C37-C38
7	D	5101	PCW	C35-C36-C37-C38
7	A	8007	PCW	O3P-C1-C2-O2
7	B	8007	PCW	O3P-C1-C2-O2
7	C	8007	PCW	O3P-C1-C2-O2
7	D	5101	PCW	O3P-C1-C2-O2
7	B	8007	PCW	C34-C35-C36-C37
7	D	5101	PCW	C34-C35-C36-C37
7	A	8007	PCW	C34-C35-C36-C37
7	C	8007	PCW	C34-C35-C36-C37
5	A	8005	ATP	PB-O3B-PG-O1G
5	B	8005	ATP	PB-O3B-PG-O1G
5	C	8005	ATP	PB-O3B-PG-O1G
5	D	5106	ATP	PB-O3B-PG-O1G
7	A	8007	PCW	C1-C2-O2-C31
7	B	8007	PCW	C1-C2-O2-C31
7	C	8007	PCW	C1-C2-O2-C31
7	D	5101	PCW	C1-C2-O2-C31
7	C	8006	PCW	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
7	A	8006	PCW	O2-C2-C3-O3
7	B	8006	PCW	O2-C2-C3-O3
7	C	8006	PCW	O2-C2-C3-O3
7	D	5107	PCW	O2-C2-C3-O3
7	A	8006	PCW	C11-C12-C13-C14
7	B	8006	PCW	C11-C12-C13-C14
7	D	5107	PCW	C11-C12-C13-C14
5	A	8003	ATP	PG-O3B-PB-O2B
5	B	8003	ATP	PG-O3B-PB-O2B
5	C	8003	ATP	PG-O3B-PB-O2B
5	D	5104	ATP	PG-O3B-PB-O2B
7	D	5107	PCW	C41-C42-C43-C44
7	A	8006	PCW	C41-C42-C43-C44
7	B	8006	PCW	C41-C42-C43-C44
7	C	8006	PCW	C41-C42-C43-C44
7	A	8006	PCW	C19-C20-C21-C22
7	C	8006	PCW	C19-C20-C21-C22
7	D	5107	PCW	C19-C20-C21-C22
7	B	8006	PCW	C19-C20-C21-C22
7	A	8006	PCW	C4-C5-N-C8
7	B	8006	PCW	C4-C5-N-C8
7	C	8006	PCW	C4-C5-N-C8
7	D	5107	PCW	C4-C5-N-C8
7	A	8007	PCW	C19-C20-C21-C22
7	B	8007	PCW	C19-C20-C21-C22
7	C	8007	PCW	C19-C20-C21-C22
7	D	5101	PCW	C19-C20-C21-C22
7	A	8006	PCW	C33-C34-C35-C36
7	D	5107	PCW	C33-C34-C35-C36
7	C	8006	PCW	C33-C34-C35-C36
7	B	8006	PCW	C33-C34-C35-C36
7	C	8007	PCW	O31-C31-O2-C2
7	D	5101	PCW	O31-C31-O2-C2
7	D	5107	PCW	C23-C24-C25-C26
7	A	8006	PCW	C23-C24-C25-C26
7	B	8006	PCW	C23-C24-C25-C26
7	C	8006	PCW	C23-C24-C25-C26
7	A	8007	PCW	O31-C31-O2-C2
7	B	8007	PCW	O31-C31-O2-C2
5	A	8003	ATP	O4'-C4'-C5'-O5'
5	B	8003	ATP	O4'-C4'-C5'-O5'
5	C	8003	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	D	5104	ATP	O4'-C4'-C5'-O5'
7	A	8006	PCW	C21-C22-C23-C24
7	B	8006	PCW	C21-C22-C23-C24
7	C	8006	PCW	C21-C22-C23-C24
7	D	5107	PCW	C21-C22-C23-C24
7	A	8007	PCW	C4-C5-N-C7
7	B	8007	PCW	C4-C5-N-C7
7	C	8007	PCW	C4-C5-N-C7
7	D	5101	PCW	C4-C5-N-C7
7	B	8007	PCW	C43-C44-C45-C46
7	A	8007	PCW	C43-C44-C45-C46
7	C	8007	PCW	C43-C44-C45-C46
7	D	5101	PCW	C43-C44-C45-C46

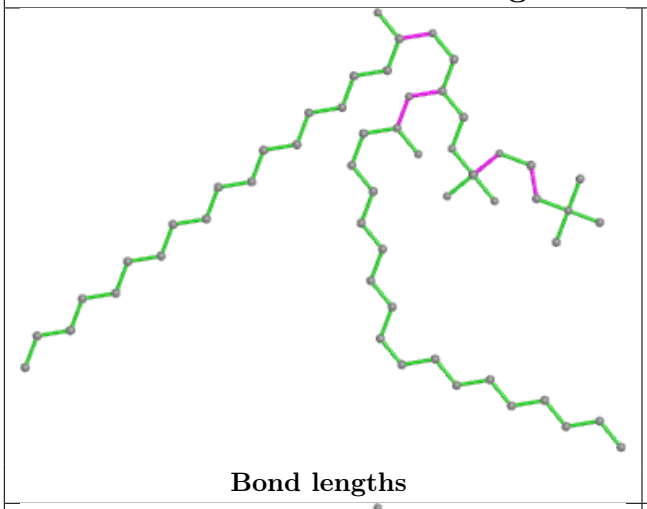
There are no ring outliers.

8 monomers are involved in 12 short contacts:

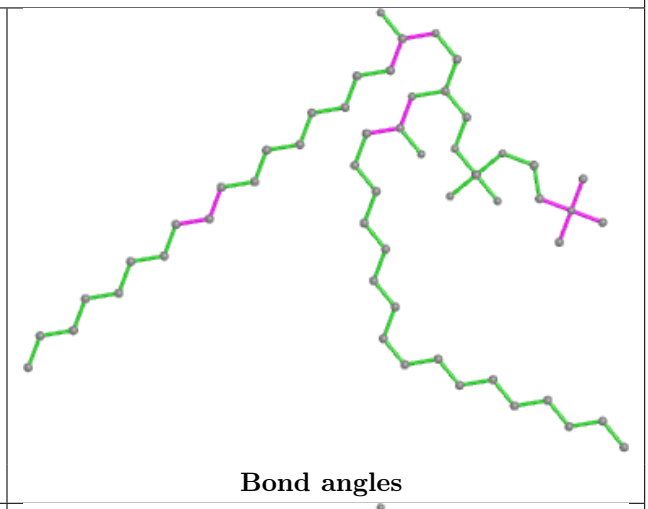
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	5107	PCW	1	0
7	A	8007	PCW	2	0
7	D	5101	PCW	2	0
7	B	8006	PCW	1	0
7	C	8007	PCW	2	0
7	C	8006	PCW	1	0
7	B	8007	PCW	2	0
7	A	8006	PCW	1	0

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

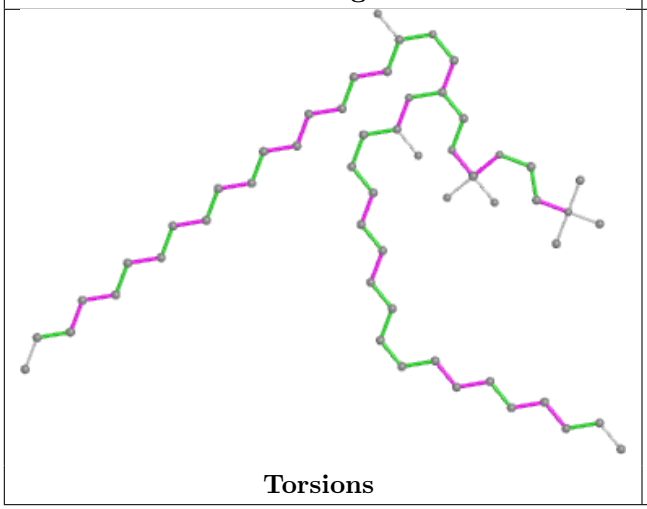
Ligand PCW D 5107



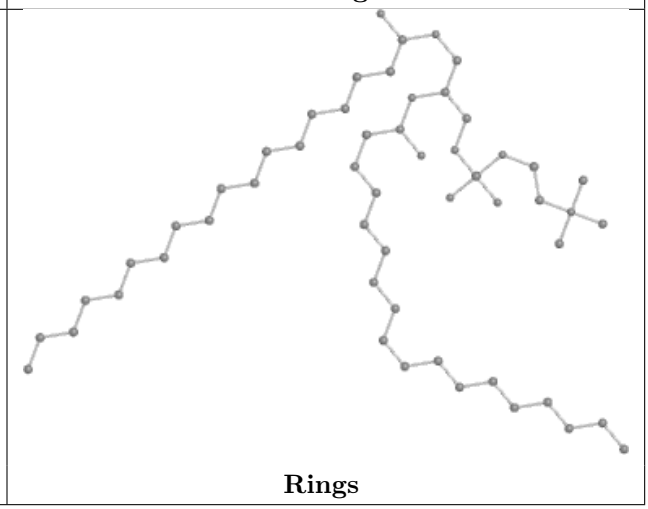
Bond lengths



Bond angles

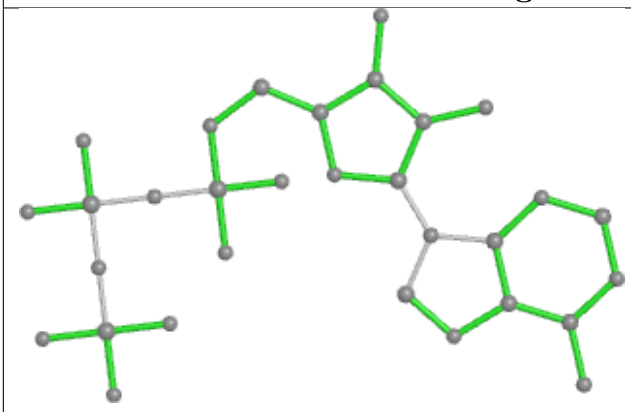


Torsions

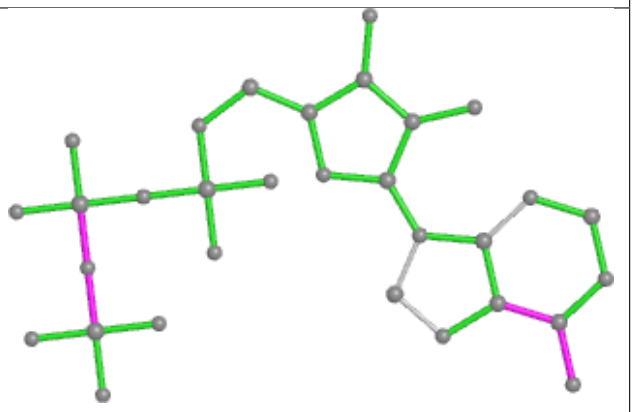


Rings

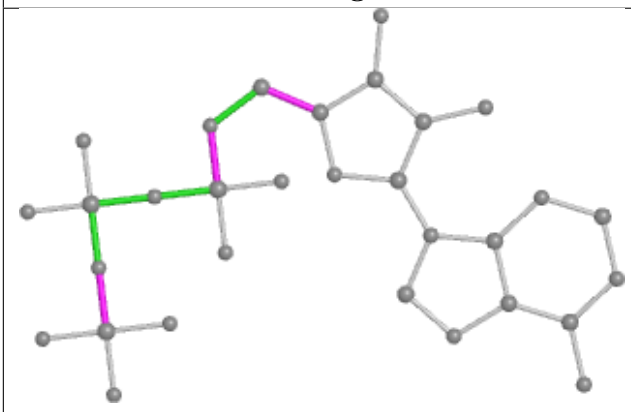
Ligand ATP A 8005



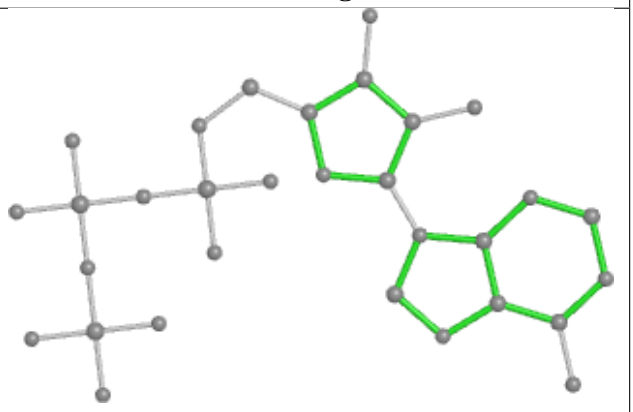
Bond lengths



Bond angles

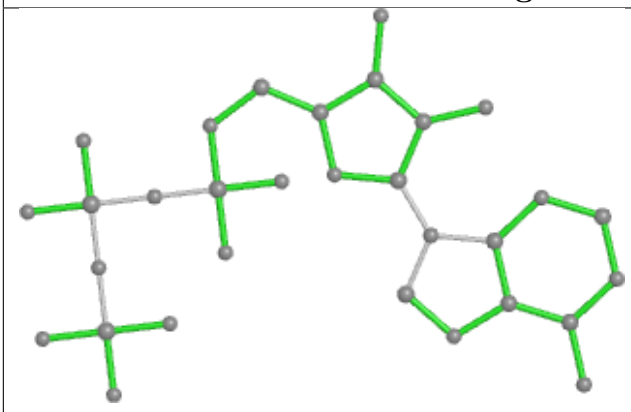


Torsions

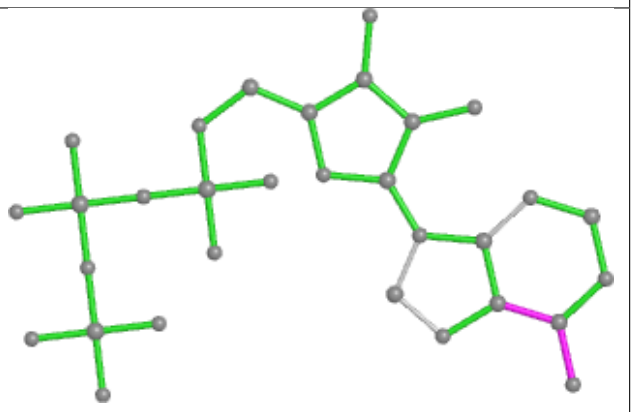


Rings

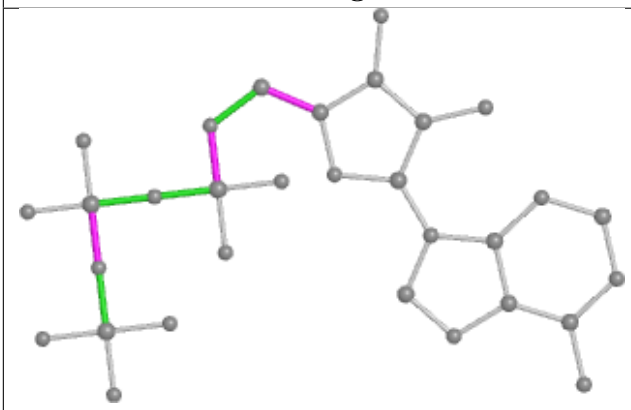
Ligand ATP A 8003



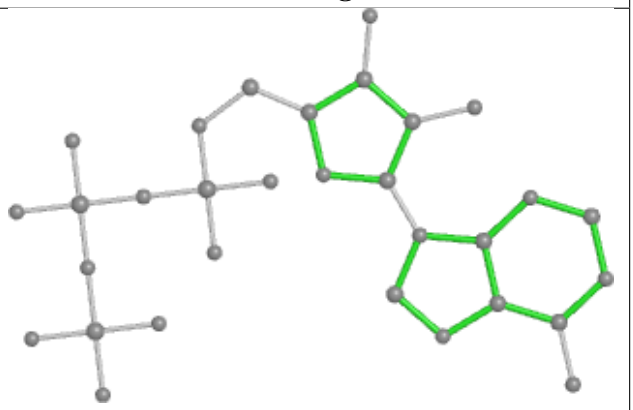
Bond lengths



Bond angles

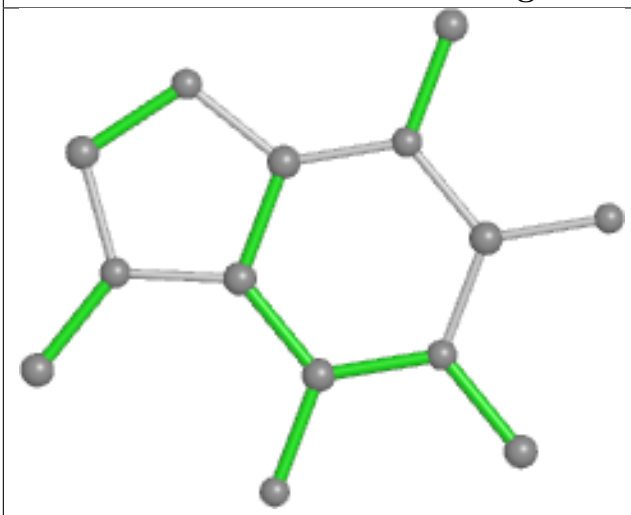


Torsions

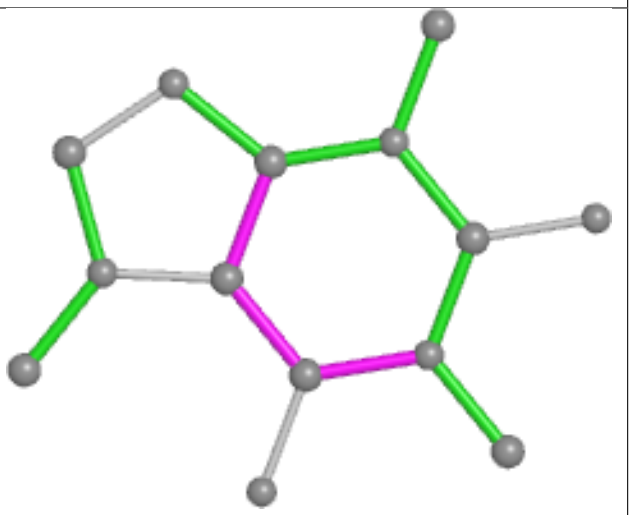


Rings

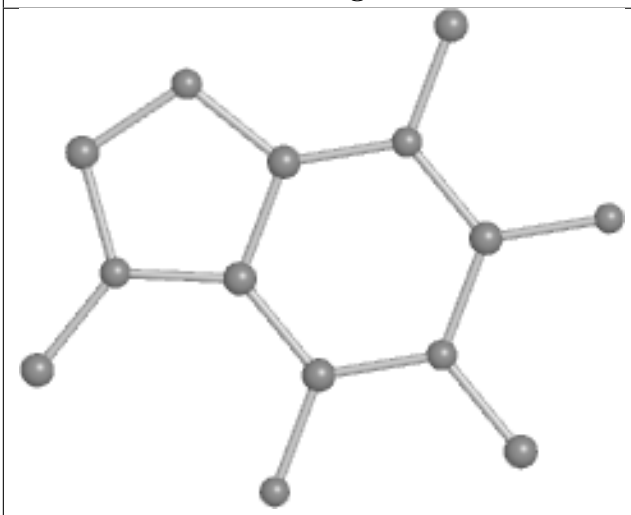
Ligand CFF B 8002



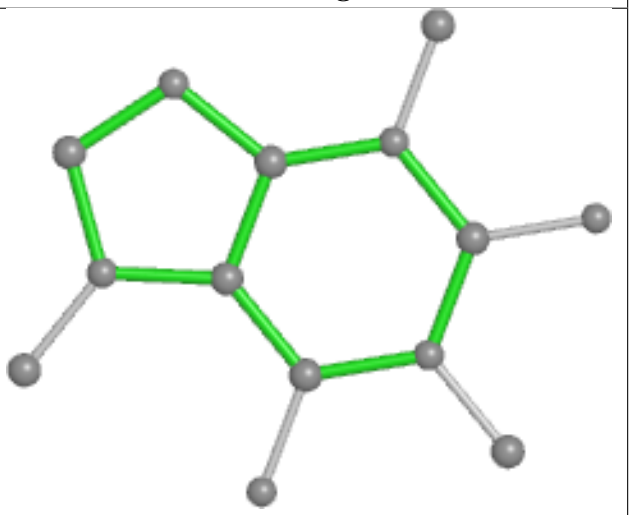
Bond lengths



Bond angles

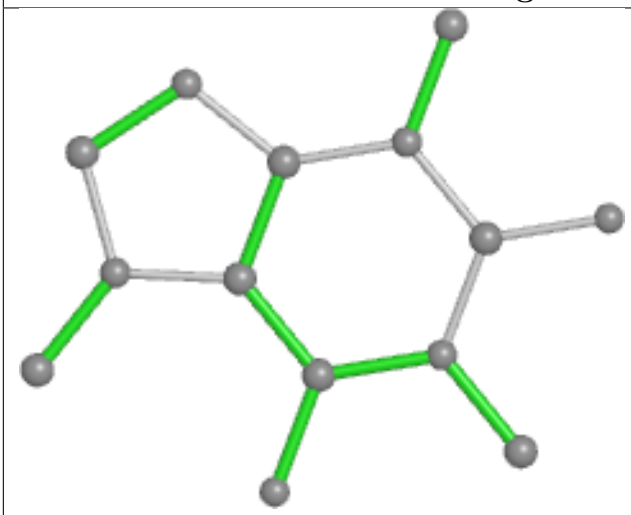


Torsions

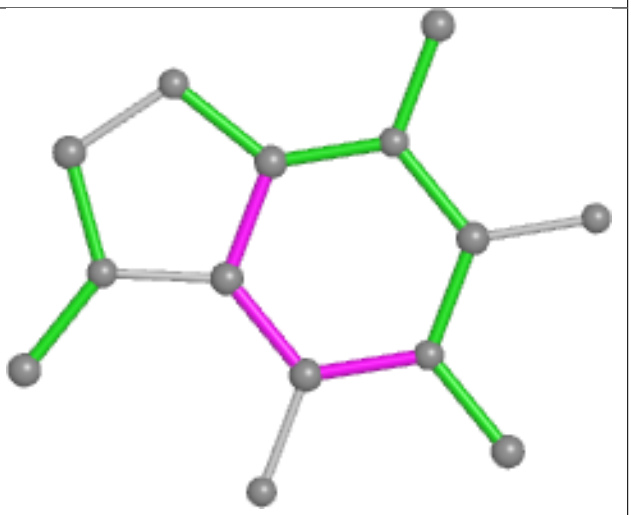


Rings

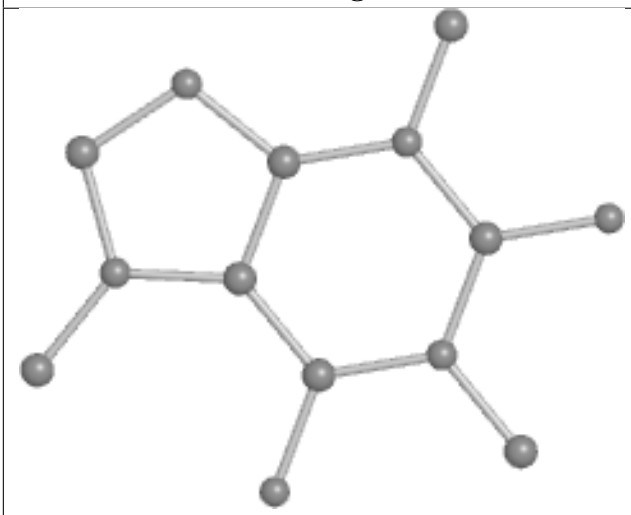
Ligand CFF A 8002



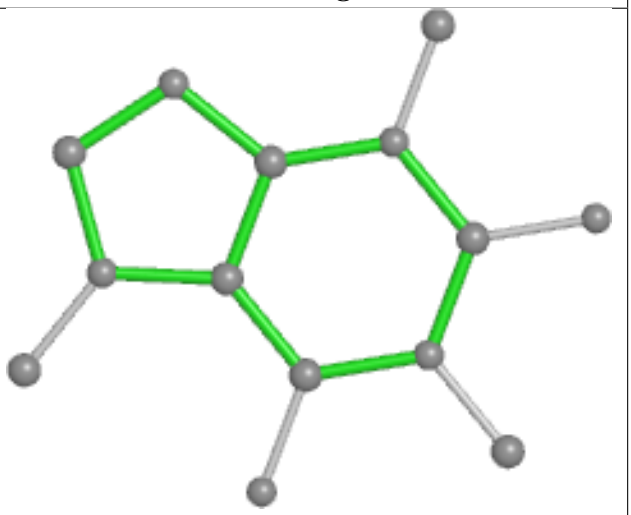
Bond lengths



Bond angles

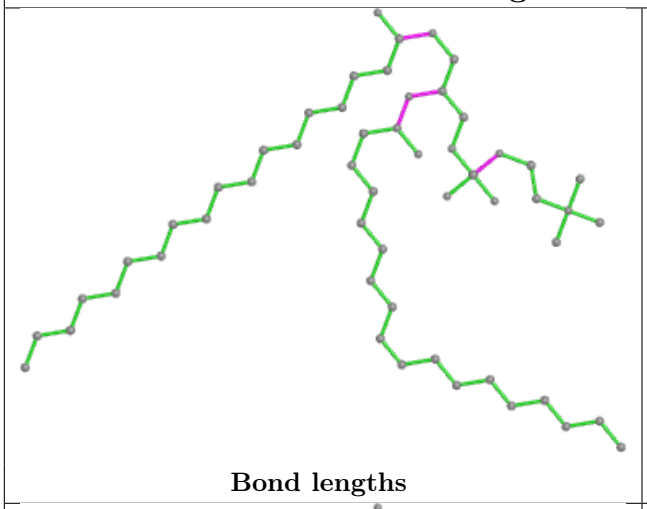


Torsions

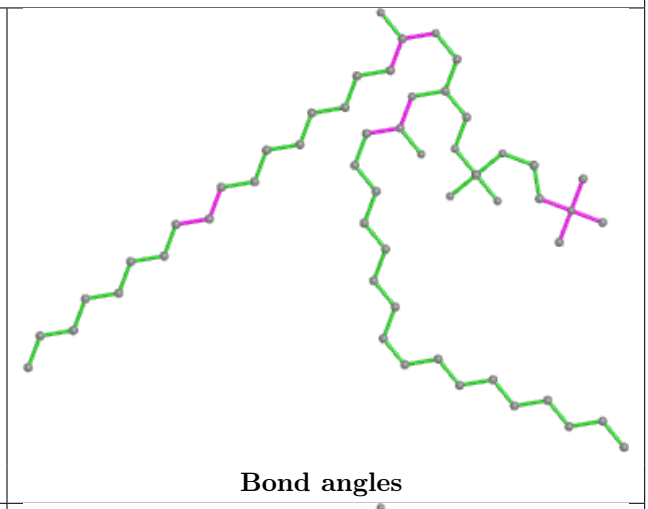


Rings

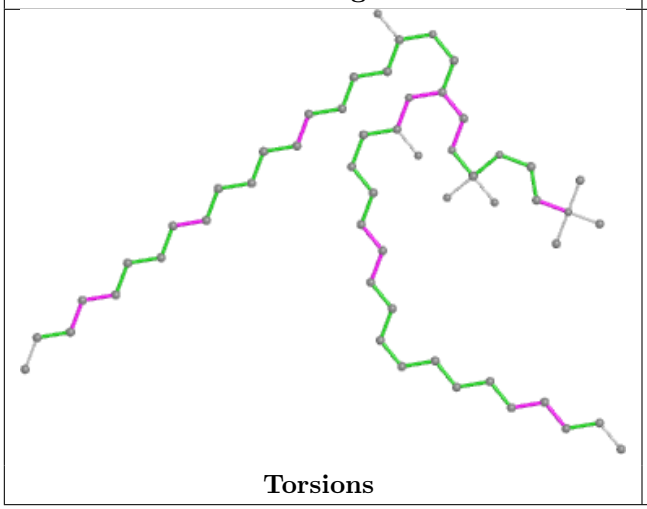
Ligand PCW A 8007



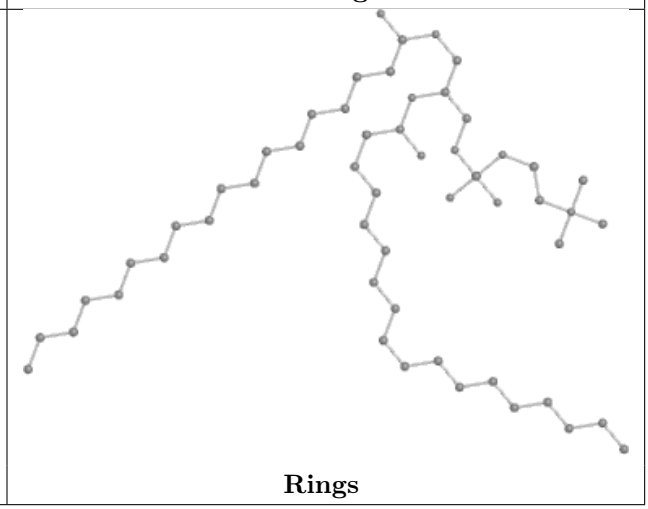
Bond lengths



Bond angles

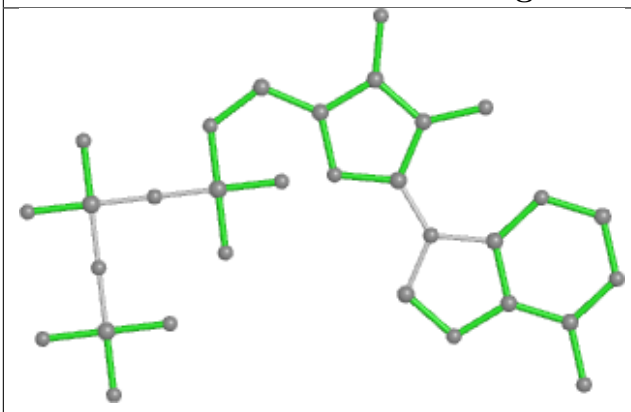


Torsions



Rings

Ligand ATP C 8005



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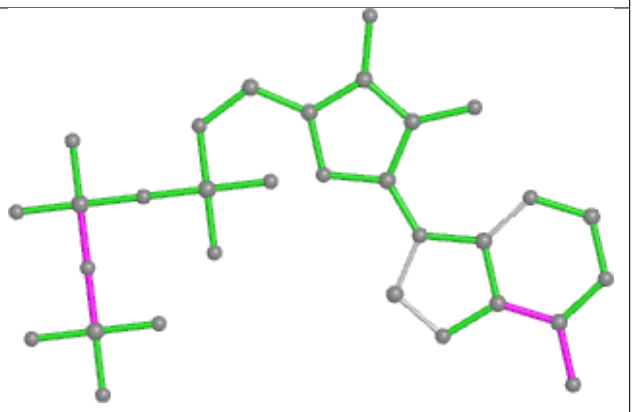
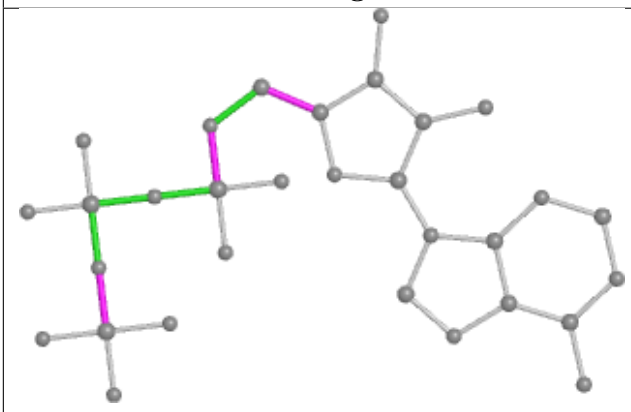


Bond angles



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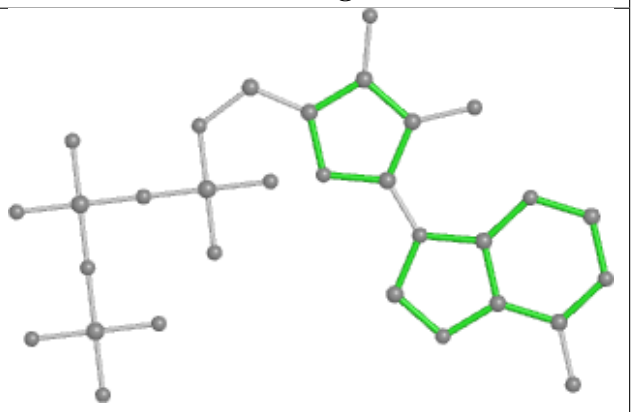
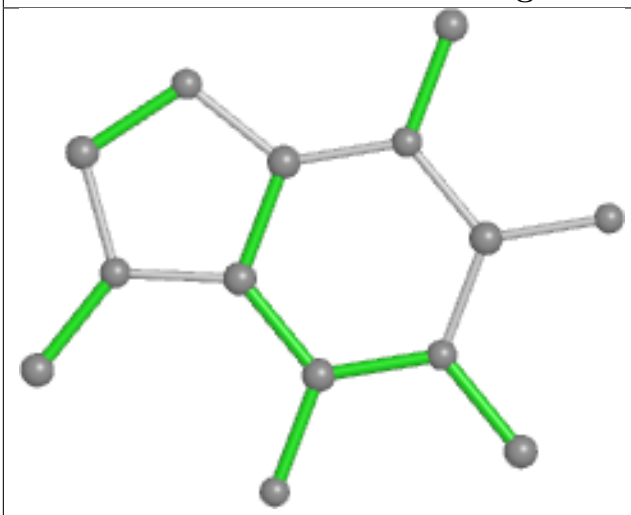


Rings

Ligand CFF D 5103



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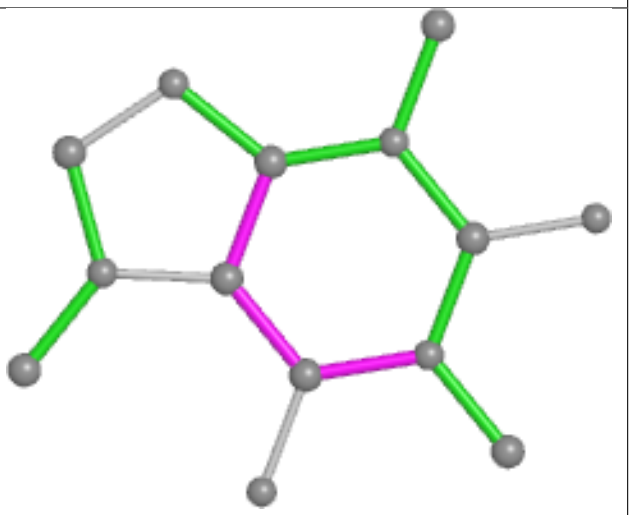
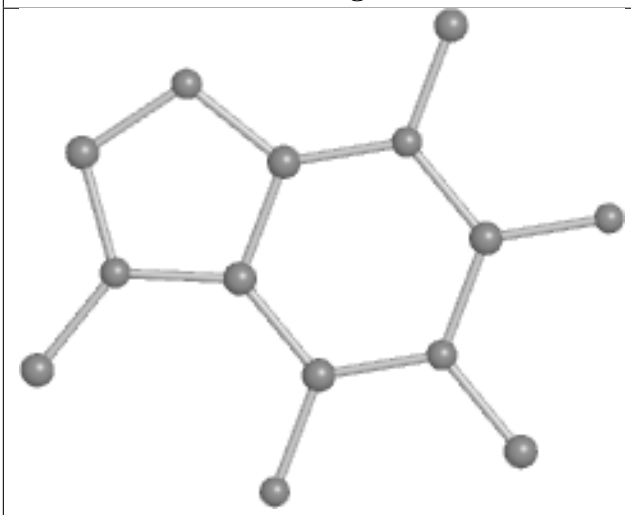
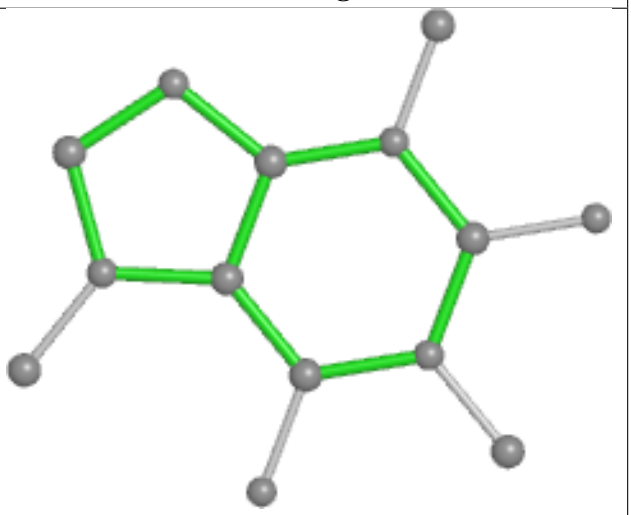


Bond angles

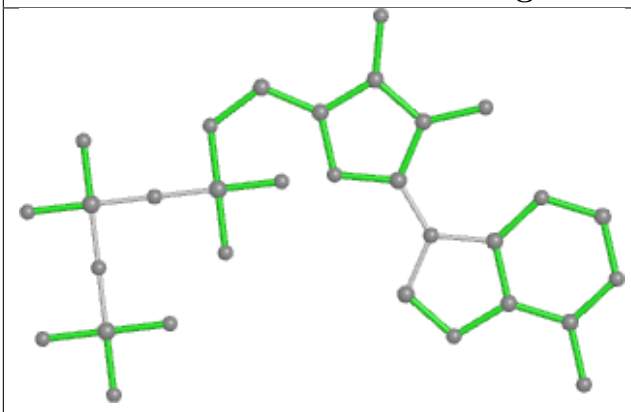


Torsions

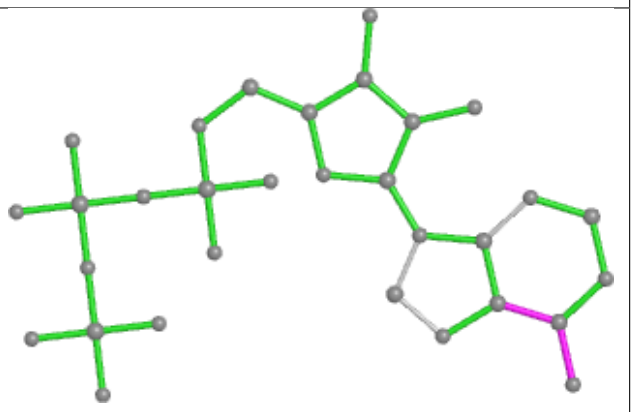


Rings

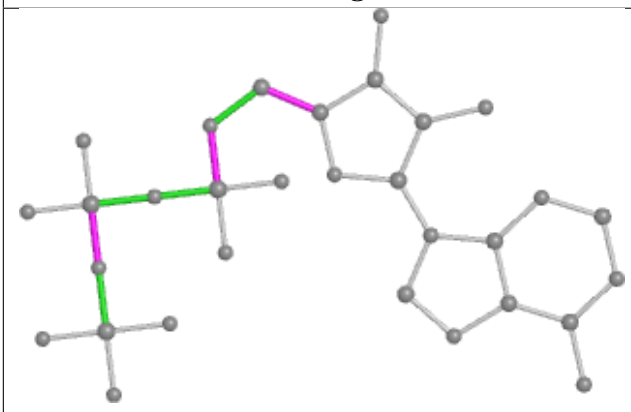
Ligand ATP B 8003



Bond lengths



Bond angles



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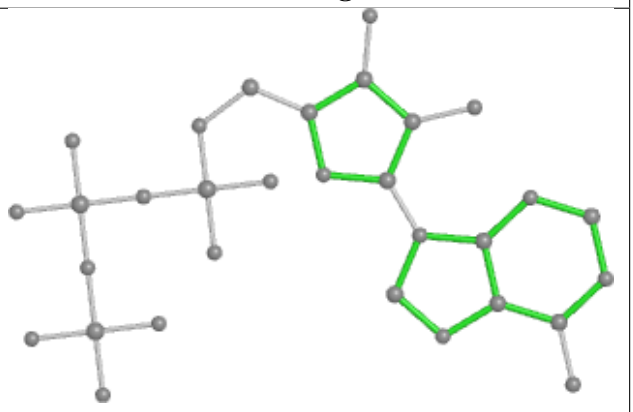
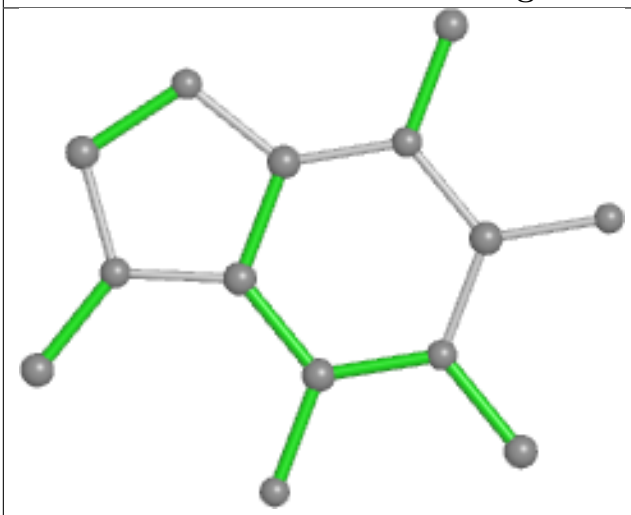
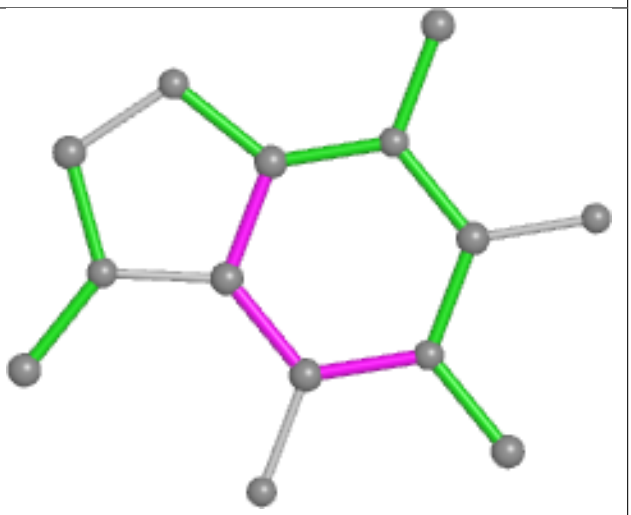


Rings

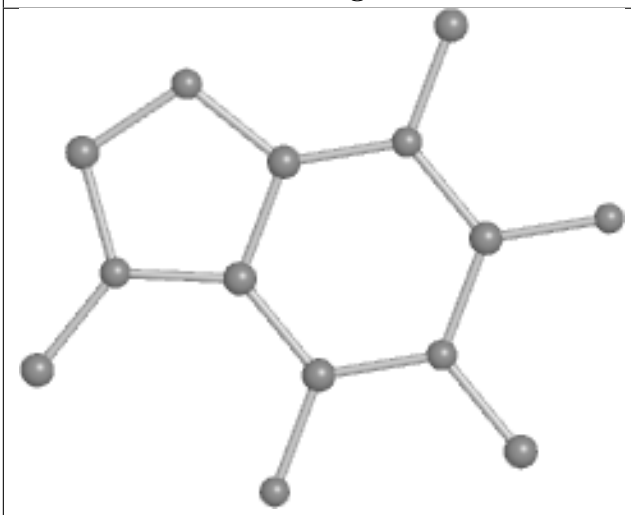
Ligand CFF C 8002



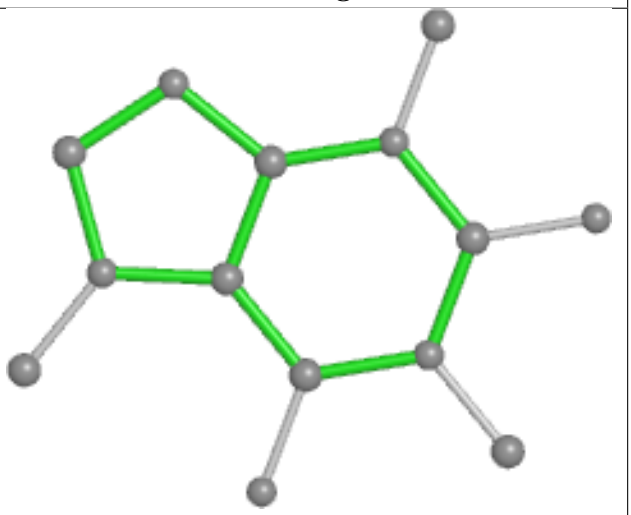
Bond lengths



Bond angles

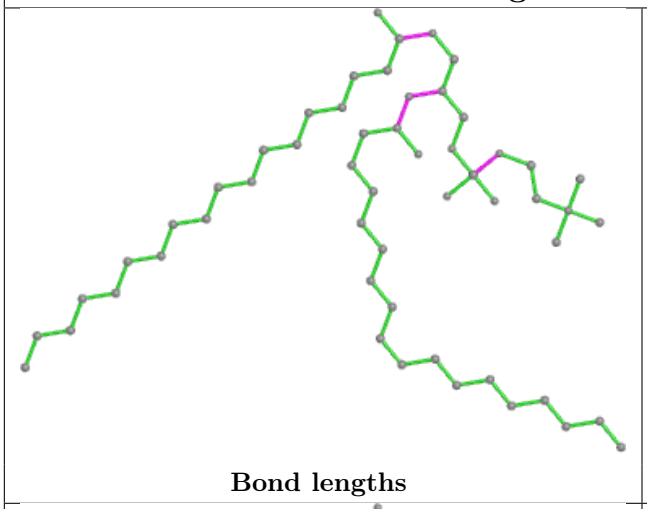


Torsions



Rings

Ligand PCW D 5101



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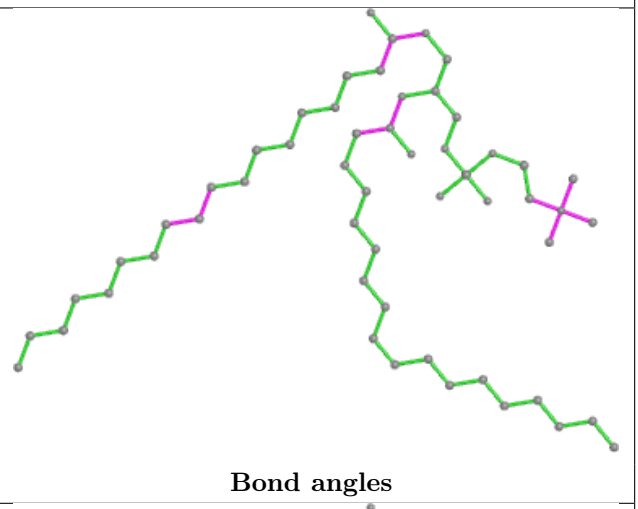
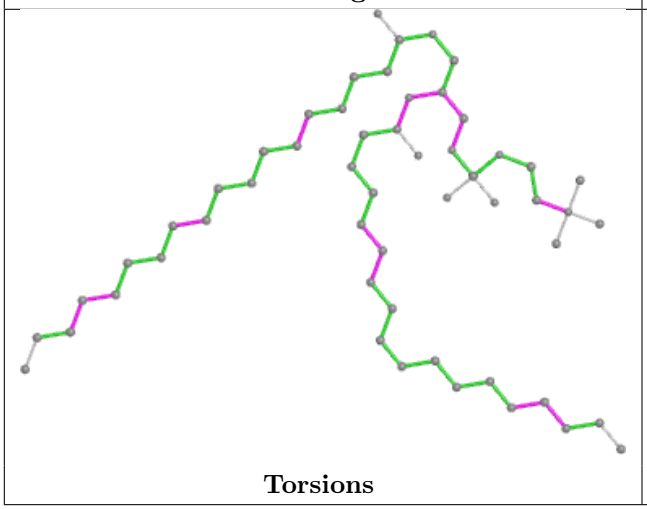
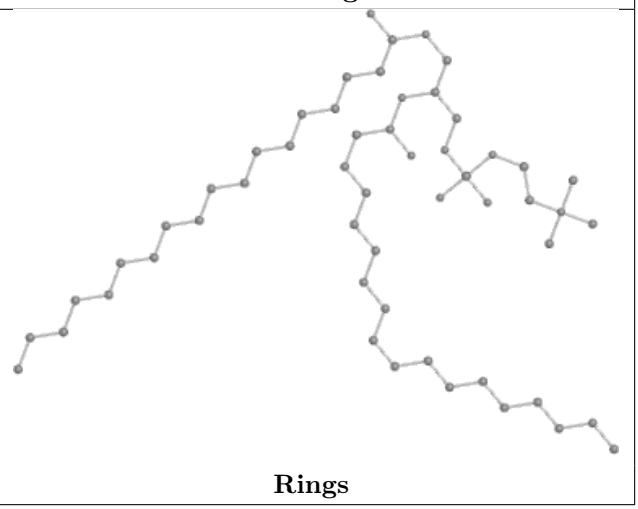


Bond angles

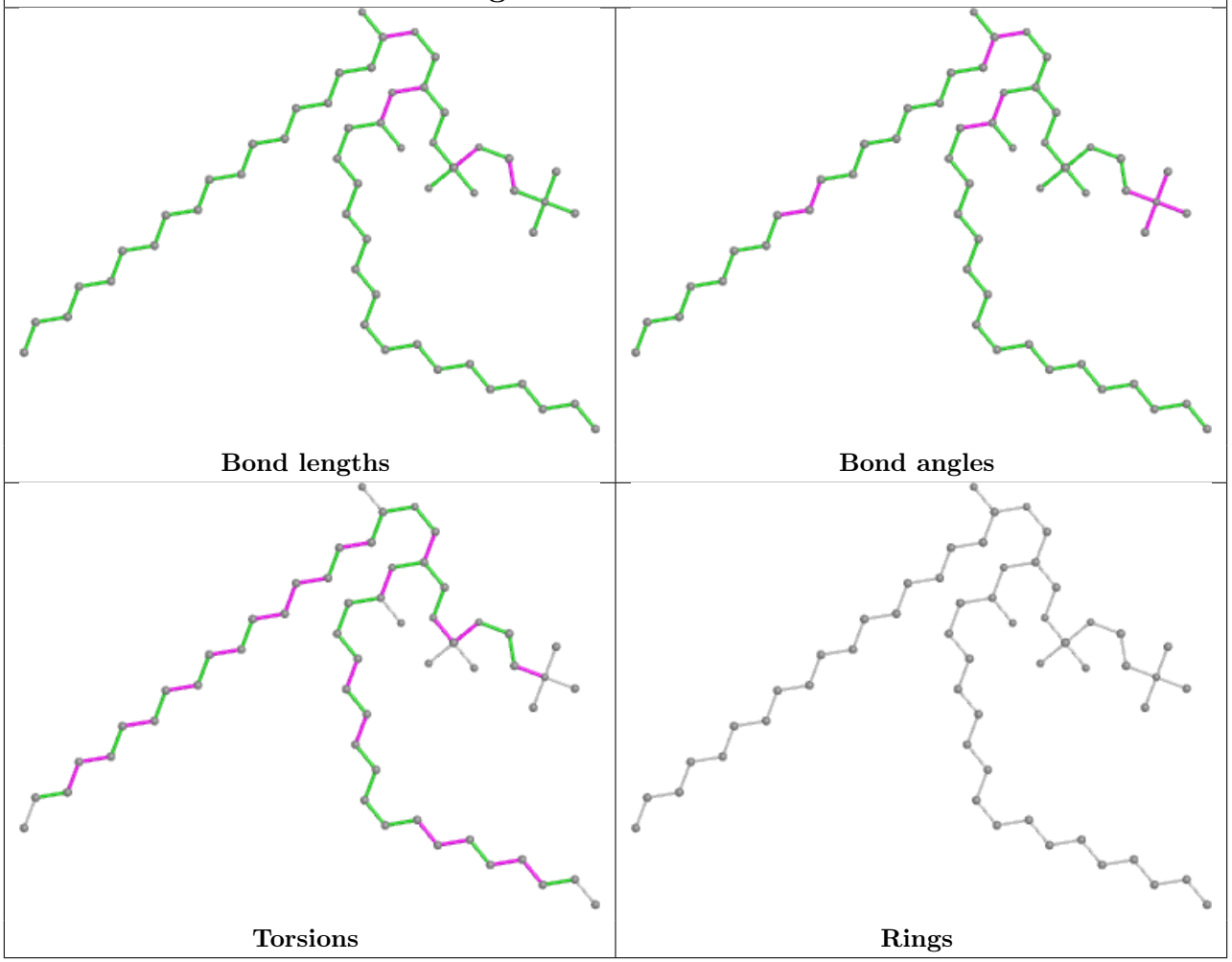


Torsions

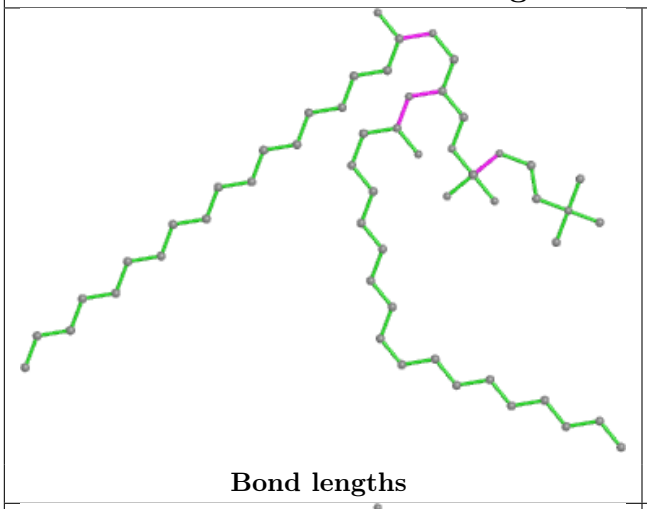


Rings

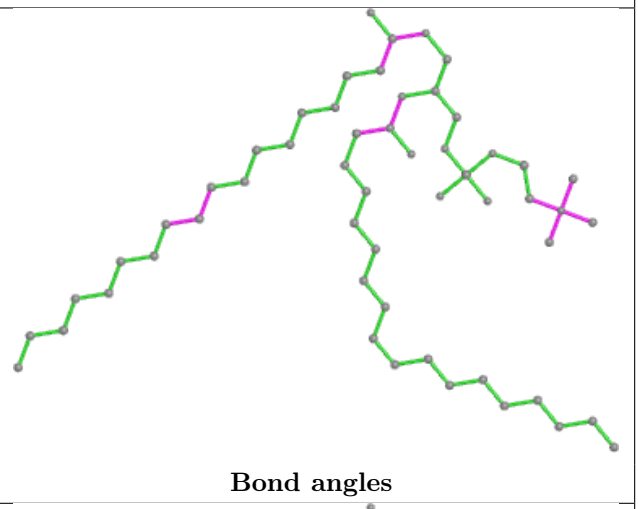
Ligand PCW B 8006



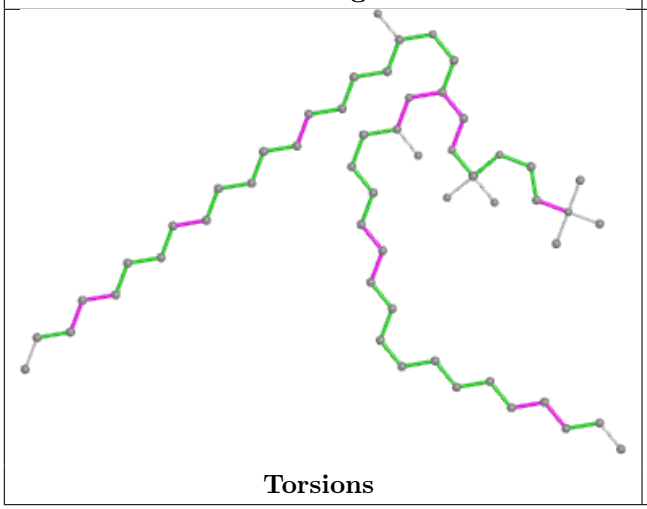
Ligand PCW C 8007



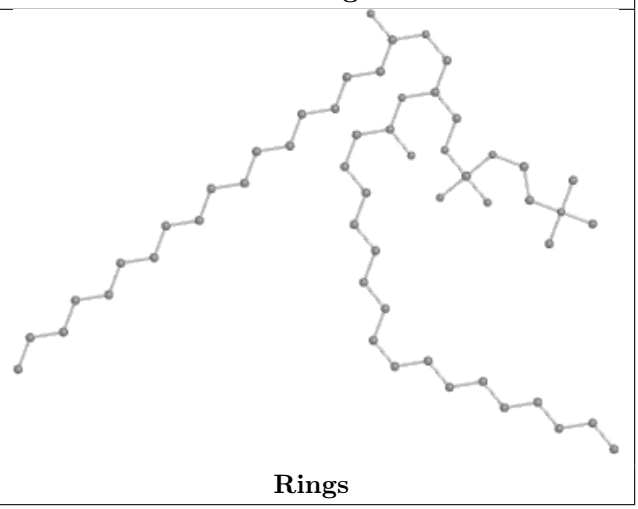
Bond lengths



Bond angles

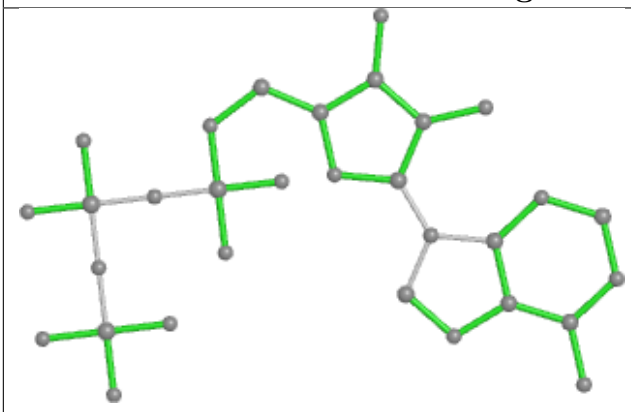


Torsions

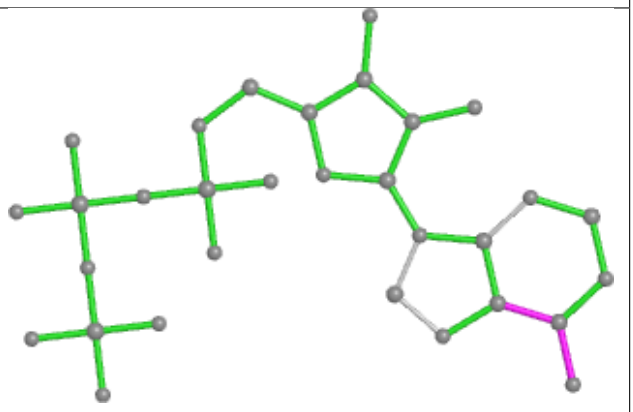


Rings

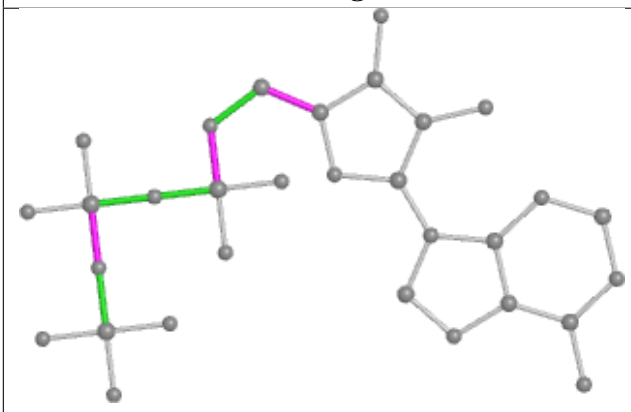
Ligand ATP C 8003



Bond lengths



Bond angles



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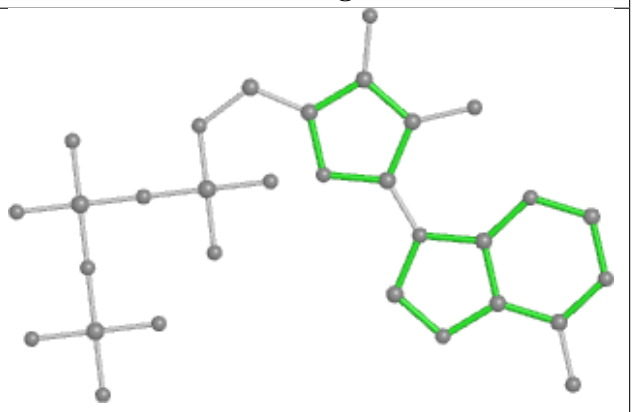
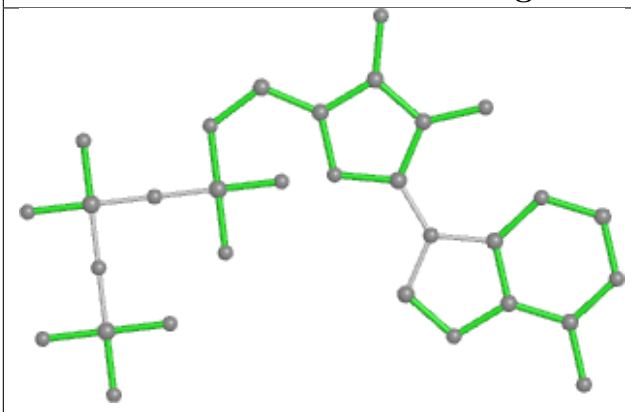
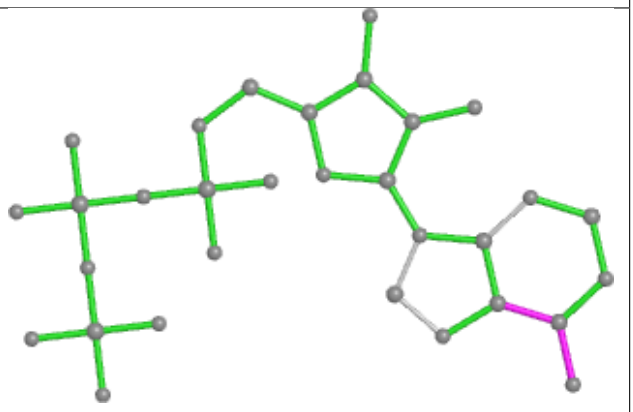


Rings

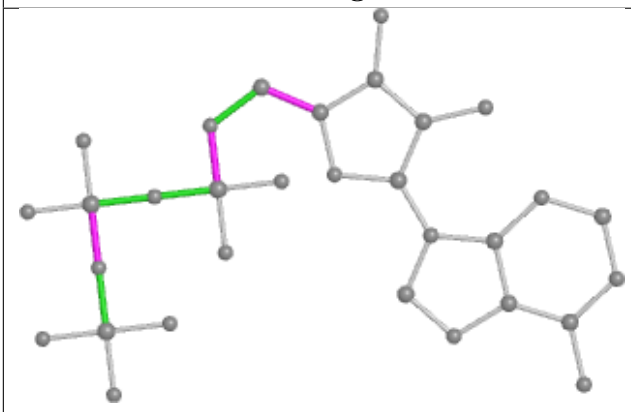
Ligand ATP D 5104



Bond lengths



Bond angles



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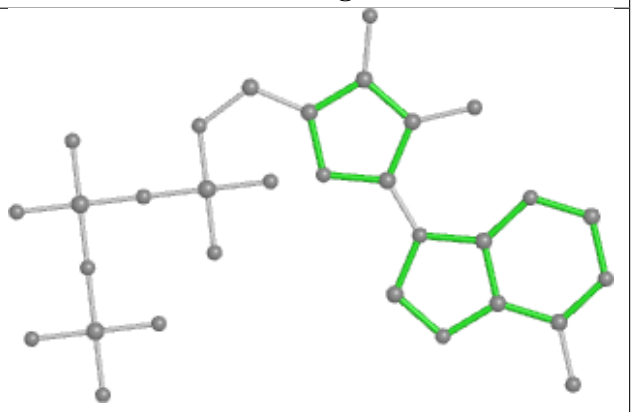
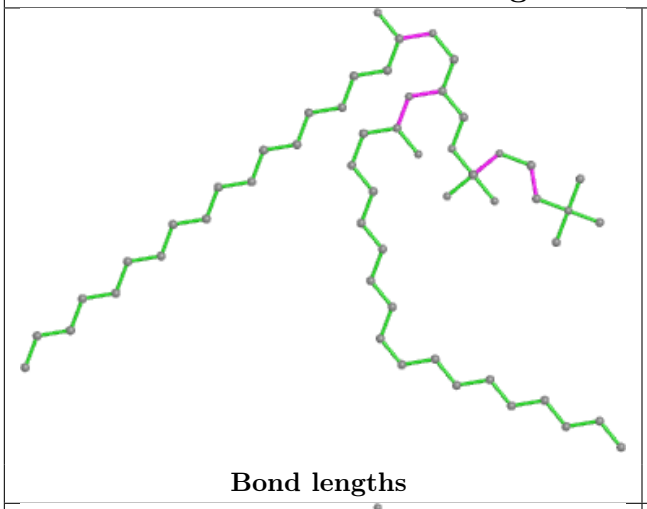
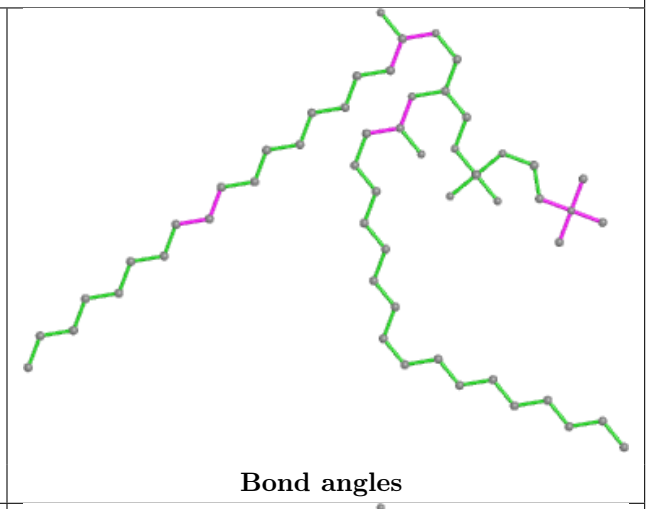


Rings

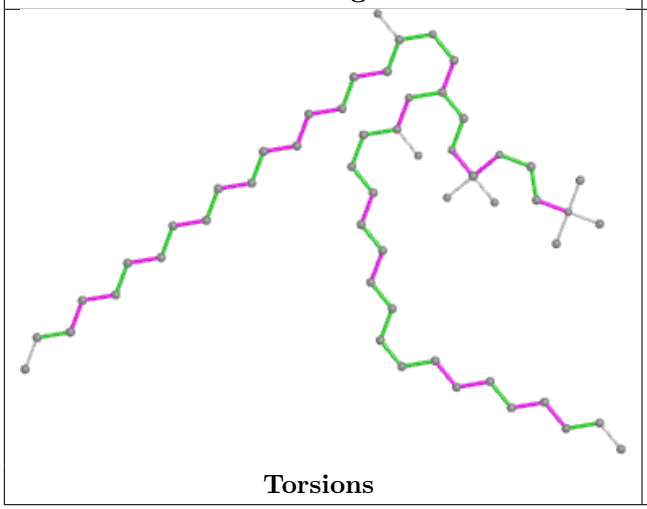
Ligand PCW C 8006



Bond lengths



Bond angles



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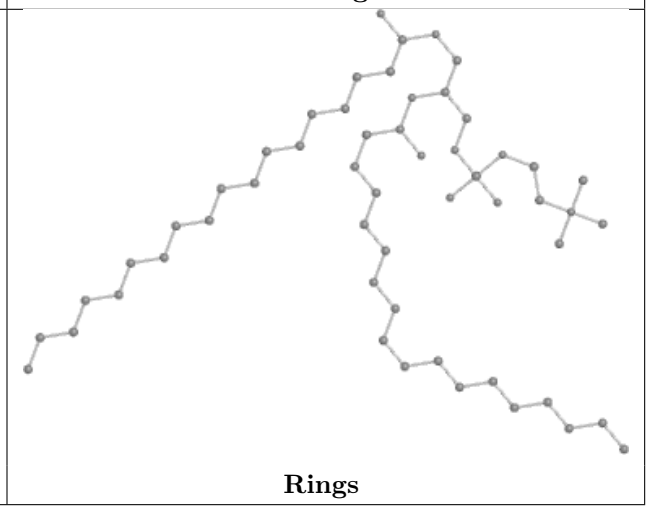
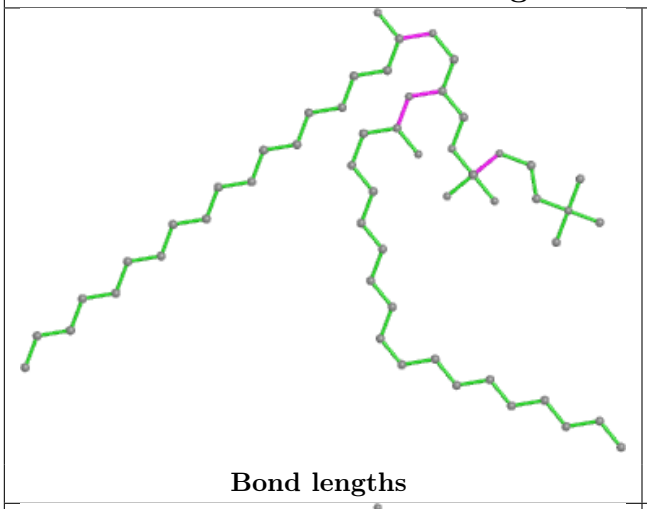


Rings

Ligand PCW B 8007



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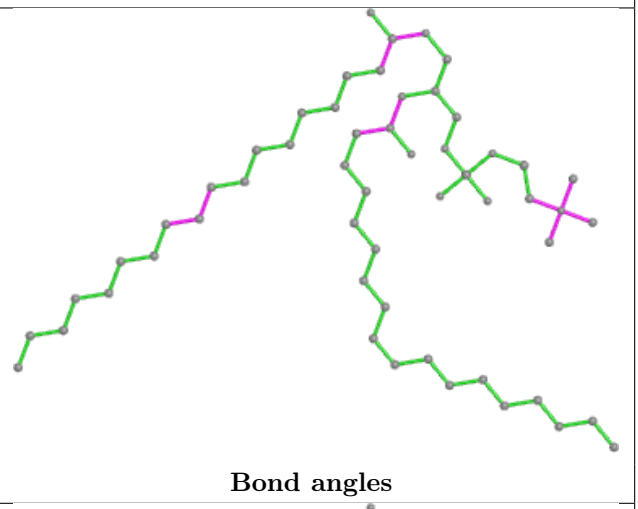
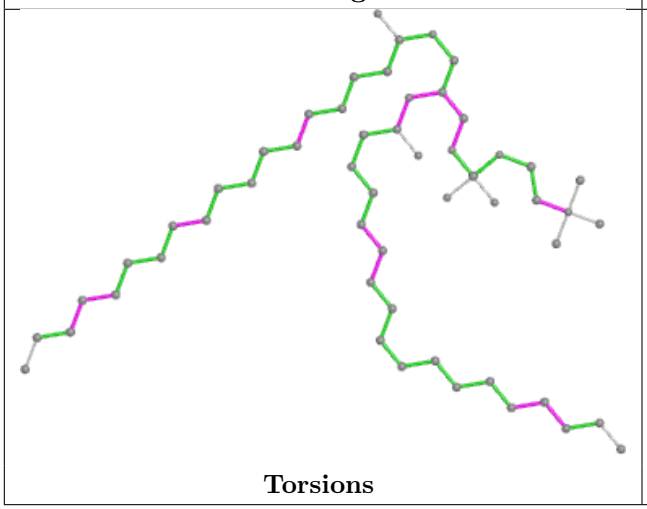
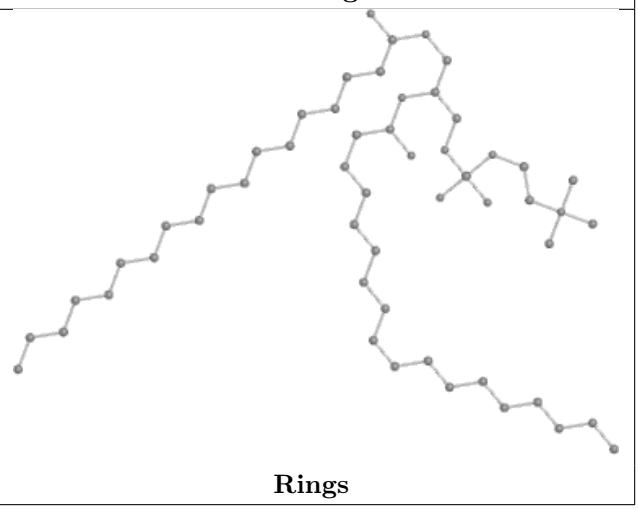


Bond angles

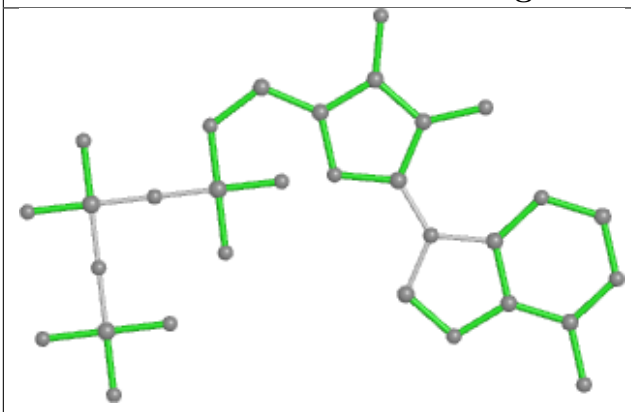


Torsions

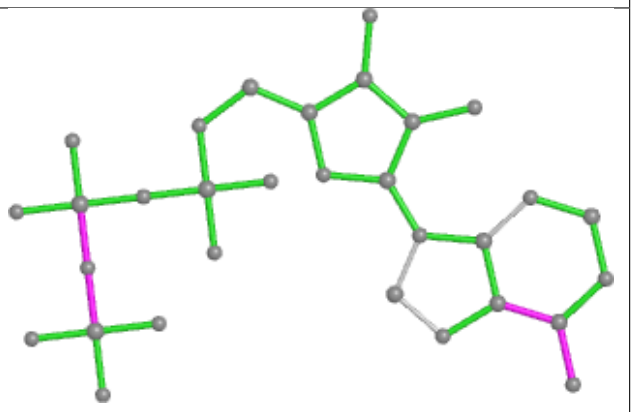


Rings

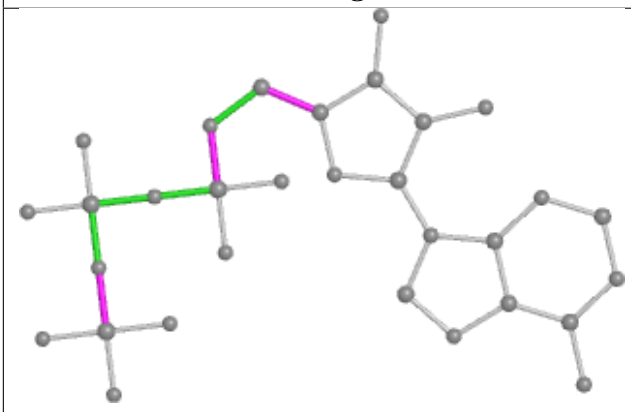
Ligand ATP D 5106



Bond lengths



Bond angles



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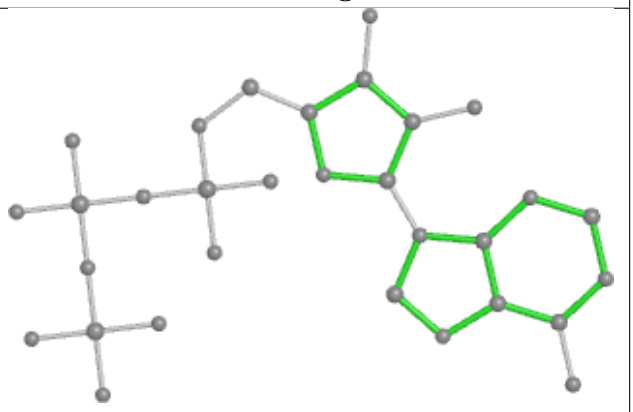
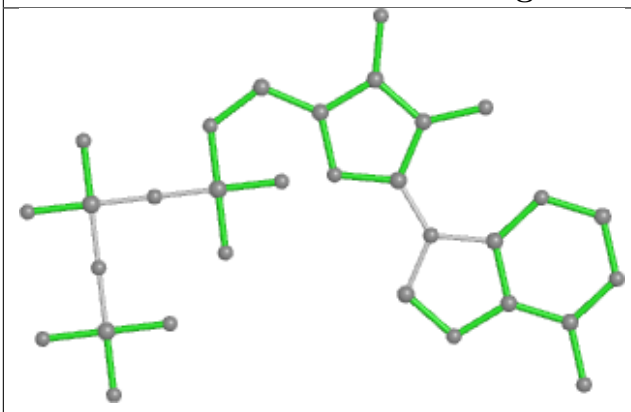
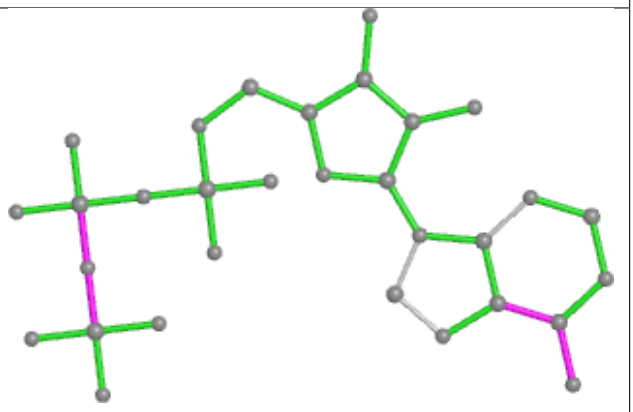


Rings

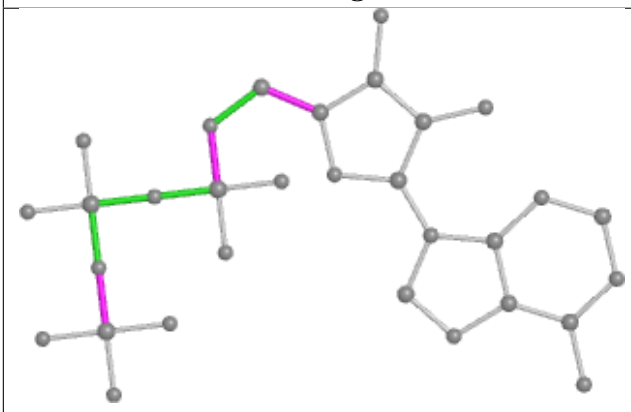
Ligand ATP B 8005



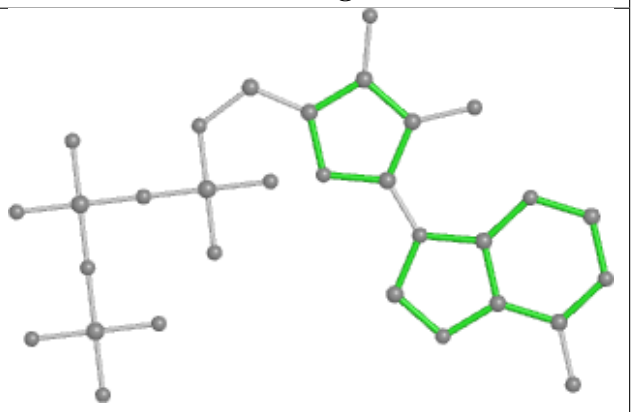
Bond lengths



Bond angles

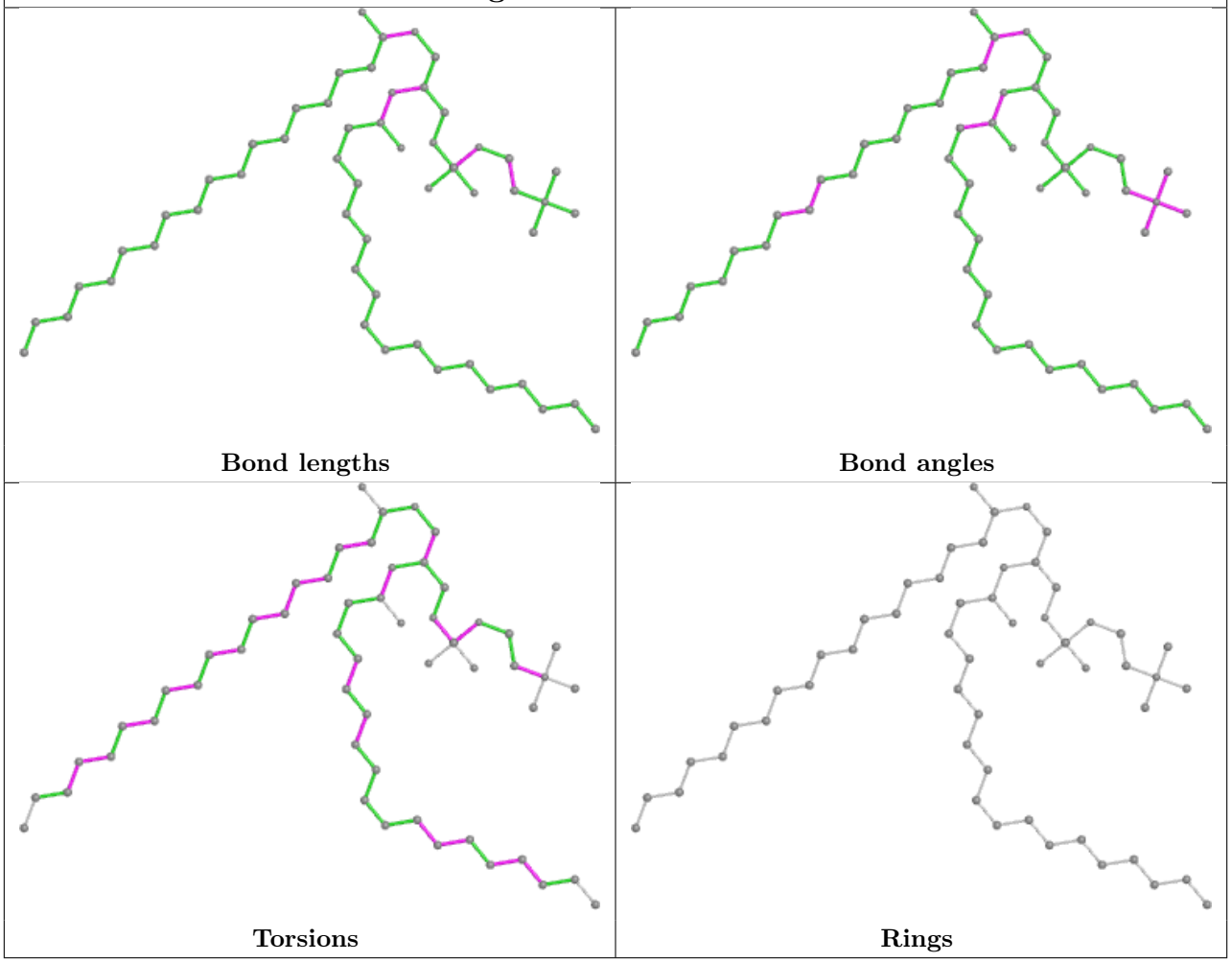


Torsions



Rings

Ligand PCW A 8006



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.

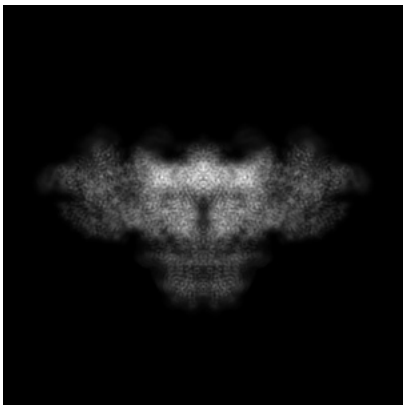
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-43284. These allow visual inspection of the internal detail of the map and identification of artifacts.

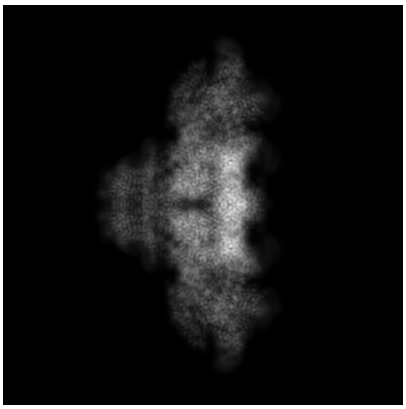
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

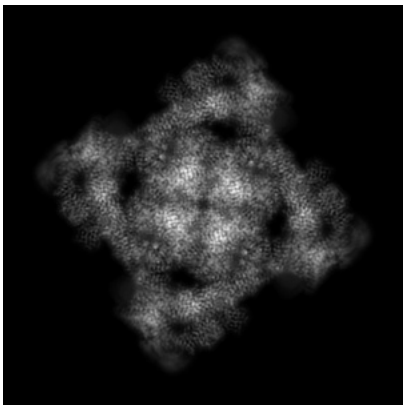
6.1.1 Primary map



X

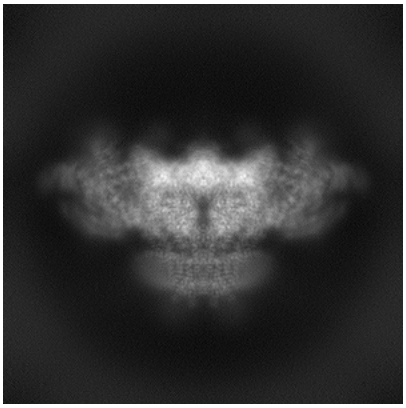


Y

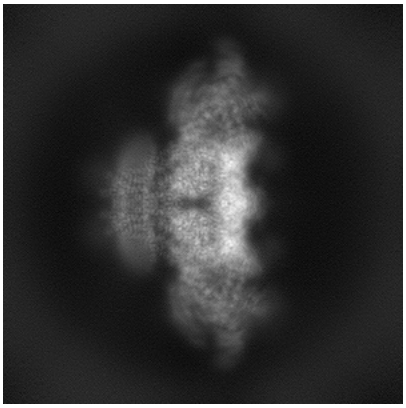


Z

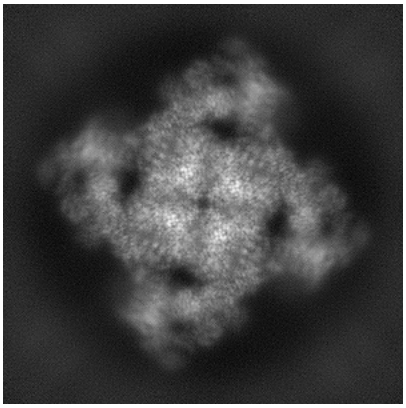
6.1.2 Raw map



X



Y

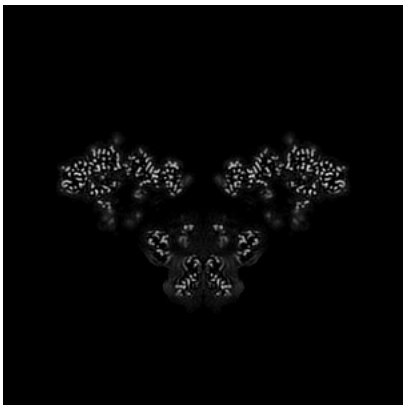


Z

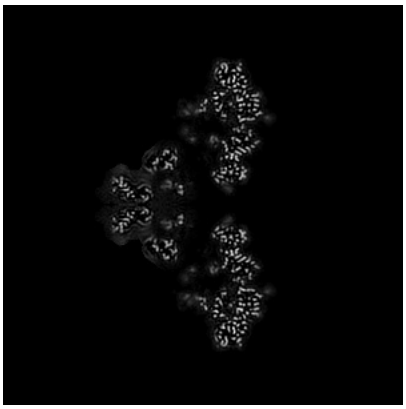
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

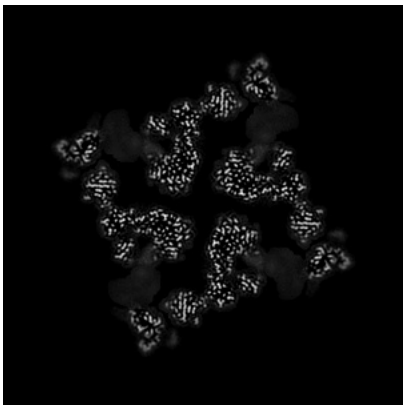
6.2.1 Primary map



X Index: 256

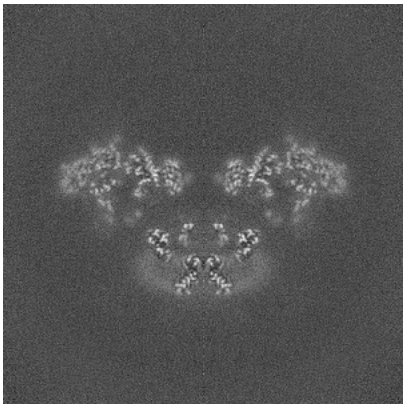


Y Index: 256

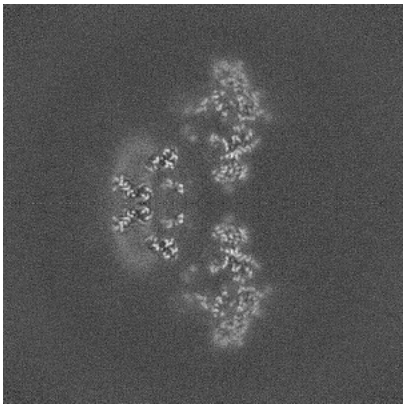


Z Index: 256

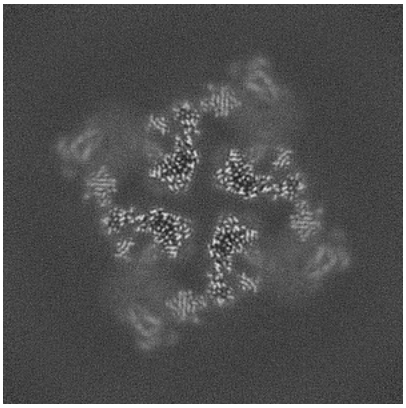
6.2.2 Raw map



X Index: 256



Y Index: 256

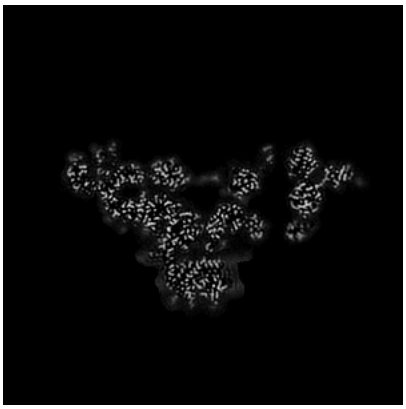


Z Index: 256

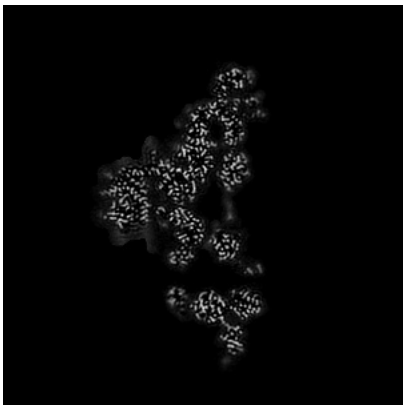
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

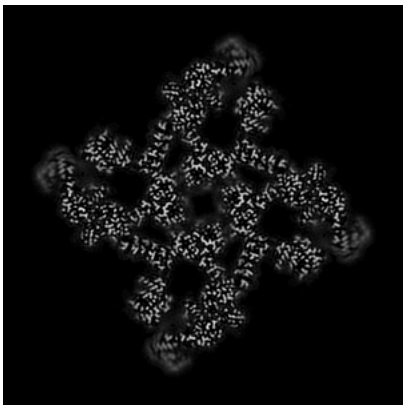
6.3.1 Primary map



X Index: 274

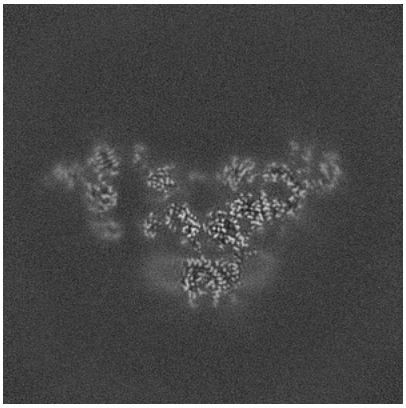


Y Index: 274

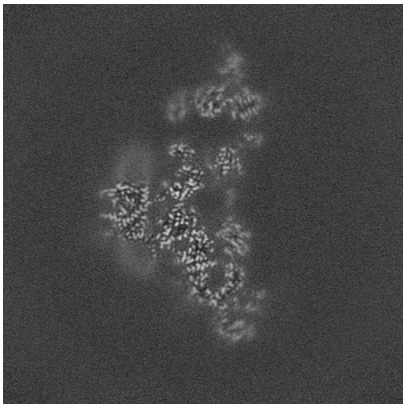


Z Index: 285

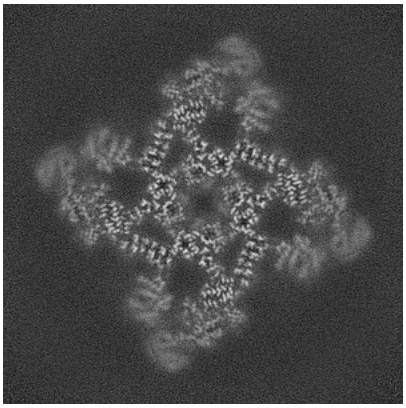
6.3.2 Raw map



X Index: 239



Y Index: 239

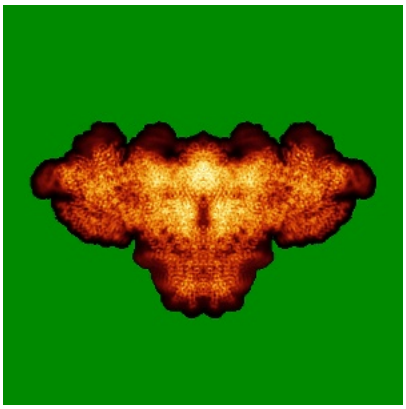


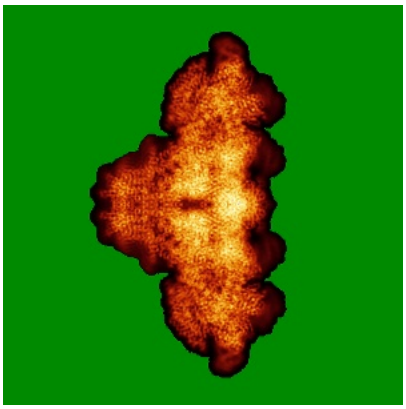
Z Index: 285

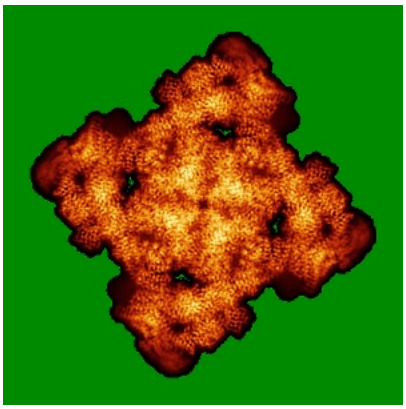
The images above show the largest variance slices of the map in three orthogonal directions.

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

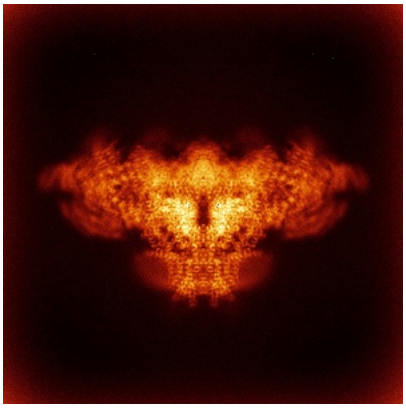
6.4.1 Primary map

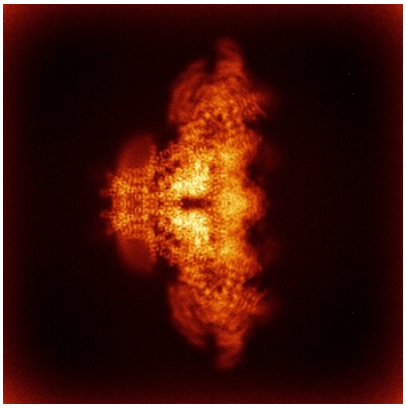

X

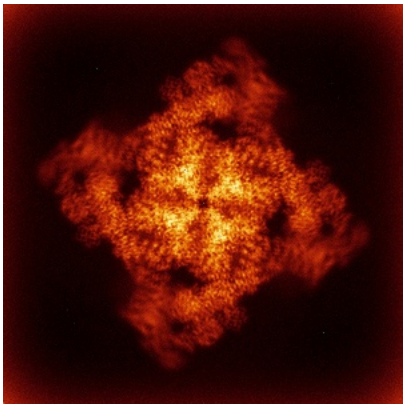

Y


Z

6.4.2 Raw map


X

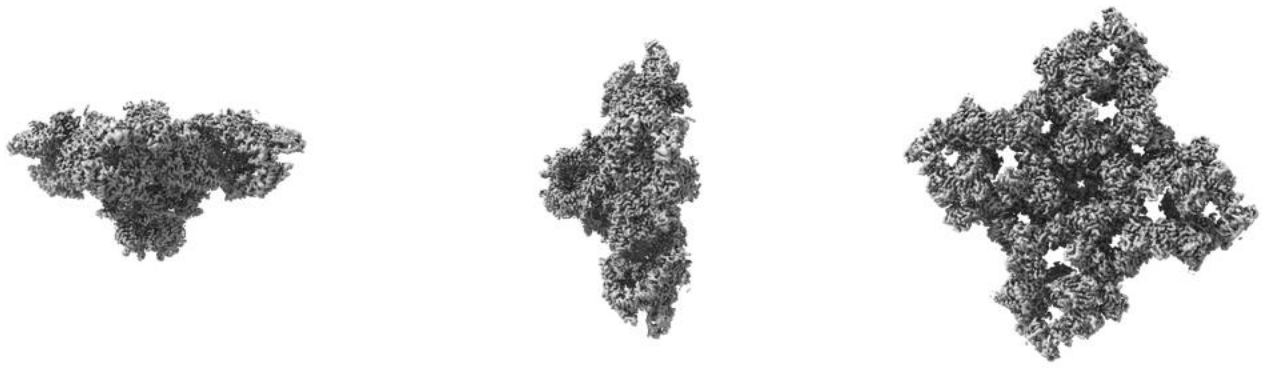

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

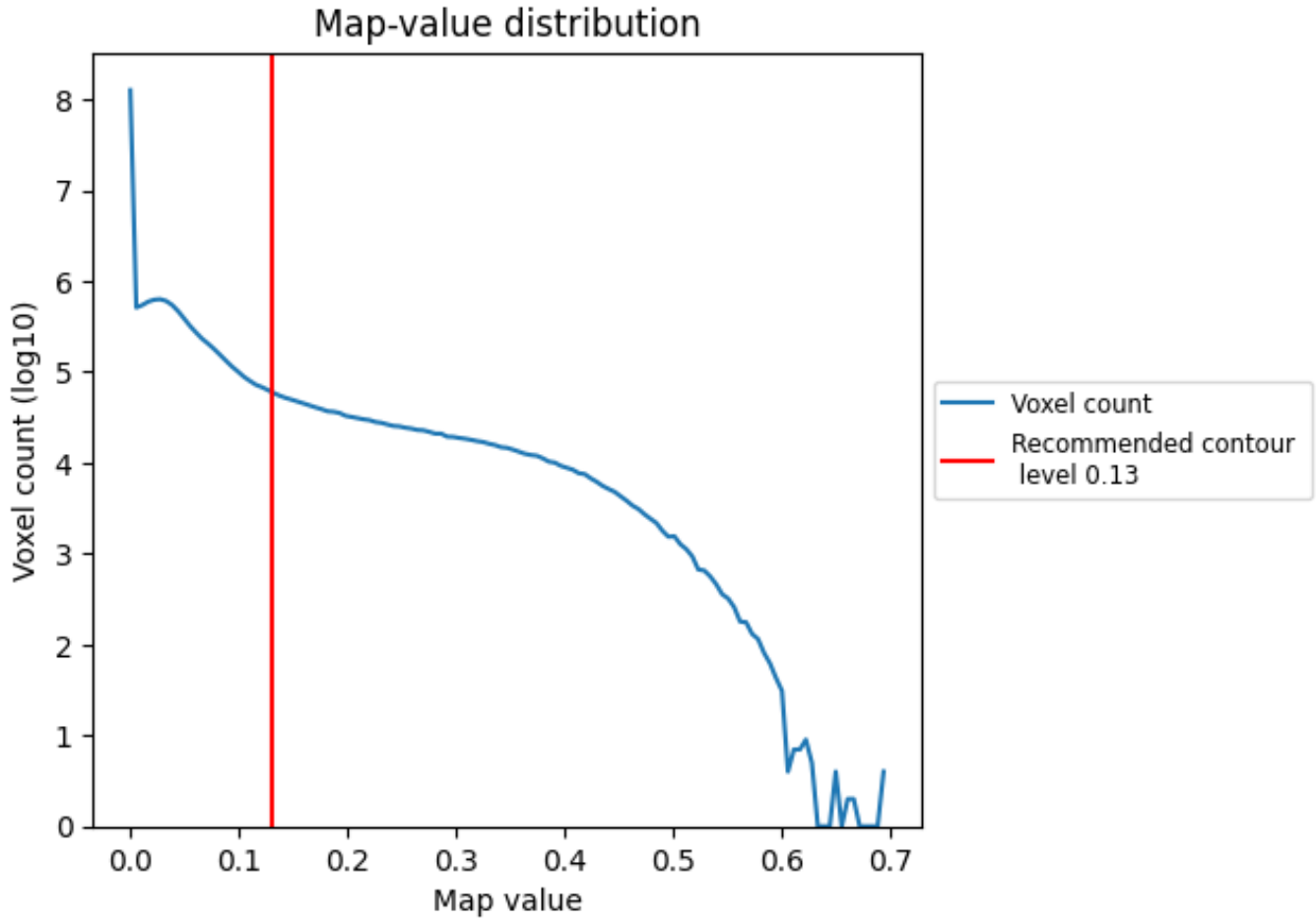
6.6 Mask visualisation (i)

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

7 Map analysis

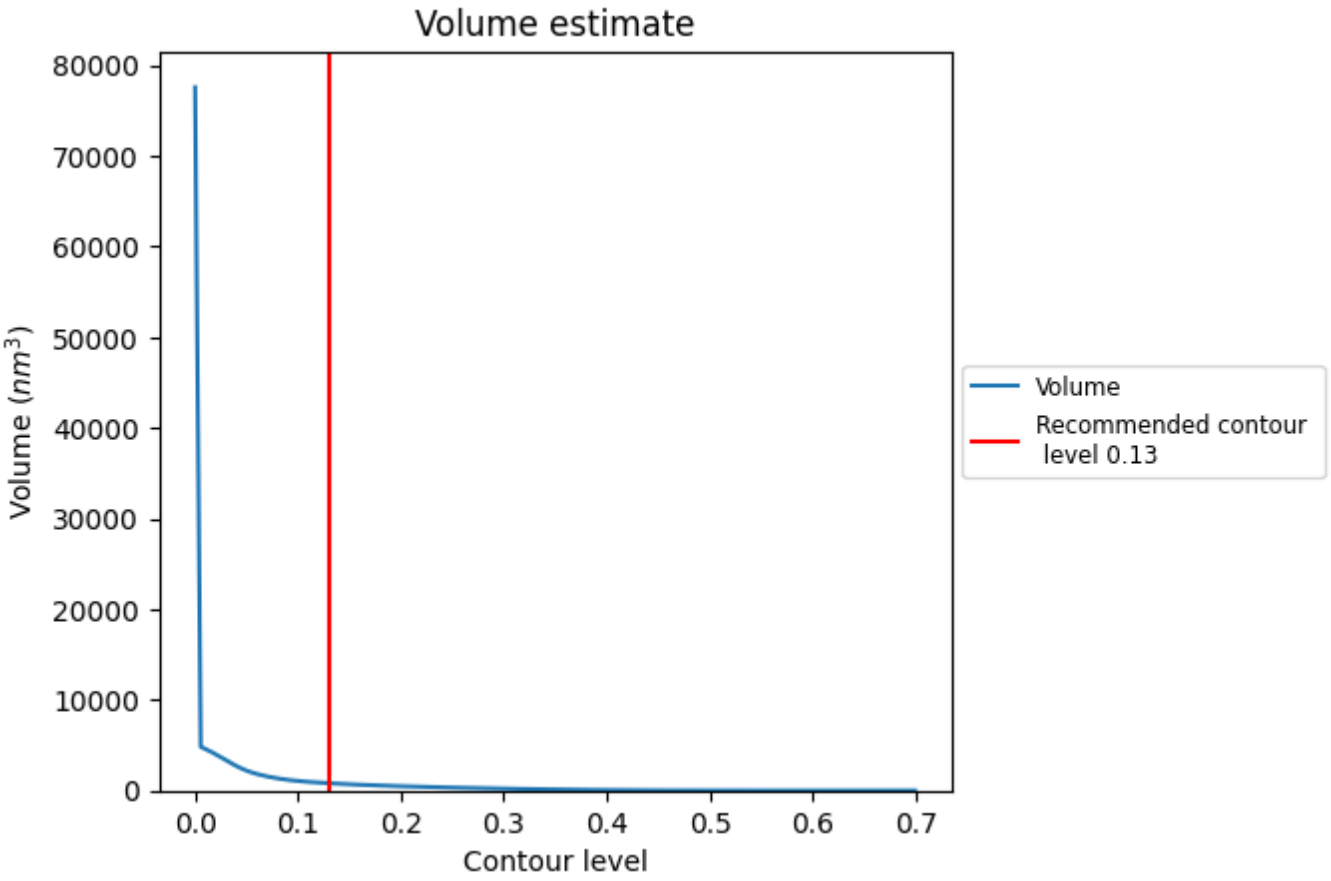
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

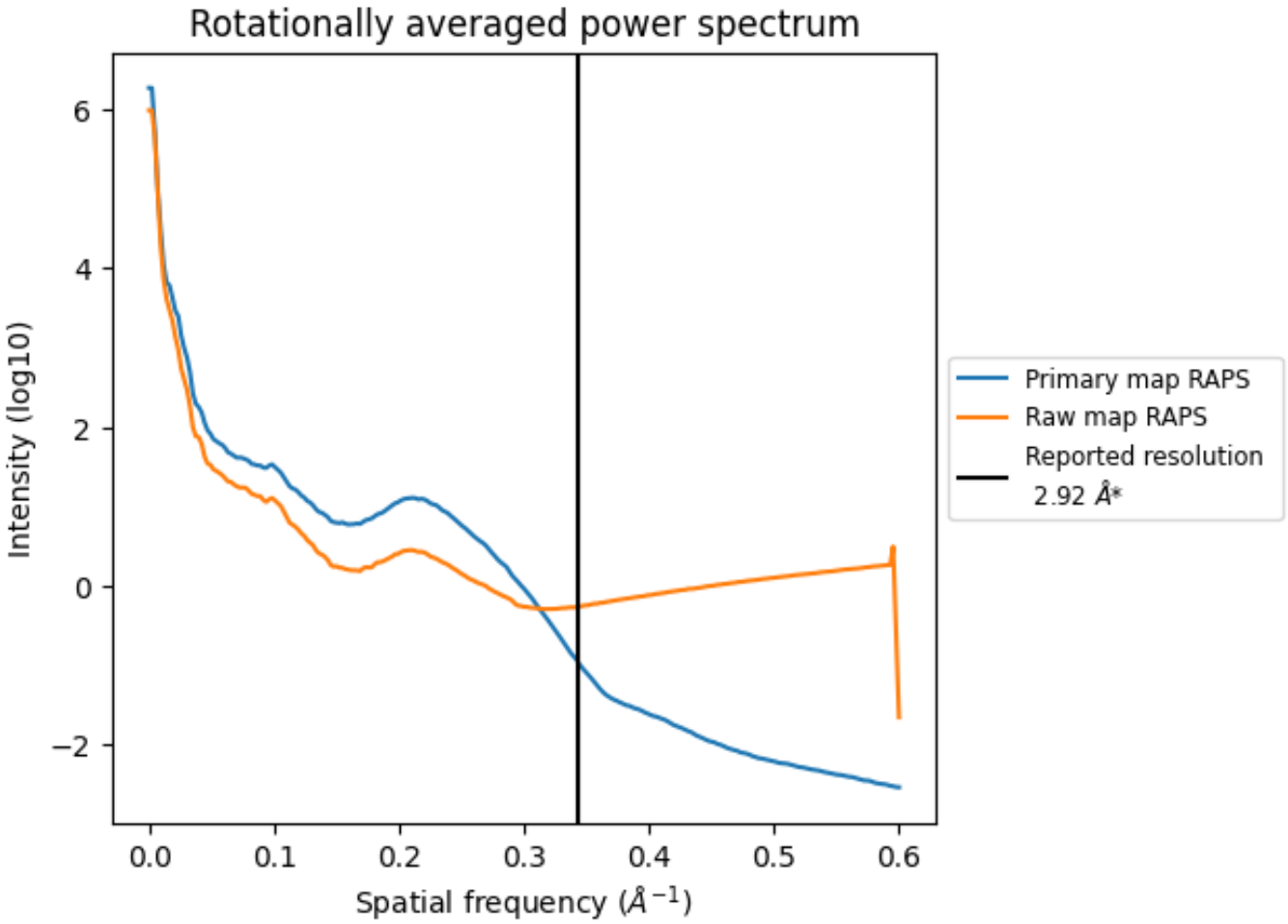
7.2 Volume estimate



The volume at the recommended contour level is 808 nm^3; this corresponds to an approximate mass of 730 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)

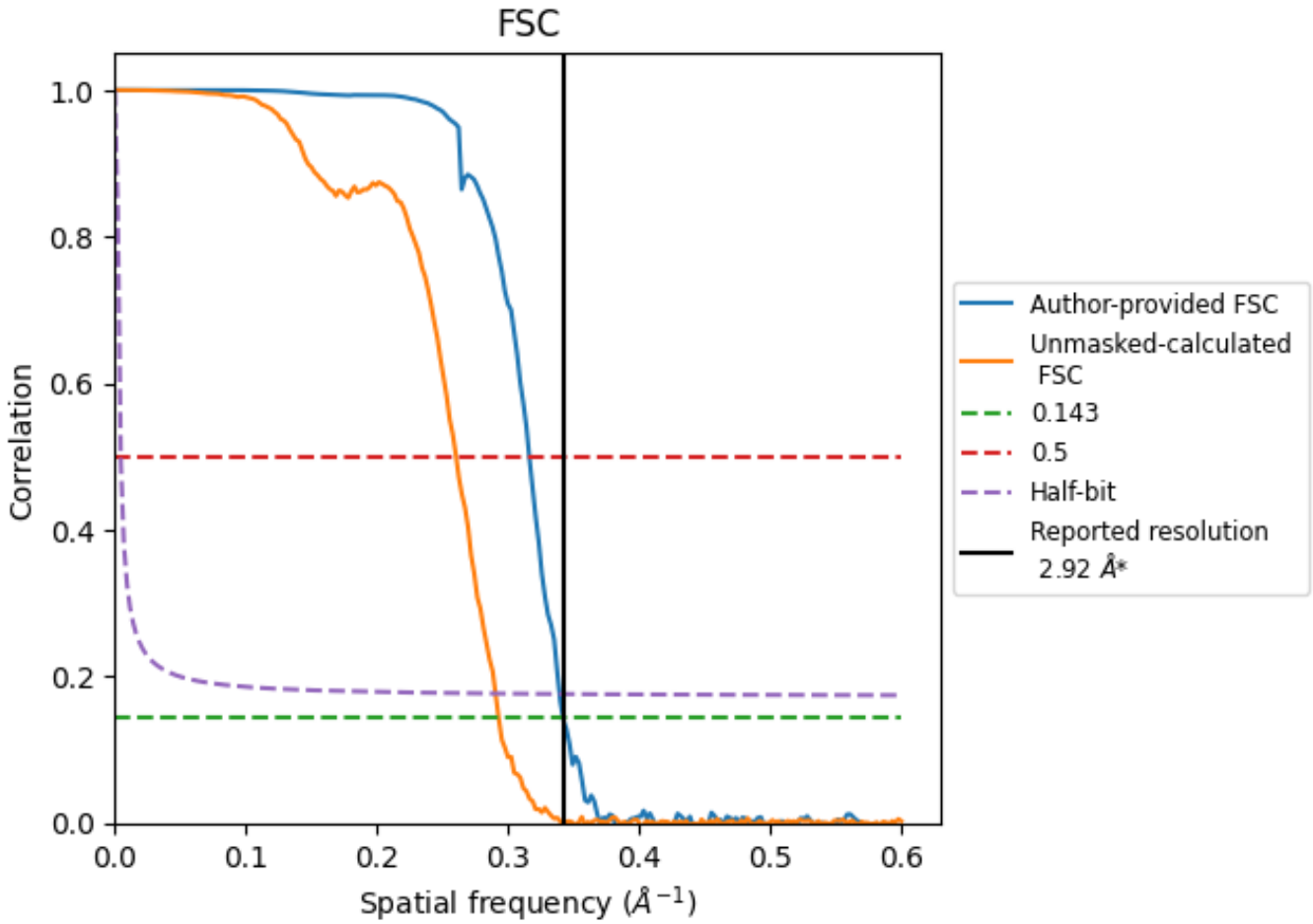


*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.342 Å^{-1}

8.2 Resolution estimates (i)

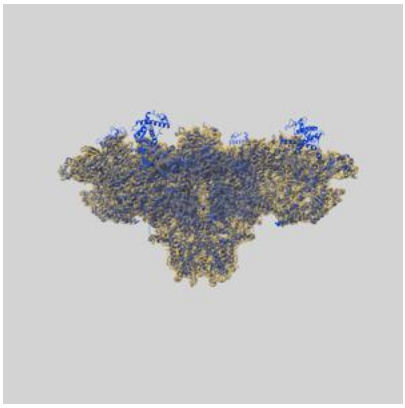
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.92	-	-
Author-provided FSC curve	2.92	3.16	2.95
Unmasked-calculated*	3.41	3.84	3.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.41 differs from the reported value 2.92 by more than 10 %

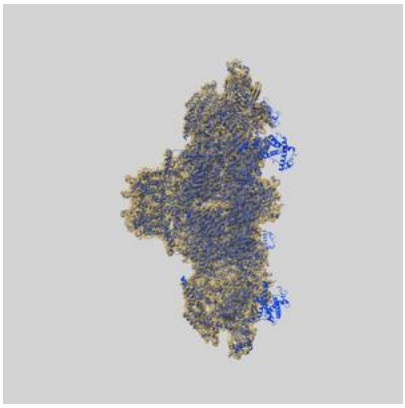
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-43284 and PDB model 8VJK. Per-residue inclusion information can be found in section 3 on page 7.

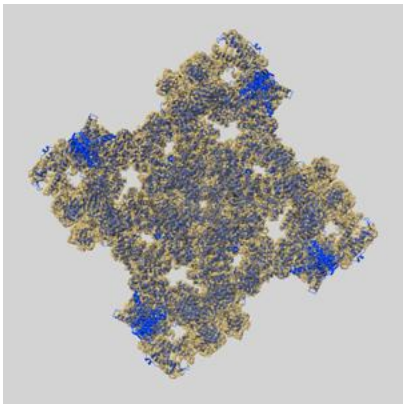
9.1 Map-model overlay



X



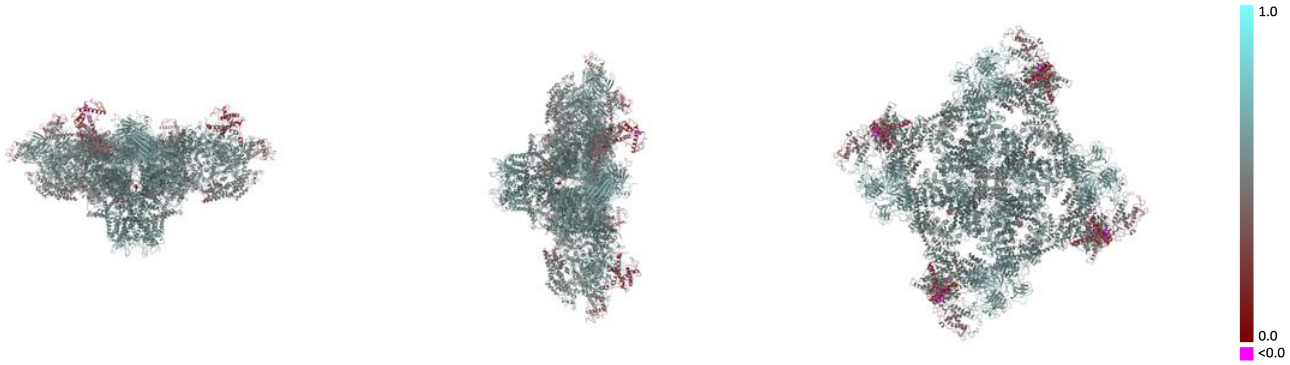
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

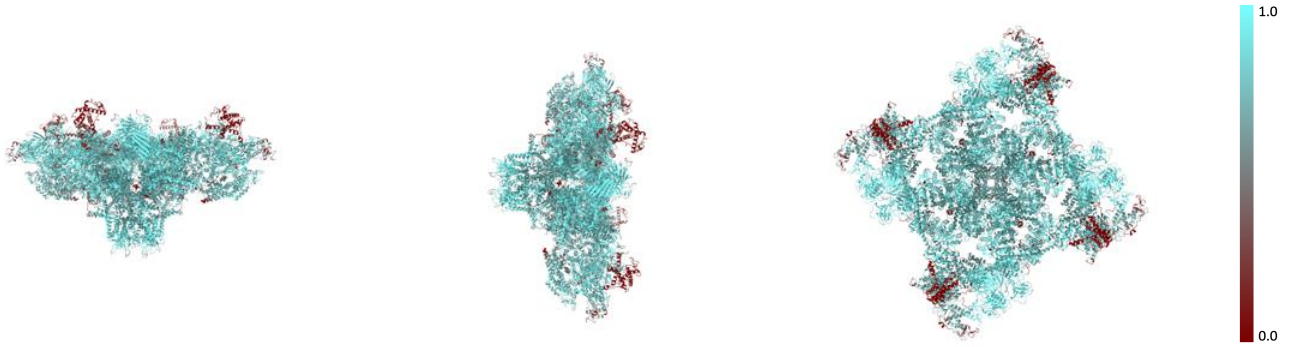
9.2 Q-score mapped to coordinate model (i)



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.

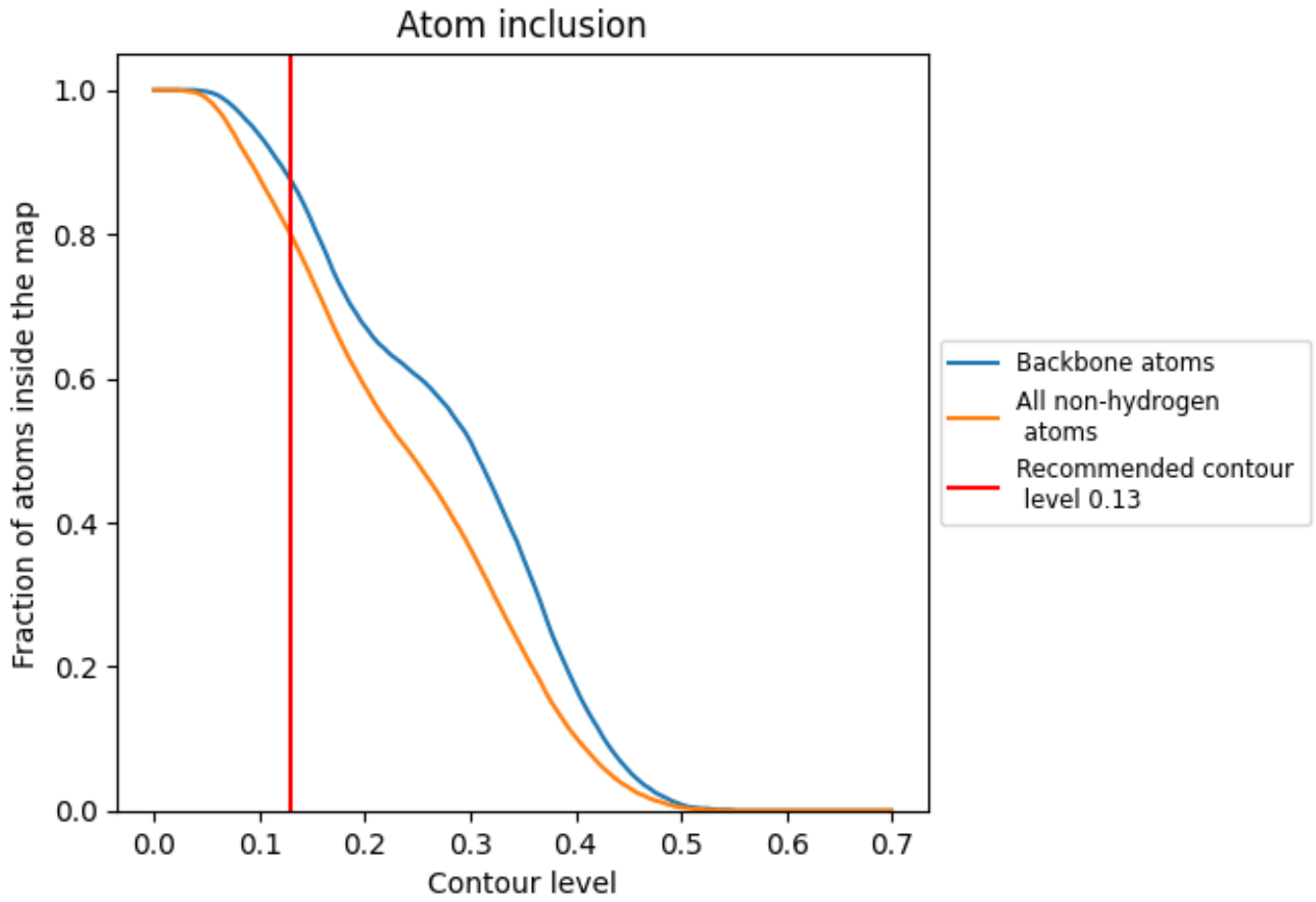
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7980	0.5330
A	0.7960	0.5320
B	0.7960	0.5320
C	0.7960	0.5310
D	0.7960	0.5310
E	0.8720	0.5840
F	0.8770	0.5840
G	0.8780	0.5830
H	0.8770	0.5840