wwPDB EM Validation Summary Report ⓘ

Oct 23, 2024 – 02:08 PM EDT

PDB ID : 9E17
EMDB ID : EMD-26205
Title : Structure of RyR1 in the primed state in the presence of caffeine (reprocessed /reanalyzed from EMPIAR-10997, 7TZC, EMD-26205)
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.45 Å(reported)
Based on initial model : 7TZC

This is a wwPDB EM Validation Summary 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:

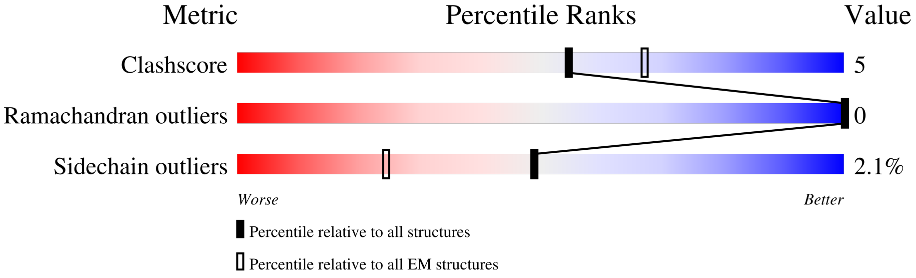
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance ⓘ

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

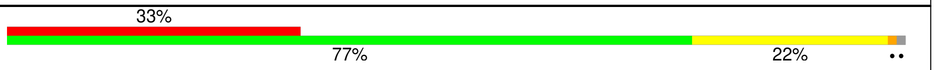
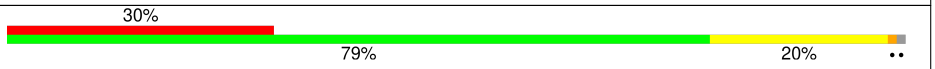
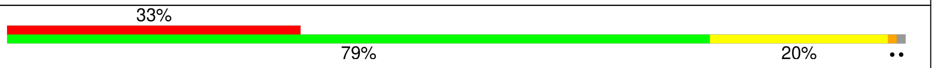
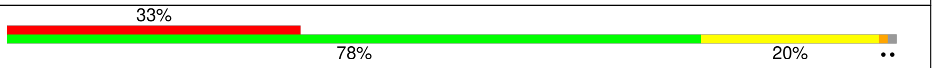
The reported resolution of this entry is 2.45 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	C	150	
1	D	150	
1	E	150	
1	K	150	
2	F	108	
2	H	108	
2	J	108	
2	O	108	

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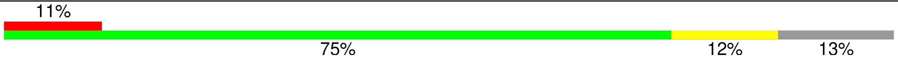
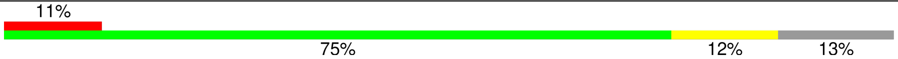
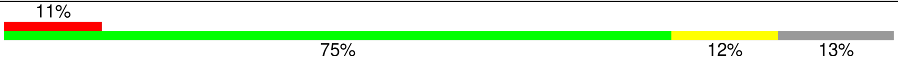
Mol	Chain	Length	Quality of chain
3	A	5037	 11% 75% 12% 13%
3	B	5037	 11% 75% 12% 13%
3	G	5037	 11% 75% 12% 13%
3	I	5037	 11% 75% 12% 13%

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 149476 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total 1174	C 719	N 190	O 255	S 10	0	0
1	D	149	Total 1174	C 719	N 190	O 255	S 10	0	0
1	E	149	Total 1174	C 719	N 190	O 255	S 10	0	0
1	C	149	Total 1174	C 719	N 190	O 255	S 10	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	H	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	J	107	Total 831	C 527	N 146	O 154	S 4	0	0
2	O	107	Total 831	C 527	N 146	O 154	S 4	0	0

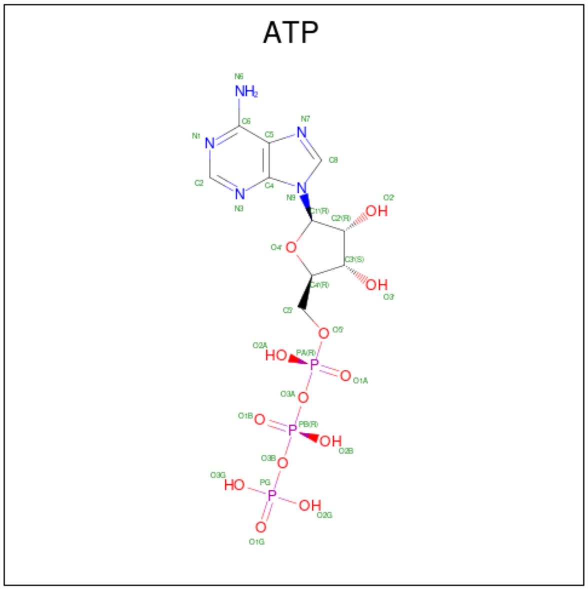
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	B	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	G	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0
3	I	4404	Total 35150	C 22365	N 6063	O 6485	S 237	9	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total 4	Ca 4	0
4	D	4	Total 4	Ca 4	0
4	E	4	Total 4	Ca 4	0
4	C	4	Total 4	Ca 4	0
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	G	1	Total 1	Ca 1	0
4	I	1	Total 1	Ca 1	0

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

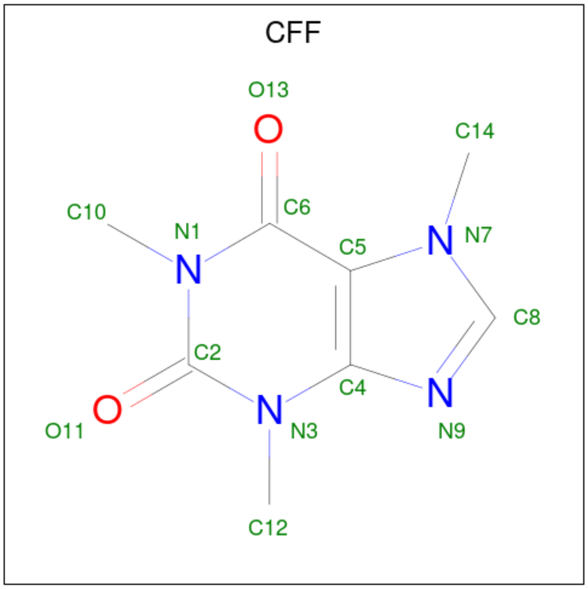


Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O P 31 10 5 13 3	0
5	A	1	Total C N O P 31 10 5 13 3	0
5	B	1	Total C N O P 31 10 5 13 3	0
5	B	1	Total C N O P 31 10 5 13 3	0
5	G	1	Total C N O P 31 10 5 13 3	0
5	G	1	Total C N O P 31 10 5 13 3	0
5	I	1	Total C N O P 31 10 5 13 3	0
5	I	1	Total C N O P 31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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

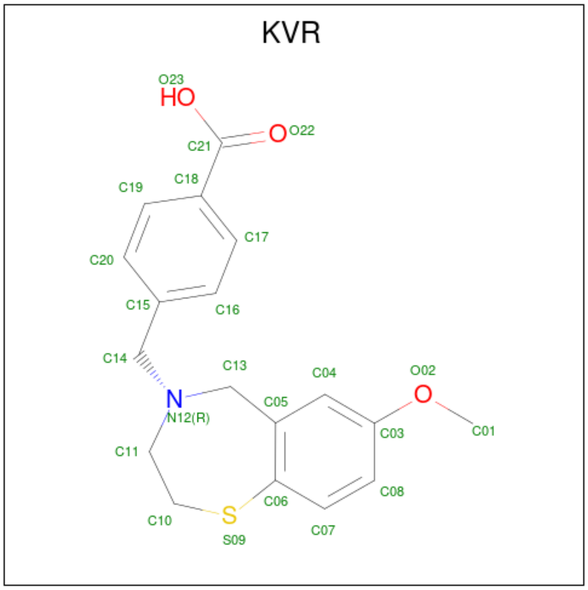
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Zn 1 1	0
6	B	1	Total Zn 1 1	0
6	G	1	Total Zn 1 1	0
6	I	1	Total Zn 1 1	0

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



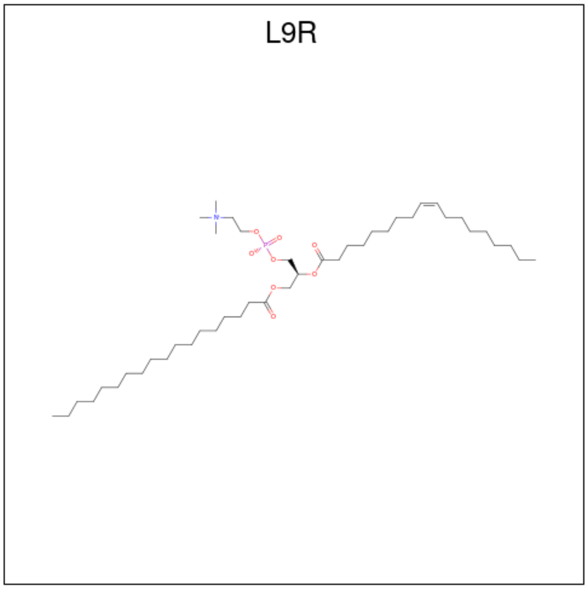
Mol	Chain	Residues	Atoms	AltConf
7	A	1	Total C N O 14 8 4 2	0
7	B	1	Total C N O 14 8 4 2	0
7	G	1	Total C N O 14 8 4 2	0
7	I	1	Total C N O 14 8 4 2	0

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (three-letter code: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
8	A	1	23	18	1	3	1	0
8	B	1	23	18	1	3	1	0
8	G	1	23	18	1	3	1	0
8	I	1	23	18	1	3	1	0

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: L9R) (formula: $C_{44}H_{86}NO_8P$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O P 54 44 1 8 1	0
9	A	1	Total C N O P 54 44 1 8 1	0
9	B	1	Total C N O P 54 44 1 8 1	0
9	B	1	Total C N O P 54 44 1 8 1	0
9	G	1	Total C N O P 54 44 1 8 1	0
9	G	1	Total C N O P 54 44 1 8 1	0
9	I	1	Total C N O P 54 44 1 8 1	0
9	I	1	Total C N O P 54 44 1 8 1	0

- Molecule 10 is water.

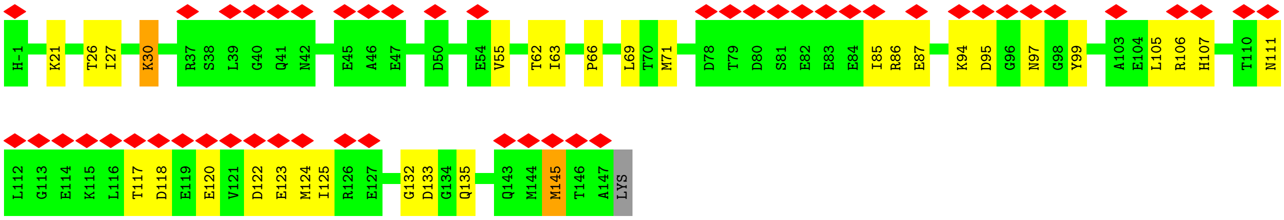
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total O 1 1	0
10	B	1	Total O 1 1	0
10	G	1	Total O 1 1	0
10	I	1	Total O 1 1	0

3 Residue-property plots ⓘ

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.

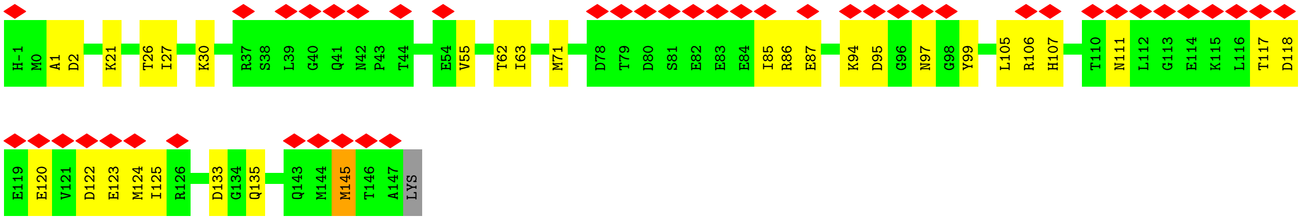
- Molecule 1: Calmodulin-1

Chain K:



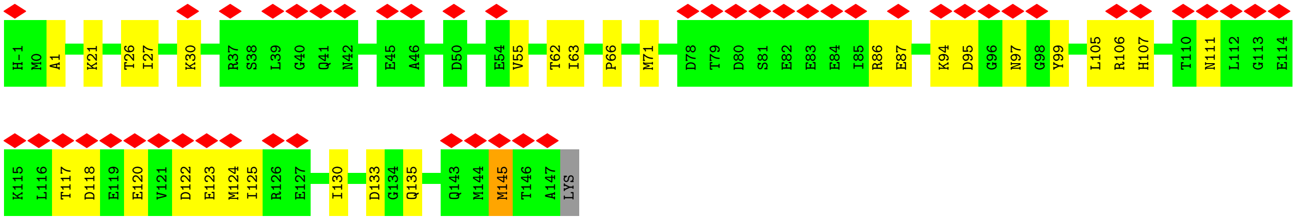
- Molecule 1: Calmodulin-1

Chain D:



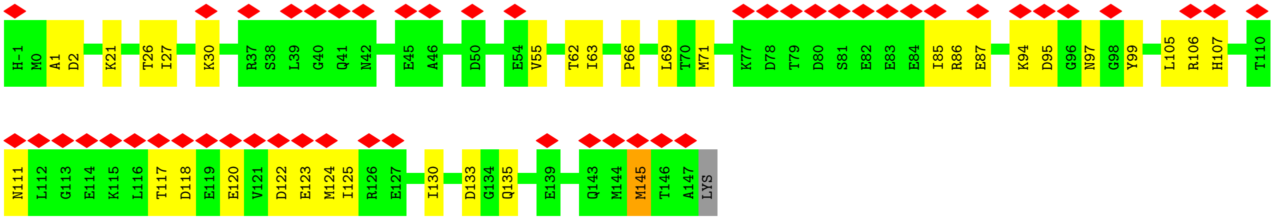
- Molecule 1: Calmodulin-1

Chain E:



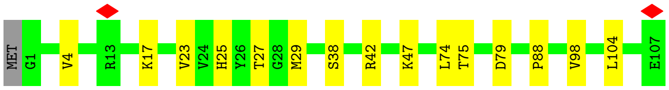
- Molecule 1: Calmodulin-1

Chain C:



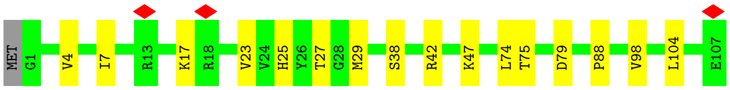
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F:



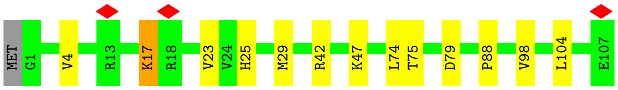
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:



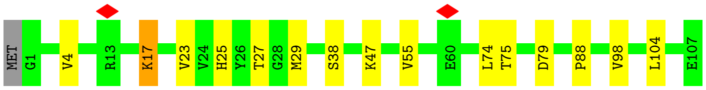
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain J:



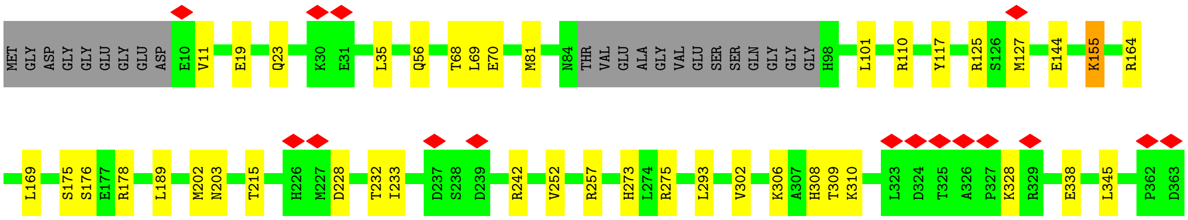
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

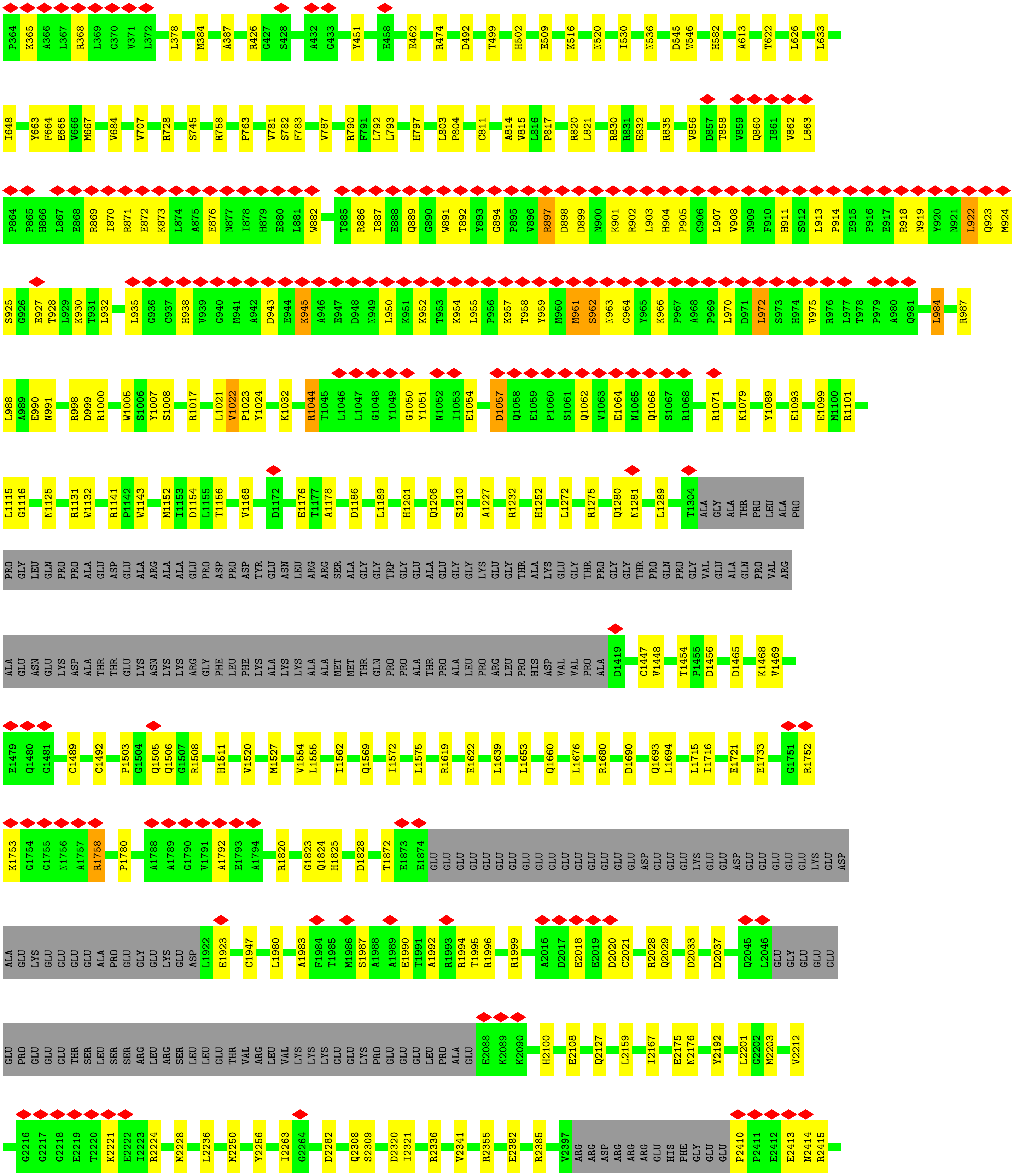
Chain O:

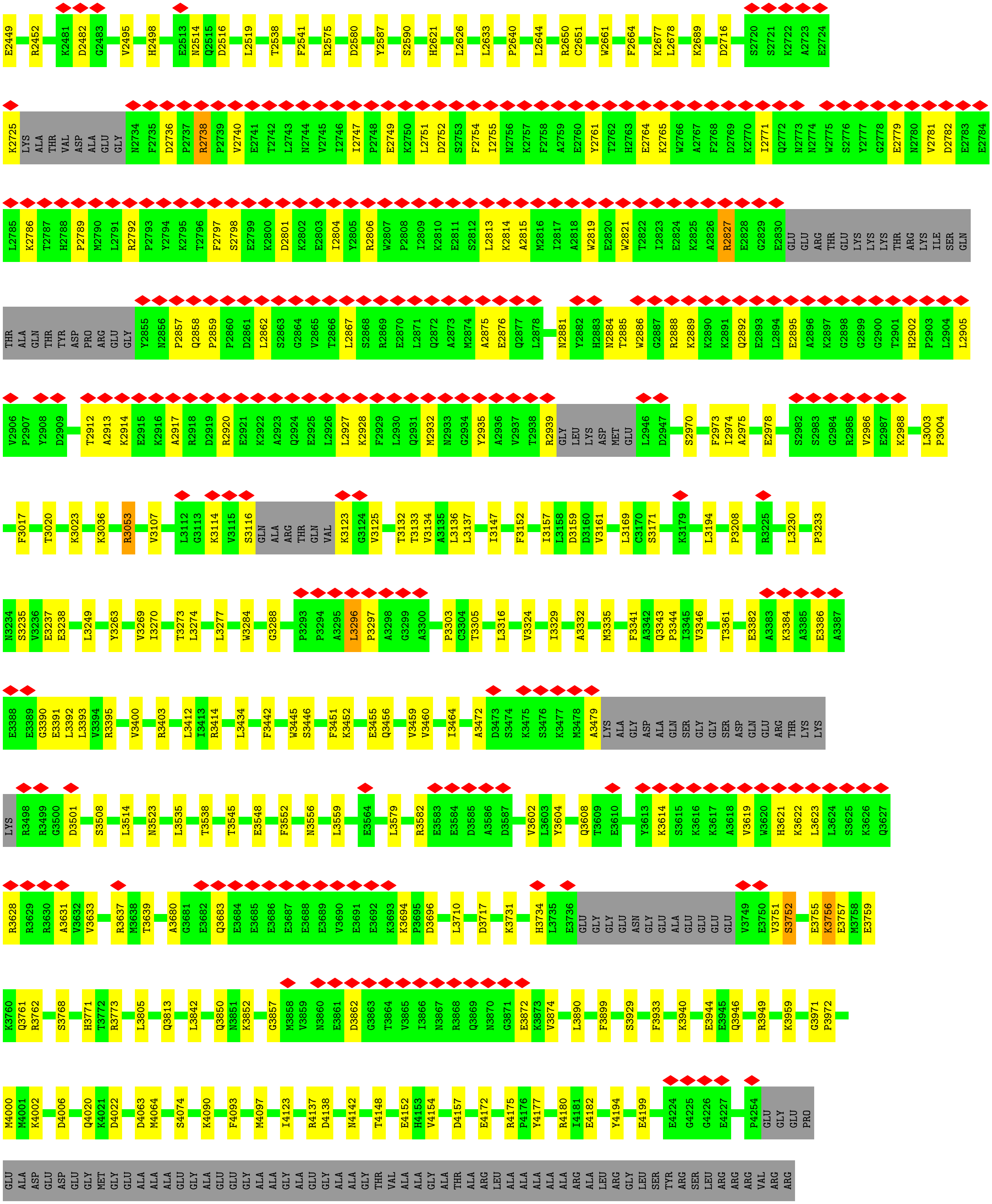


- Molecule 3: Ryanodine receptor 1

Chain A:




P364 K365 A366 L367 R368 L369 G370 V371 L372 L378 M384 A387 R426 G427 S428 A432 G433 Y451 E458 E462 R474 D492 T499 H502 E509 K516 N520 I530 N536 D545 W546 H582 A613 T622 L626 L633
I648 Y663 F664 E665 V666 M667 V684 V707 R728 S745 R758 P763 V781 S782 F783 V787 R790 F791 L792 L793 H797 L803 P804 C811 A814 V815 L816 P817 R820 L821 R830 R831 E832 R835 V856 D857 T858 V859 Q860 I861 V862 L863
P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917 R918 N919 Y920 N921 L922 Q923 M924
S925 G926 E927 T928 L929 K930 T931 L932 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 Q981 L984 R987
L988 A989 E990 N991 R998 D999 R1000 W1005 S1006 Y1007 S1008 R1017 L1021 V1022 P1023 Y1024 K1032 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 K1079 Y1089 E1093 E1099 M1100 R1101
L1115 G1116 N1125 R1131 W1132 R1141 P1142 W1143 M1152 I1153 D1154 L1155 T1156 V1168 D1172 E1176 T1177 A1178 D1186 L1189 H1201 Q1206 S1210 A1227 R1232 H1252 L1272 R1275 Q1280 N1281 L1289 T1304 ALA GLY ALA THR PRO LEU ALA PRO
PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 C1447 V1448 T1454 P1455 D1456 D1465 K1468 V1469
E1479 Q1480 G1481 C1489 C1492 P1503 G1504 Q1505 Q1506 G1507 R1508 H1511 V1520 M1527 V1554 L1555 I1562 Q1569 I1572 L1575 R1619 E1622 L1639 L1653 Q1660 L1676 R1680 D1690 Q1693 L1694 L1715 I1716 E1721 E1733 G1751 R1752
K1753 G1754 G1755 N1756 A1757 R1758 P1780 A1788 A1789 G1790 V1791 A1792 E1793 A1794 R1820 G1823 Q1824 H1825 D1828 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP
ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 C1947 L1980 A1983 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 R1999 A2016 D2017 E2018 E2019 D2020 C2021 R2028 Q2029 D2033 D2037 Q2045 L2046 GLU GLY GLU GLU GLU
GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 H2100 E2108 Q2127 L2159 I2167 E2175 N2176 Y2192 L2201 G2202 M2203 V2212
G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 L2236 M2250 Y2256 I2263 G2264 D2282 Q2308 S2309 D2320 I2321 R2336 V2341 R2355 E2382 R2385 V2397 ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415


E2449
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D2482
G2483
V2495
H2498
E2513
N2514
Q2515
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F2541
R2575
D2580
Y2587
S2590
H2621
L2626
L2633
P2640
L2644
R2650
C2651
W2661
F2664
K2677
L2678
K2689
D2716
S2720
S2721
K2722
A2723
E2724
K2725
LYS
ALA
THR
VAL
ASP
ALA
GLU
GLY
N2734
F2735
D2736
P2737
R2738
P2739
V2740
E2741
T2742
L2743
N2744
V2745
I2746
I2747
P2748
E2749
K2750
L2751
D2752
S2753
F2754
I2755
N2756
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G2778
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L2785
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M2790
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R2792
P2793
Y2794
K2795
T2796
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S2798
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GLN
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TYR
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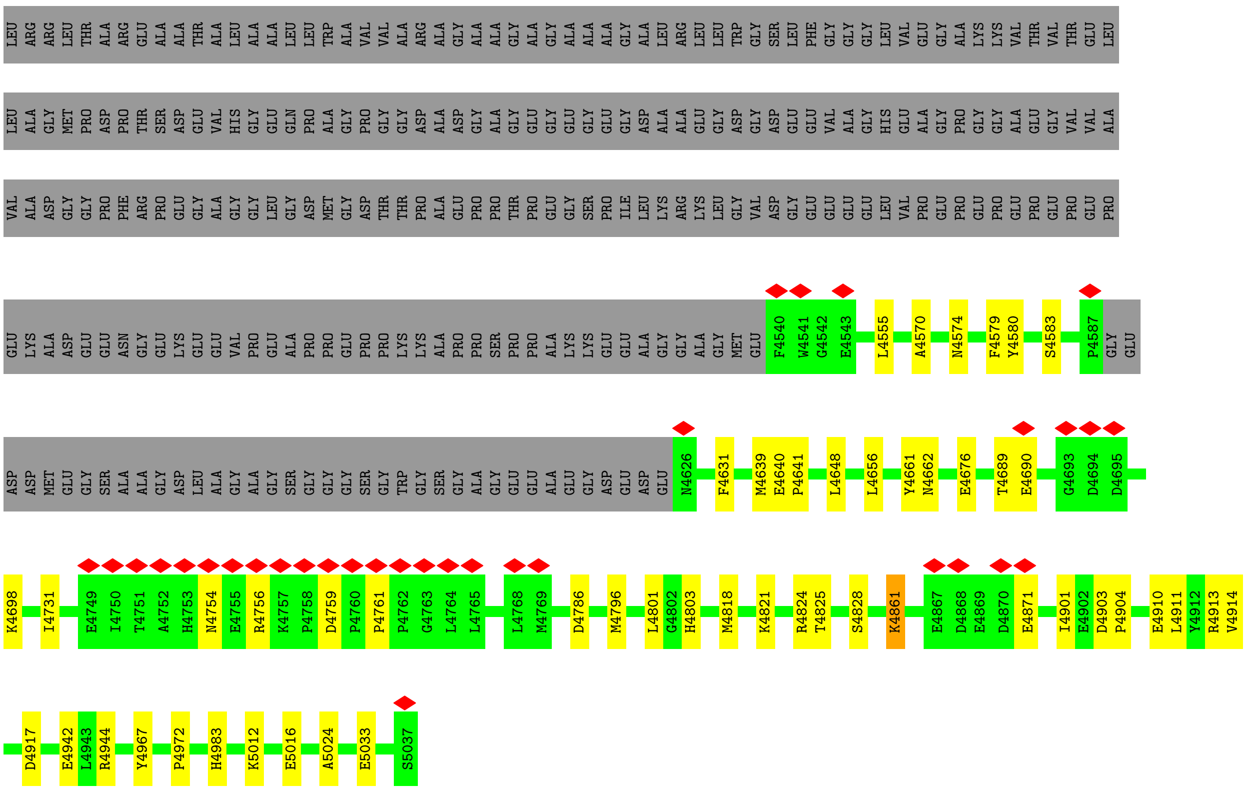
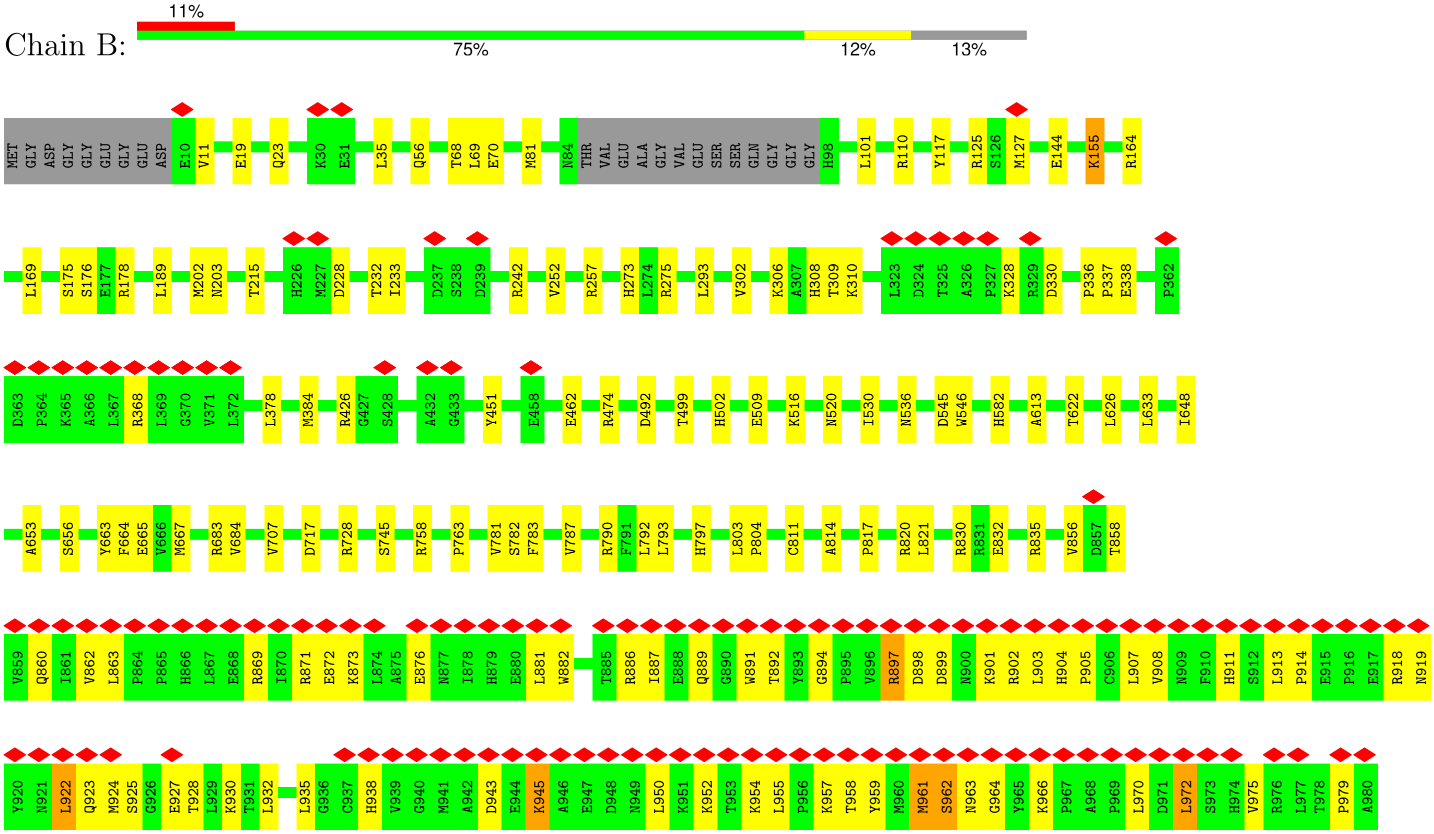
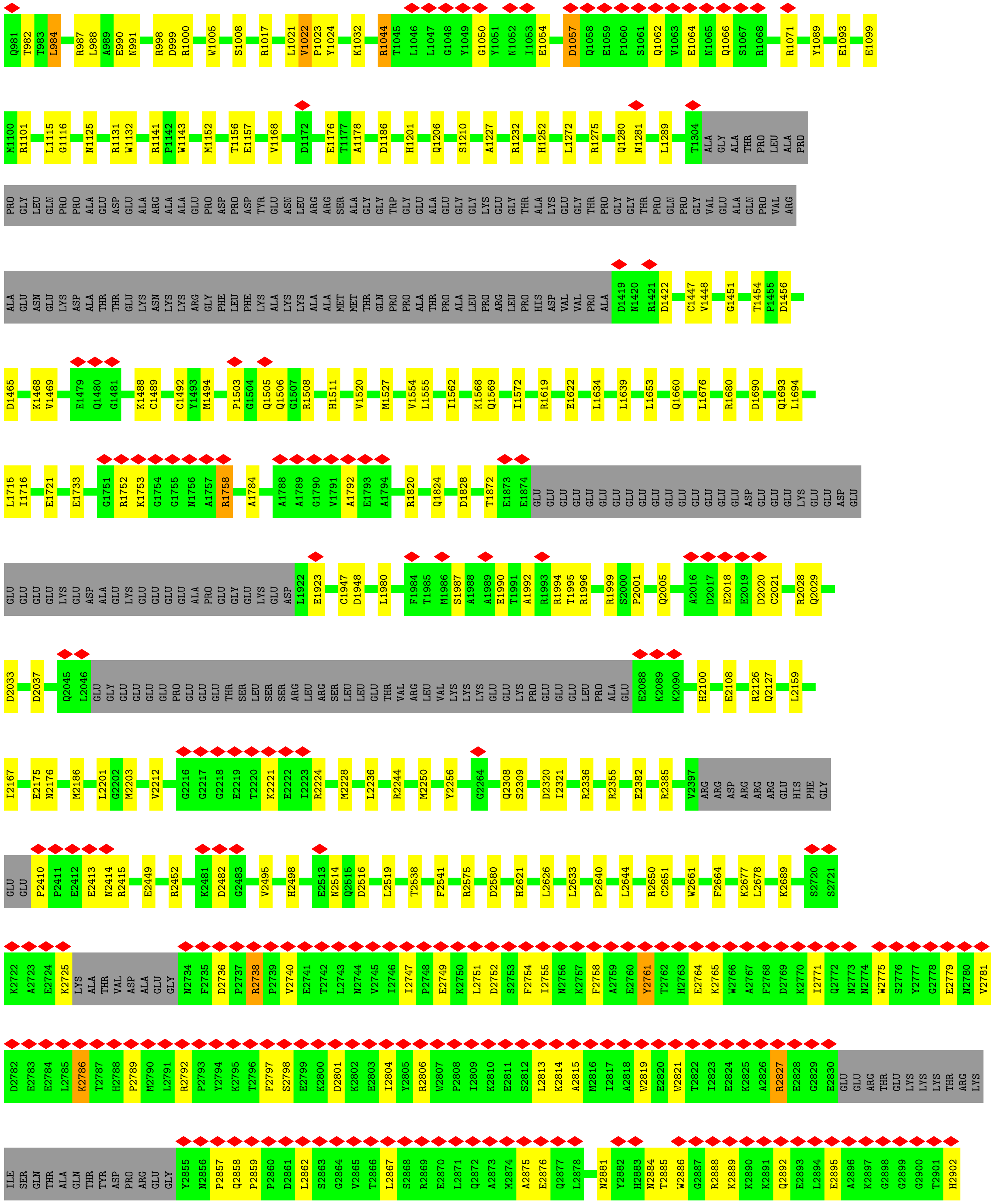


- Molecule 3: Ryanodine receptor 1

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PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 D1422 C1447 V1448 G1451 T1454 P1455 D1456
D1465 K1468 V1469 E1479 Q1480 G1481 K1488 C1489 C1492 Y1493 M1494 P1503 G1504 Q1505 Q1506 G1507 R1508 H1511 V1520 M1527 V1554 L1555 I1562 K1568 Q1569 I1572 R1619 E1622 L1634 L1639 L1653 Q1660 L1676 R1680 D1690 Q1693 L1694
L1715 I1716 E1721 E1733 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 A1784 A1788 A1789 G1790 V1791 A1792 E1793 A1794 R1820 Q1824 D1828 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU
GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 C1947 D1948 L1980 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 R1999 S2000 P2001 Q2005 A2016 D2017 E2018 E2019 D2020 C2021 R2028 Q2029
D2033 D2037 Q2045 L2046 GLU GLY GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 H2100 E2108 R2126 Q2127 L2159
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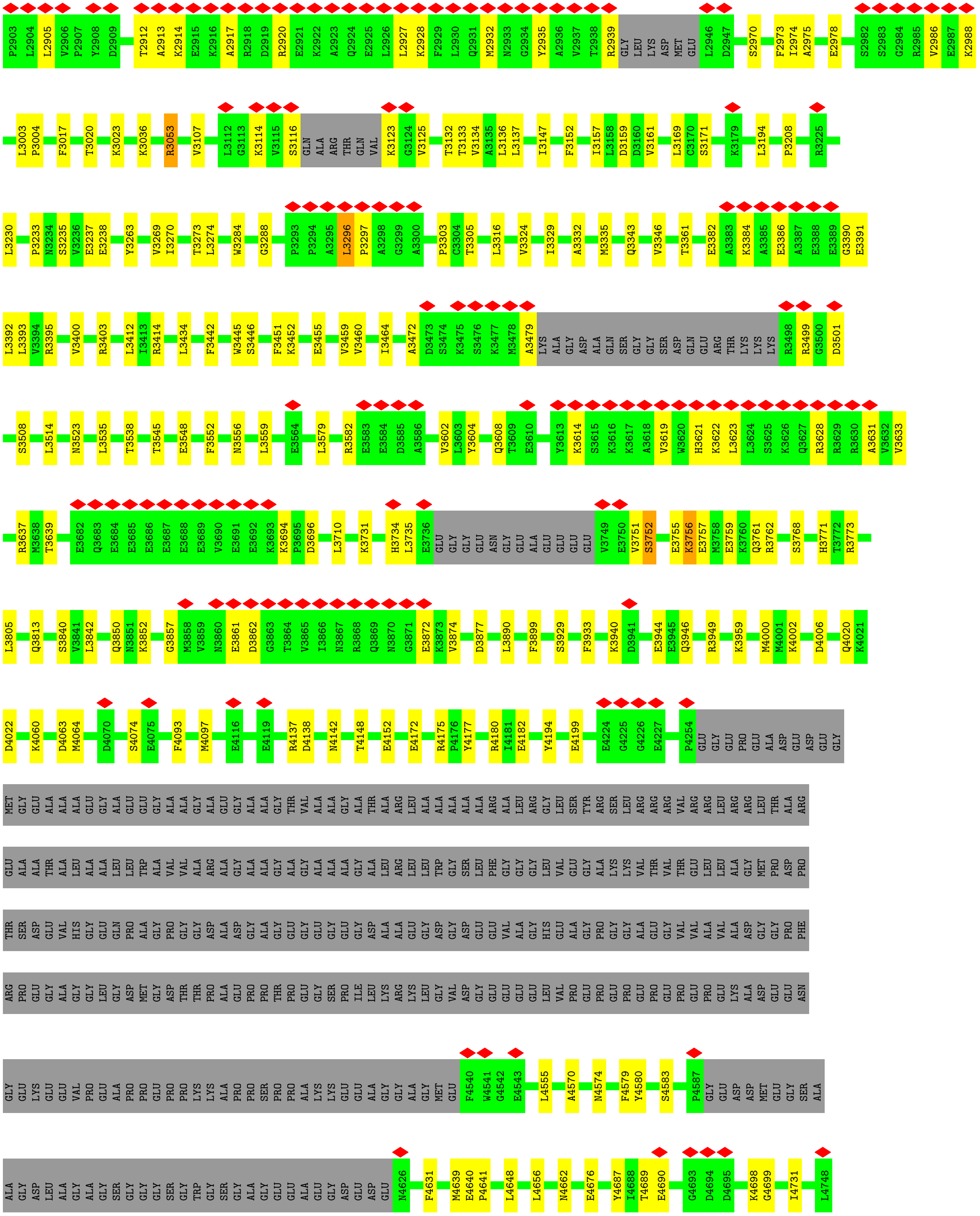
ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902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L3392 L3393 V3394 R3395 V3400 R3403 L3412 I3413 R3414 L3434 F3442 W3445 S3446 F3451 K3452 E3455 V3459 V3460 I3464 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501
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L3805 Q3813 S3840 V3841 L3842 Q3850 N3851 K3852 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 D3877 L3890 F3899 S3929 F3933 K3940 D3941 E3944 E3945 Q3946 R3949 K3959 M4000 M4001 K4002 D4006 Q4020 K4021
D4022 K4060 D4063 M4064 D4070 S4074 E4075 F4093 M4097 E4116 E4119 R4137 D4138 N4142 T4148 E4152 E4172 R4175 P4176 Y4177 R4180 I4181 E4182 Y4194 E4199 E4224 G4225 G4226 E4227 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY
MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG LEU ARG ARG LEU THR ALA ARG
GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO
THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE
ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN
GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4555 A4570 N4574 F4579 Y4580 S4583 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA
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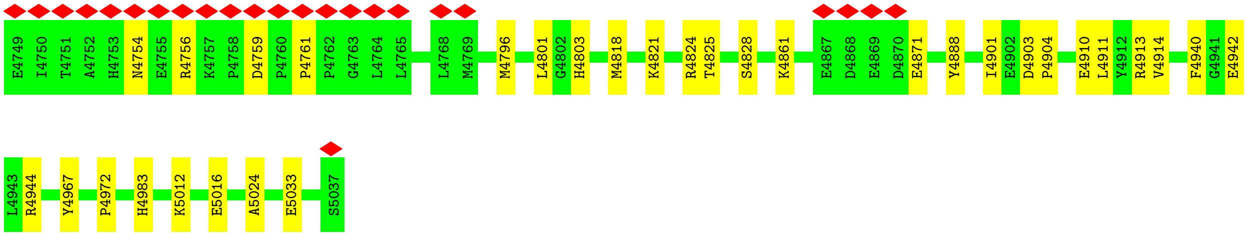
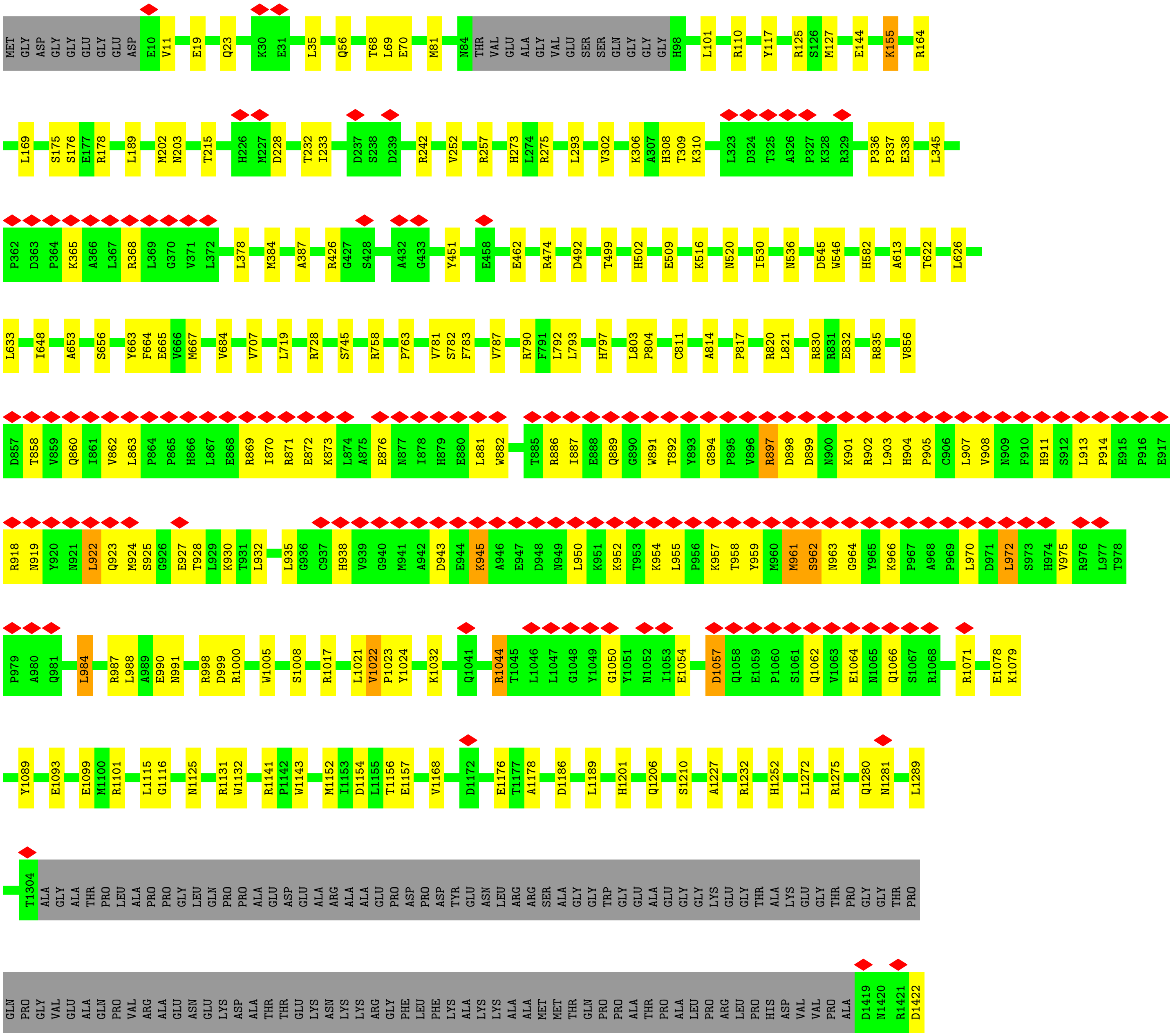
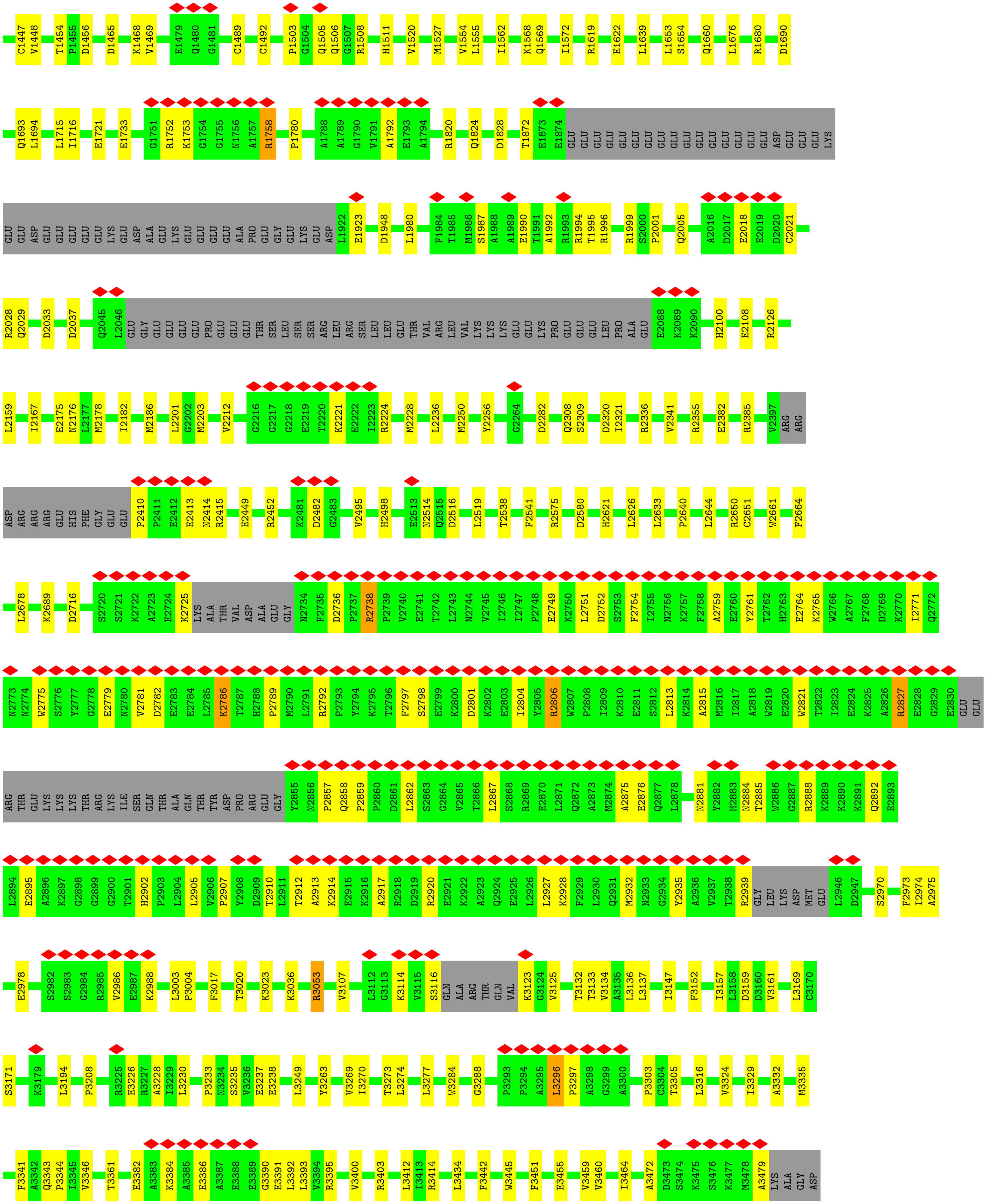


- Molecule 3: Ryanodine receptor 1

Chain G:

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GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 D1948 L1980 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 R1999 S2000 P2001 Q2005 A2016 D2017 E2018 E2019 D2020 C2021
R2028 Q2029 D2033 D2037 Q2045 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 H2100 E2108 R2126
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ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415 E2449 R2452 K2481 D2482 G2483 V2495 H2498 E2513 N2514 Q2515 D2516 L2519 T2538 F2541 R2575 D2580 H2621 L2626 L2633 P2640 L2644 R2650 C2651 W2661 F2664
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ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893
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E2978 S2982 S2983 G2984 R2985 V2986 E2987 K2988 L3003 P3004 F3017 T3020 K3023 K3036 R3053 V3107 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 T3132 T3133 V3134 A3135 L3136 L3137 I3147 F3152 I3157 L3158 D3159 D3160 V3161 L3169 C3170
S3171 K3179 L3194 P3208 R3225 E3226 R3227 A3228 I3229 L3230 P3233 N3234 S3235 V3236 E3237 E3238 L3249 Y3263 V3269 I3270 T3273 L3274 L3277 W3284 G3288 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3303 C3304 T3305 L3316 V3324 I3329 A3332 M3335
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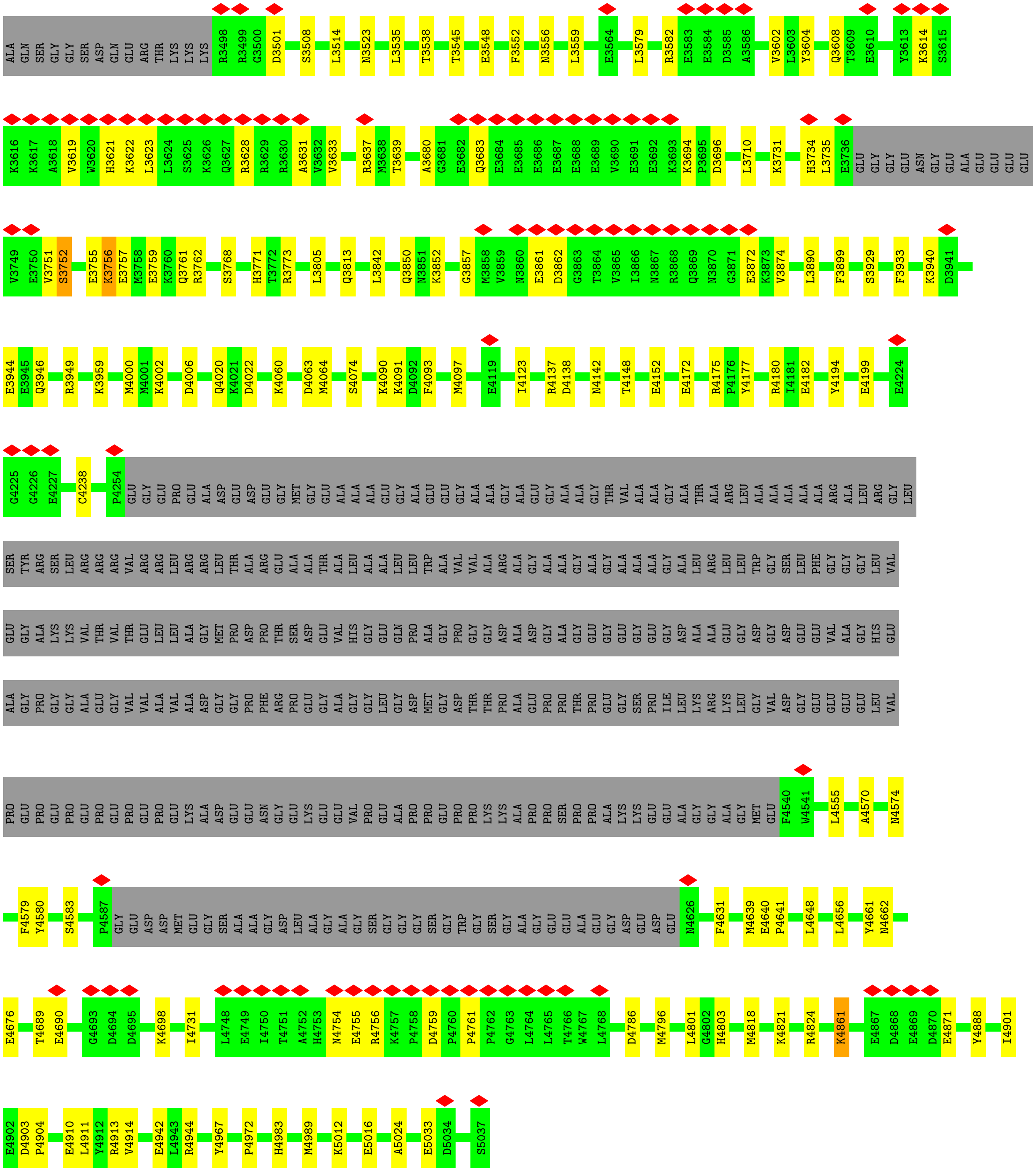
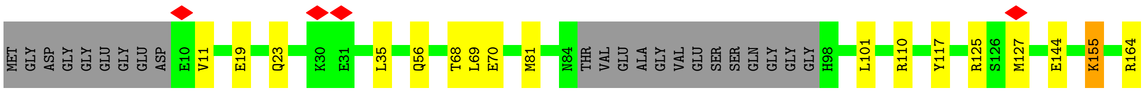
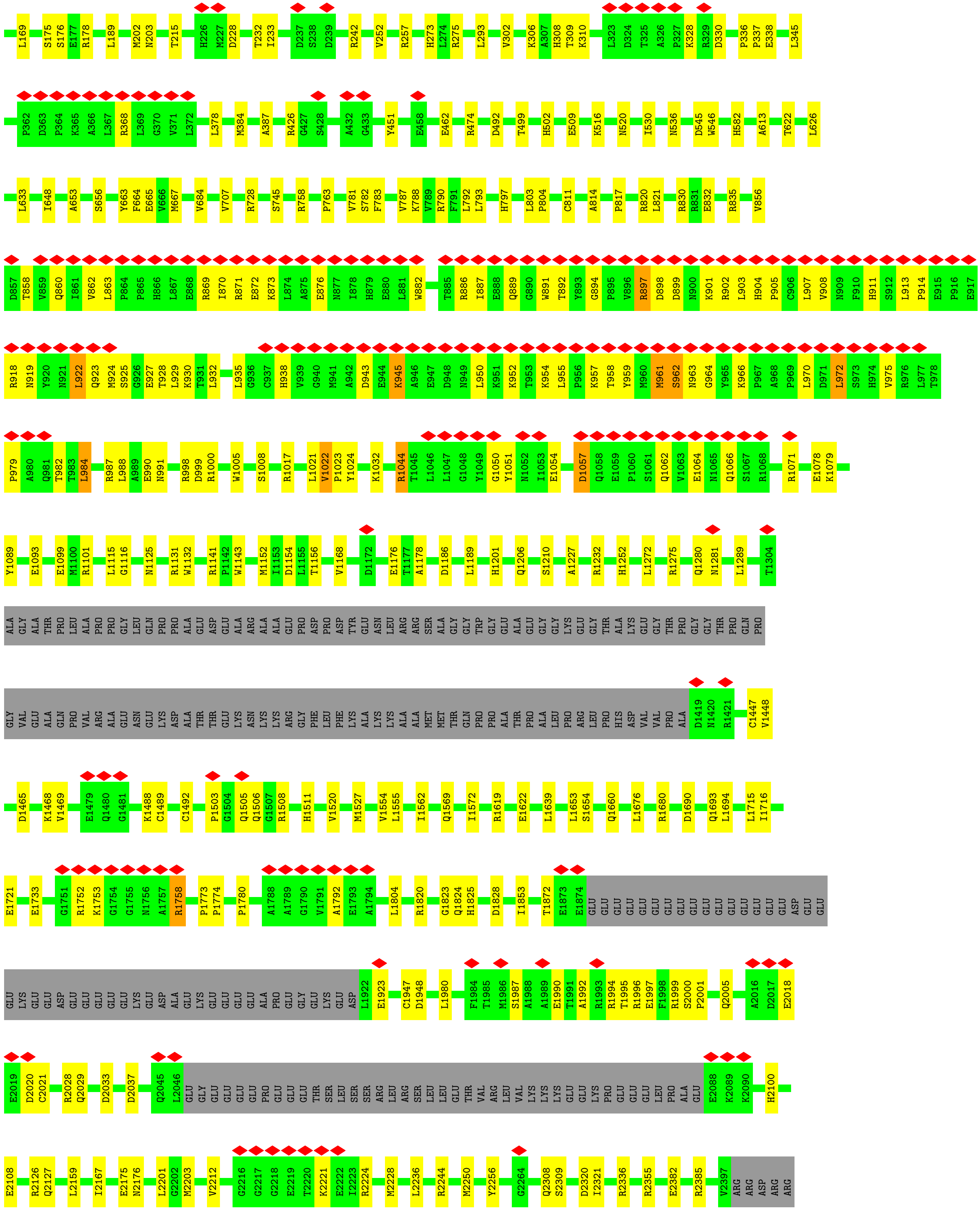


- Molecule 3: Ryanodine receptor 1

Chain I:

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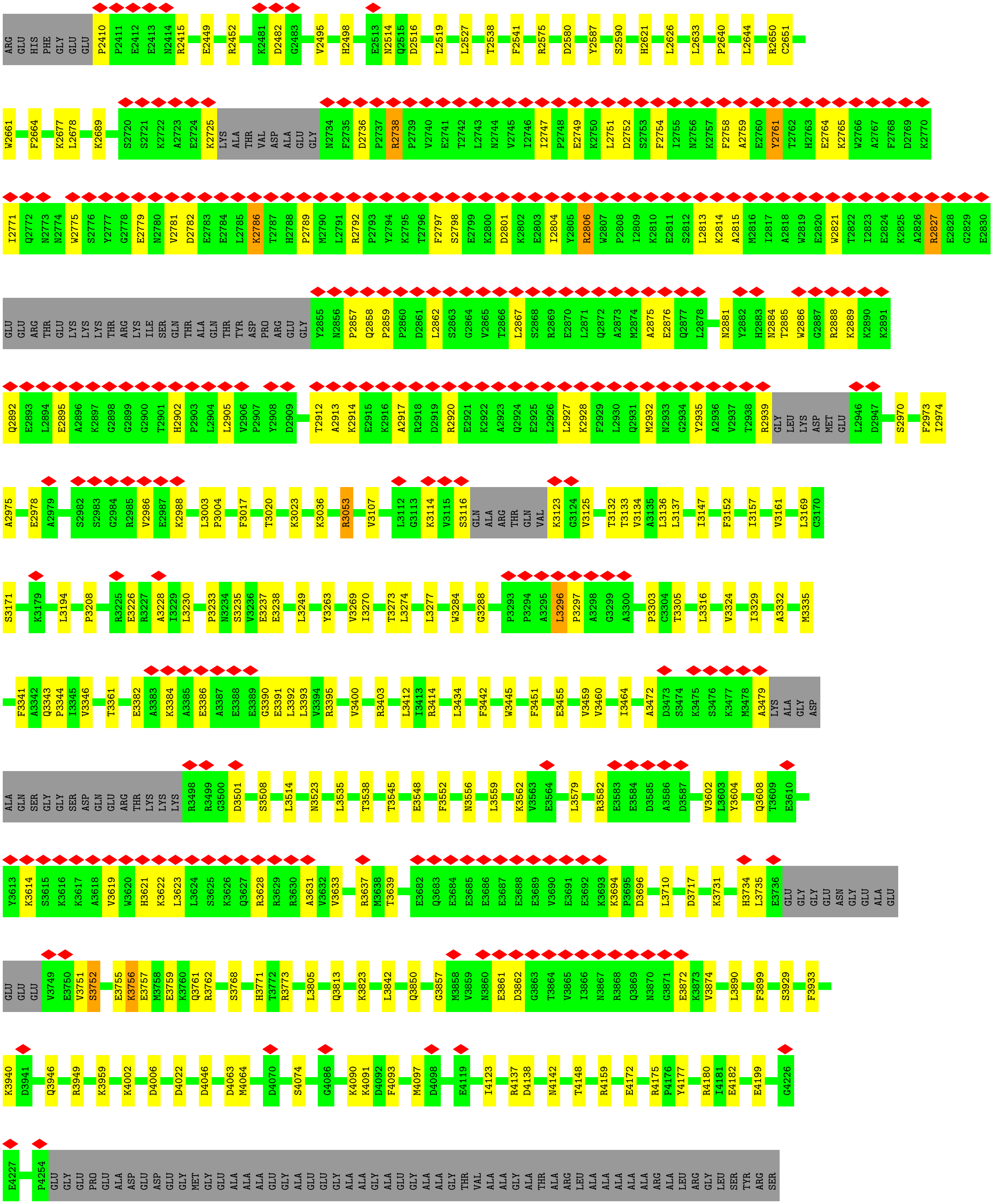
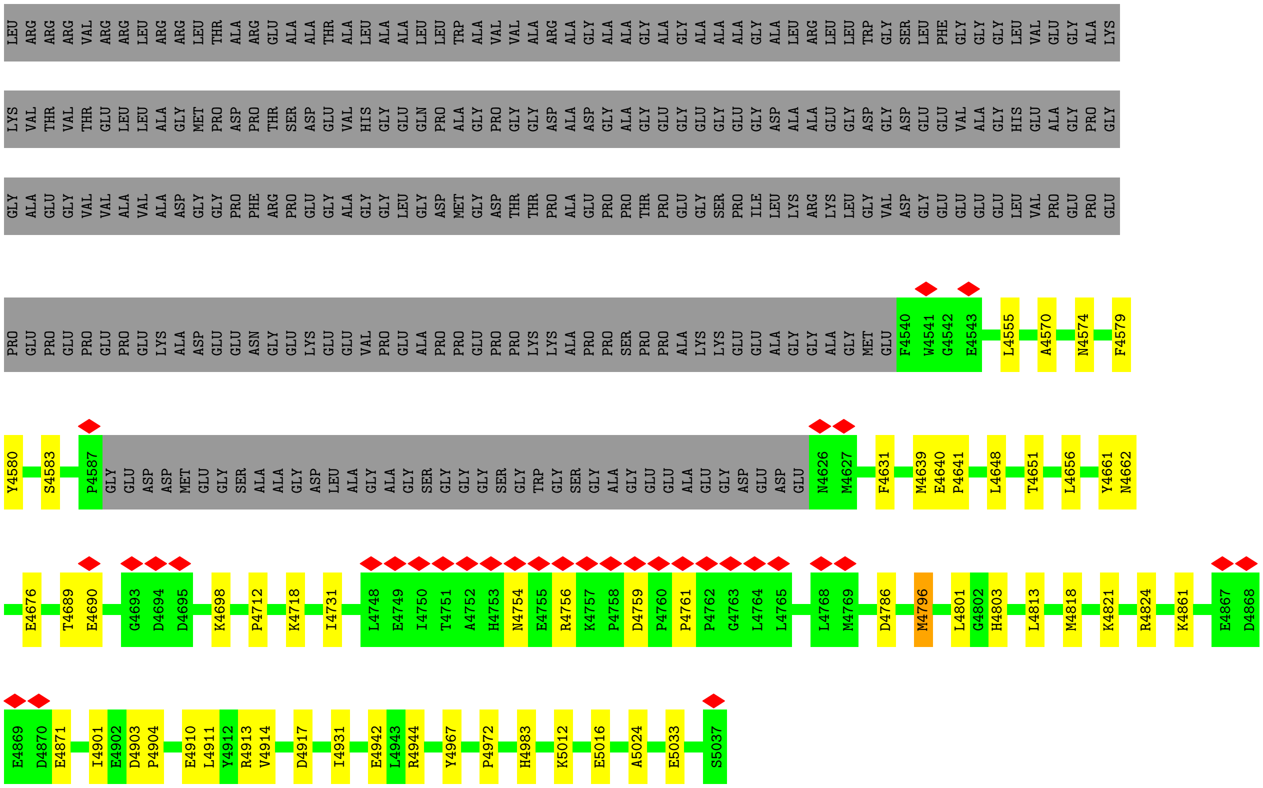
P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 L378 M384 A387 R426 G427 S428 A432 G433 Y451 E458 E462 R474 D492 T499 H502 E509 K516 N520 I530 N536 D545 W546 H582 A613 T622 L626
L633 I648 A653 S656 Y663 F664 E665 V666 M667 V684 V707 R728 S745 R758 P763 V781 S782 F783 V787 K788 V789 R790 F791 L792 L793 H797 L803 P804 C811 A814 P817 R820 L821 R830 R831 E832 R835 V856
D857 T858 V859 Q860 I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 A875 E876 N877 I878 H879 E880 L881 W882 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 H911 S912 L913 P914 E915 P916 E917
R918 N919 Y920 N921 L922 Q923 M924 S925 G926 E927 T928 L929 K930 T931 L932 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966 P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978
P979 A980 Q981 T982 T983 L984 R987 L988 A989 E990 N991 R998 D999 R1000 W1005 S1008 R1017 L1021 V1022 P1023 Y1024 K1032 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 D1057 Q1058 E1059 P1060 S1061 Q1062 V1063 E1064 N1065 Q1066 S1067 R1068 R1071 E1078 K1079
Y1089 E1093 E1099 M1100 R1101 L1115 G1116 N1125 R1131 W1132 R1141 P1142 W1143 M1152 I1153 D1154 L1155 T1156 V1168 D1172 E1176 T1177 A1178 D1186 L1189 H1201 Q1206 S1210 A1227 R1232 H1252 L1272 R1275 Q1280 N1281 L1289 T1304
ALA GLY ALA THR PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO
GLY VAL GLU ALA GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA D1419 N1420 R1421 C1447 V1448
D1465 K1468 V1469 E1479 Q1480 G1481 K1488 C1489 C1492 P1503 G1504 Q1505 Q1506 G1507 R1508 H1511 V1520 M1527 V1554 L1555 I1562 Q1569 I1572 R1619 E1622 L1639 L1653 S1654 Q1660 L1676 R1680 D1690 Q1693 L1694 L1715 I1716
E1721 E1733 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 P1773 P1774 P1780 A1788 A1789 G1790 V1791 A1792 E1793 A1794 L1804 R1820 G1823 Q1824 H1825 D1828 I1853 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU
GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 C1947 D1948 L1980 F1984 T1985 M1986 S1987 A1988 A1989 E1990 T1991 A1992 R1993 R1994 T1995 R1996 E1997 F1998 R1999 S2000 P2001 Q2005 A2016 D2017 E2018
E2019 D2020 C2021 R2028 Q2029 D2033 D2037 Q2045 L2046 GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU E2088 K2089 K2090 H2100
E2108 R2126 Q2127 L2159 I2167 E2175 N2176 L2201 G2202 M2203 V2212 G2216 G2217 G2218 E2219 T2220 K2221 E2222 I2223 R2224 M2228 L2236 R2244 M2250 Y2256 G2264 Q2308 S2309 D2320 I2321 R2336 R2355 E2382 R2385 V2397 ARG ARG ASP ARG ARG


ARG GLU HIS PHE GLY GLU GLU P2410 P2411 E2412 E2413 N2414 R2415 E2449 R2452 K2481 D2482 G2483 V2495 H2498 E2513 N2514 Q2515 D2516 L2519 L2527 T2538 F2541 R2575 D2580 Y2587 S2590 H2621 L2626 L2633 P2640 L2644 R2650 C2651
W2661 F2664 K2677 L2678 K2689 S2720 S2721 K2722 A2723 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY N2734 F2735 D2736 P2737 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758 A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770
I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830
GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891
Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU L2946 D2947 S2970 F2973 I2974
A2975 E2978 A2979 S2982 S2983 G2984 R2985 V2986 E2987 K2988 L3003 P3004 F3017 T3020 K3023 K3036 R3053 V3107 L3112 G3113 K3114 V3115 S3116 GLN ALA ARG THR GLN VAL K3123 G3124 V3125 T3132 T3133 V3134 A3135 L3136 L3137 I3147 F3152 I3157 V3161 L3169 C3170
S3171 K3179 L3194 P3208 R3225 E3226 R3227 A3228 I3229 L3230 P3233 N3234 S3235 V3236 E3237 E3238 L3249 Y3263 V3269 I3270 T3273 L3274 L3277 W3284 G3288 P3293 P3294 A3295 L3296 P3297 A3298 G3299 A3300 P3303 C3304 T3305 L3316 V3324 I3329 A3332 M3335
F3341 A3342 Q3343 P3344 I3345 V3346 T3361 E3382 A3383 K3384 A3385 E3386 A3387 E3388 E3389 G3390 E3391 L3392 L3393 V3394 R3395 V3400 R3403 L3412 I3413 R3414 L3434 F3442 W3445 F3451 E3455 V3459 V3460 I3464 A3472 D3473 S3474 K3475 S3476 K3477 M3478 A3479 LYS ALA GLY ASP
ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS R3498 R3499 G3500 D3501 S3508 L3514 N3523 L3535 T3538 T3545 E3548 F3552 N3556 L3559 K3562 V3563 E3564 L3579 R3582 E3583 E3584 D3585 A3586 D3587 V3602 L3603 Y3604 Q3608 T3609 E3610
Y3613 K3614 S3615 K3616 K3617 A3618 V3619 W3620 H3621 K3622 L3623 L3624 S3625 K3626 Q3627 R3628 R3629 R3630 A3631 V3632 V3633 R3637 M3638 T3639 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 K3694 P3695 D3696 L3710 D3717 K3731 H3734 L3735 E3736 GLU GLY GLY GLU ASN GLY GLU ALA GLU
GLU GLU GLU V3749 E3750 V3751 S3752 E3755 K3756 E3757 M3758 E3759 K3760 Q3761 R3762 S3768 H3771 T3772 R3773 L3805 Q3813 K3823 L3842 Q3850 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 V3874 L3890 F3899 S3929 F3933
K3940 D3941 Q3946 R3949 K3959 K4002 D4006 D4022 D4046 D4063 M4064 D4070 S4074 G4086 K4090 K4091 D4092 F4093 M4097 D4098 E4119 I4123 R4137 D4138 N4142 T4148 R4159 E4172 R4175 P4176 Y4177 R4180 I4181 E4182 E4199 G4226
E4227 P4254 GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA 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 LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS
LYS VAL THR VAL THR GLU LEU LEU ALA GLY MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY
GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU
PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 W4541 G4542 E4543 L4555 A4570 N4574 F4579
Y4580 S4583 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 M4627 F4631 M4639 E4640 P4641 L4648 T4651 L4656 Y4661 N4662
E4676 T4689 E4690 G4693 D4694 D4695 K4698 P4712 K4718 I4731 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 L4768 M4769 D4786 M4796 L4801 G4802 H4803 L4813 M4818 K4821 R4824 K4861 E4867 D4868
E4869 D4870 E4871 I4901 E4902 D4903 P4904 E4910 L4911 Y4912 R4913 V4914 D4917 I4931 E4942 L4943 R4944 Y4967 P4972 H4983 K5012 E5016 A5024 E5033 S5037

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	333010	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^{-}/\text{Å}^2)$	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.887	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	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: L9R, KVR, CFF, CA, ZN, 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	C	0.24	0/1187	0.44	0/1594
1	D	0.24	0/1187	0.44	0/1594
1	E	0.24	0/1187	0.44	0/1594
1	K	0.24	0/1187	0.44	0/1594
2	F	0.32	0/850	0.52	0/1146
2	H	0.32	0/850	0.52	0/1146
2	J	0.32	0/850	0.52	0/1146
2	O	0.32	0/850	0.52	0/1146
3	A	0.25	0/35977	0.46	0/48726
3	B	0.25	0/35977	0.46	0/48726
3	G	0.25	0/35977	0.46	0/48726
3	I	0.25	0/35977	0.46	0/48726
All	All	0.25	0/152056	0.46	0/205864

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	C	1174	0	1099	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1174	0	1099	17	0
1	E	1174	0	1099	17	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	347	0
3	B	35150	0	34797	347	0
3	G	35150	0	34797	345	0
3	I	35150	0	34797	352	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0
9	B	108	0	172	5	0
9	G	108	0	172	8	0
9	I	108	0	172	7	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	1	0	0	0	0
All	All	149476	0	147732	1458	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.

The worst 5 of 1458 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	C	147/150 (98%)	146 (99%)	1 (1%)	0	100 100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100 100
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100 100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100 100
2	F	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
2	H	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
2	J	105/108 (97%)	103 (98%)	2 (2%)	0	100 100
2	O	105/108 (97%)	103 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21180 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	C	127/128 (99%)	122 (96%)	5 (4%)	27	41
1	D	127/128 (99%)	122 (96%)	5 (4%)	27	41
1	E	127/128 (99%)	122 (96%)	5 (4%)	27	41
1	K	127/128 (99%)	122 (96%)	5 (4%)	27	41
2	F	89/90 (99%)	86 (97%)	3 (3%)	32	46
2	H	89/90 (99%)	86 (97%)	3 (3%)	32	46
2	J	89/90 (99%)	86 (97%)	3 (3%)	32	46
2	O	89/90 (99%)	86 (97%)	3 (3%)	32	46
3	A	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
3	B	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
3	G	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
3	I	3836/4276 (90%)	3760 (98%)	76 (2%)	50	65
All	All	16208/17976 (90%)	15872 (98%)	336 (2%)	49	64

5 of 336 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	2761	TYR

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Mol	Chain	Res	Type
3	I	1021	LEU
3	G	2914	LYS
3	I	81	MET
3	I	2100[A]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	3761	GLN
3	G	991	ASN
3	I	2881	ASN
3	I	991	ASN
3	I	2180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	CFF	A	5304	-	8,15,15	0.82	0	8,23,23	2.80	2 (25%)
9	L9R	B	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	B	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
7	CFF	G	5304	-	8,15,15	0.82	0	8,23,23	2.79	2 (25%)
9	L9R	A	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	I	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	ATP	I	5301	-	28,33,33	0.63	0	34,52,52	0.85	2 (5%)
9	L9R	I	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	G	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	B	5304	-	8,15,15	0.85	0	8,23,23	2.80	2 (25%)
8	KVR	G	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.56	4 (12%)
9	L9R	B	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	A	5301	-	28,33,33	0.62	0	34,52,52	0.85	2 (5%)
9	L9R	A	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
7	CFF	I	5304	-	8,15,15	0.83	0	8,23,23	2.80	3 (37%)
8	KVR	A	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	I	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	A	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
8	KVR	B	5306	-	24,25,25	1.42	3 (12%)	31,34,34	1.55	4 (12%)
5	ATP	G	5301	-	28,33,33	0.61	0	34,52,52	0.85	2 (5%)
8	KVR	I	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	G	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	G	5305	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
5	ATP	B	5301	-	28,33,33	0.62	0	34,52,52	0.85	2 (5%)

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	CFF	A	5304	-	-	-	0/2/2/2
9	L9R	B	5307	-	-	30/57/57/57	-
5	ATP	B	5305	-	-	6/18/38/38	0/3/3/3
7	CFF	G	5304	-	-	-	0/2/2/2
9	L9R	A	5308	-	-	34/57/57/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	I	5305	-	-	6/18/38/38	0/3/3/3
5	ATP	I	5301	-	-	8/18/38/38	0/3/3/3
9	L9R	I	5307	-	-	30/57/57/57	-
9	L9R	G	5308	-	-	34/57/57/57	-
7	CFF	B	5304	-	-	-	0/2/2/2
8	KVR	G	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
5	ATP	A	5301	-	-	8/18/38/38	0/3/3/3
9	L9R	A	5307	-	-	30/57/57/57	-
7	CFF	I	5304	-	-	-	0/2/2/2
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	I	5308	-	-	34/57/57/57	-
5	ATP	A	5305	-	-	6/18/38/38	0/3/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
5	ATP	G	5301	-	-	8/18/38/38	0/3/3/3
8	KVR	I	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	G	5307	-	-	30/57/57/57	-
5	ATP	G	5305	-	-	6/18/38/38	0/3/3/3
5	ATP	B	5301	-	-	8/18/38/38	0/3/3/3

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.92	1.82	1.77
8	I	5306	KVR	C06-S09	4.91	1.82	1.77
8	A	5306	KVR	C06-S09	4.88	1.82	1.77
8	G	5306	KVR	C06-S09	4.86	1.82	1.77
9	A	5307	L9R	O2-C31	3.60	1.44	1.34

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	5304	CFF	C5-C6-N1	-6.38	111.72	118.20
7	A	5304	CFF	C5-C6-N1	-6.37	111.73	118.20
7	I	5304	CFF	C5-C6-N1	-6.35	111.76	118.20
7	G	5304	CFF	C5-C6-N1	-6.30	111.80	118.20
8	G	5306	KVR	C10-S09-C06	5.26	110.17	102.71

There are no chirality outliers.

5 of 320 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5301	ATP	C5'-O5'-PA-O3A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A

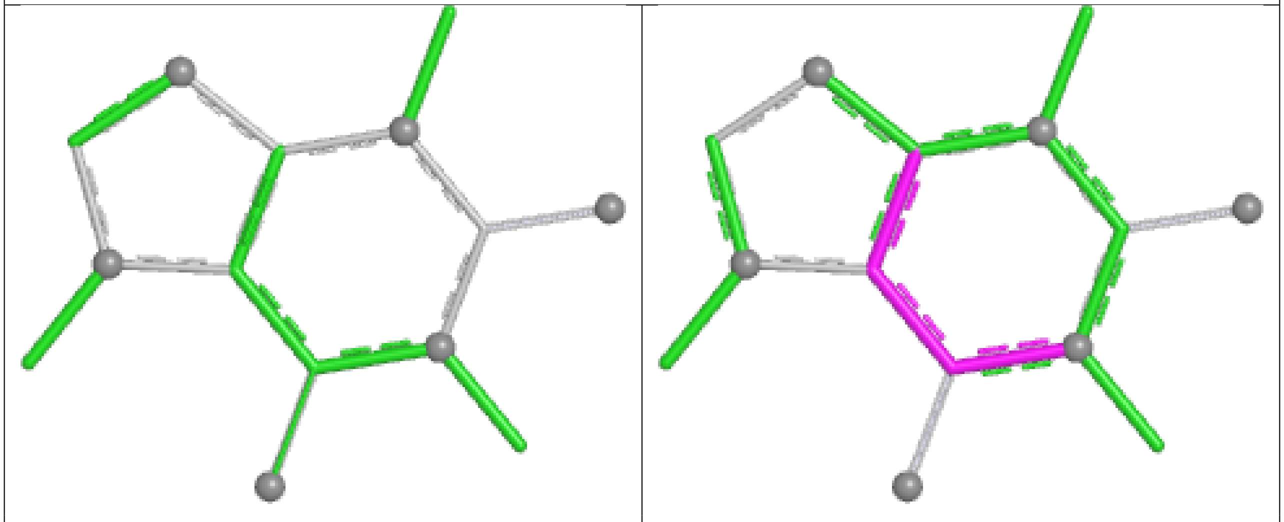
There are no ring outliers.

16 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	5307	L9R	2	0
5	B	5305	ATP	1	0
9	A	5308	L9R	6	0
5	I	5305	ATP	1	0
5	I	5301	ATP	1	0
9	I	5307	L9R	2	0
9	G	5308	L9R	5	0
9	B	5308	L9R	3	0
5	A	5301	ATP	1	0
9	A	5307	L9R	3	0
9	I	5308	L9R	5	0
5	A	5305	ATP	1	0
5	G	5301	ATP	1	0
9	G	5307	L9R	3	0
5	G	5305	ATP	1	0
5	B	5301	ATP	1	0

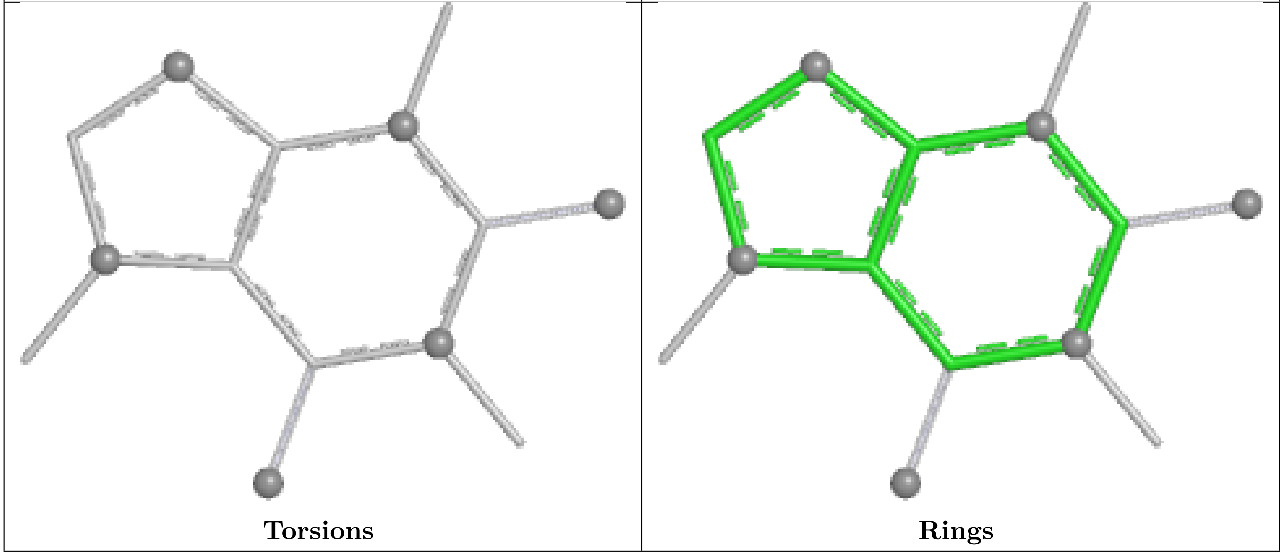
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CFF A 5304



Bond lengths

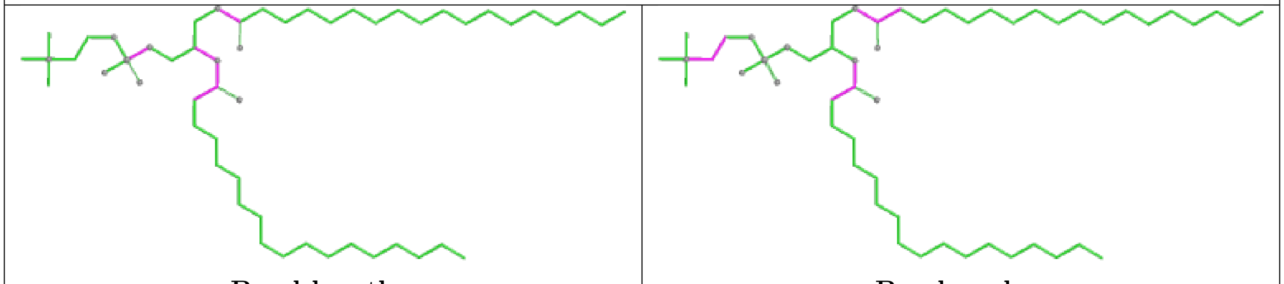
Bond angles



Torsions

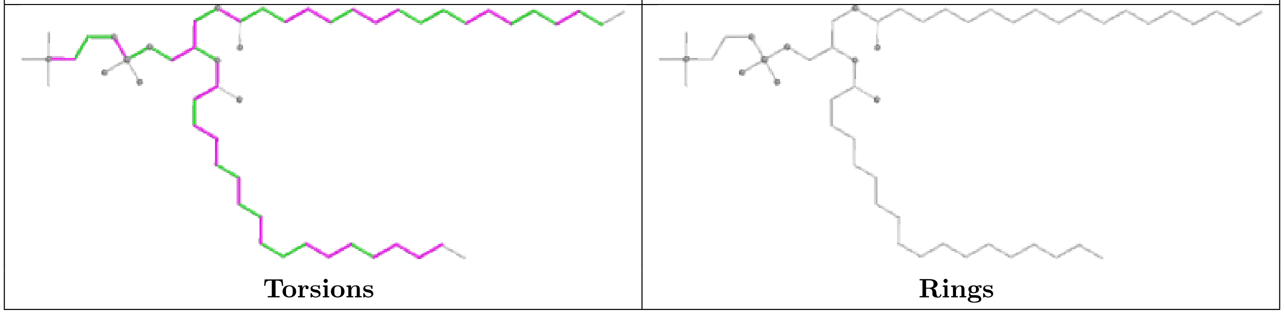
Rings

Ligand L9R B 5307



Bond lengths

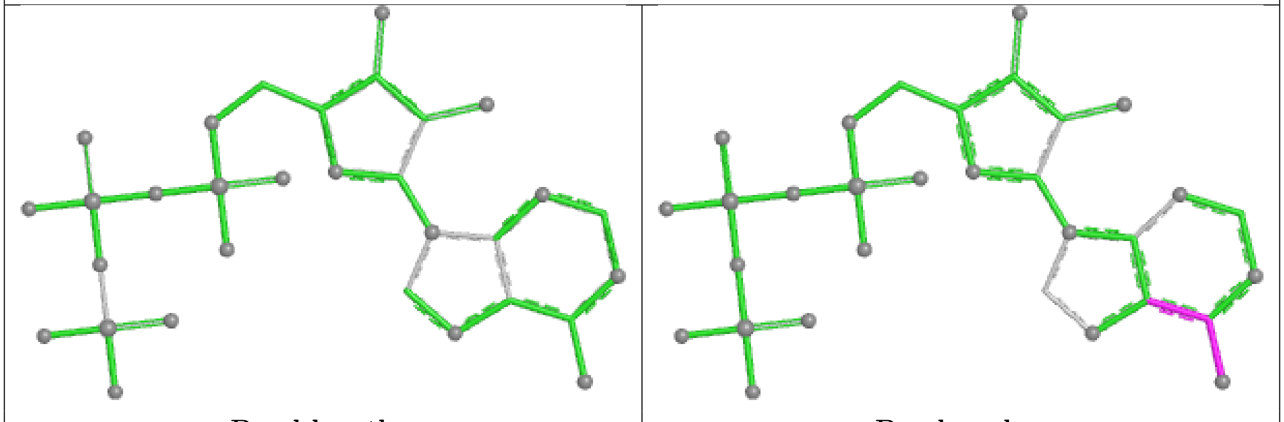
Bond angles



Torsions

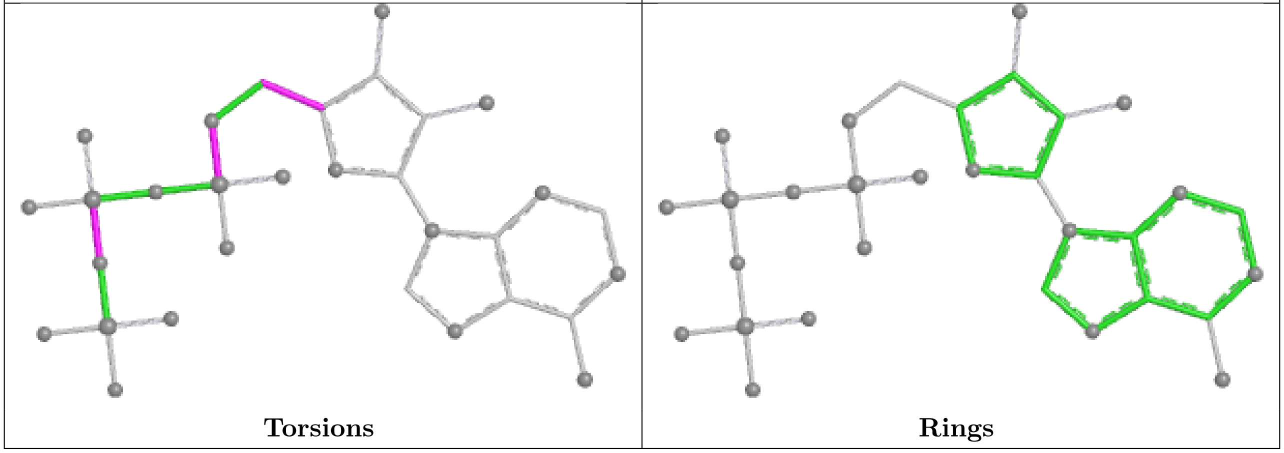
Rings

Ligand ATP B 5305



Bond lengths

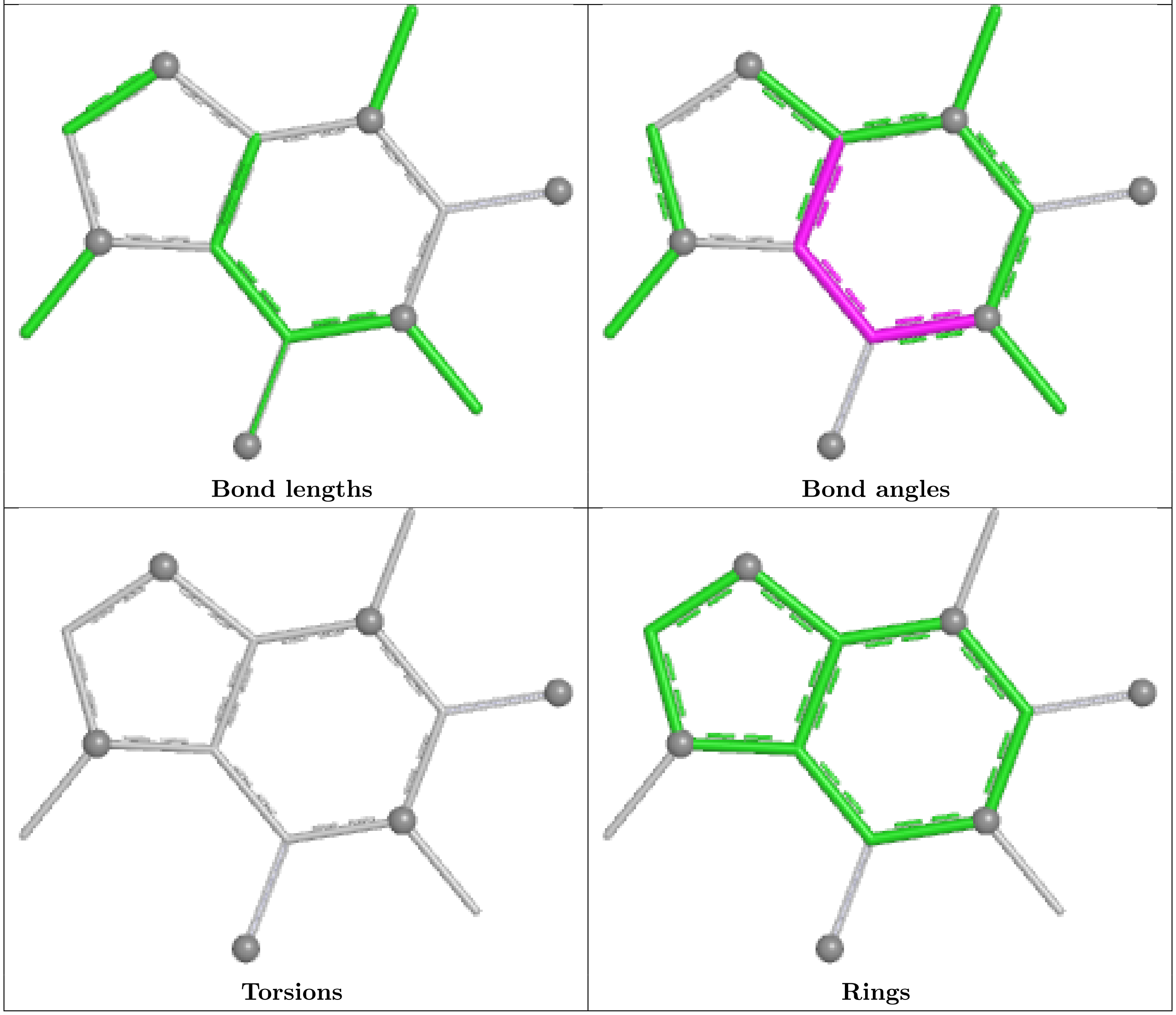
Bond angles



Torsions

Rings

Ligand CFF G 5304



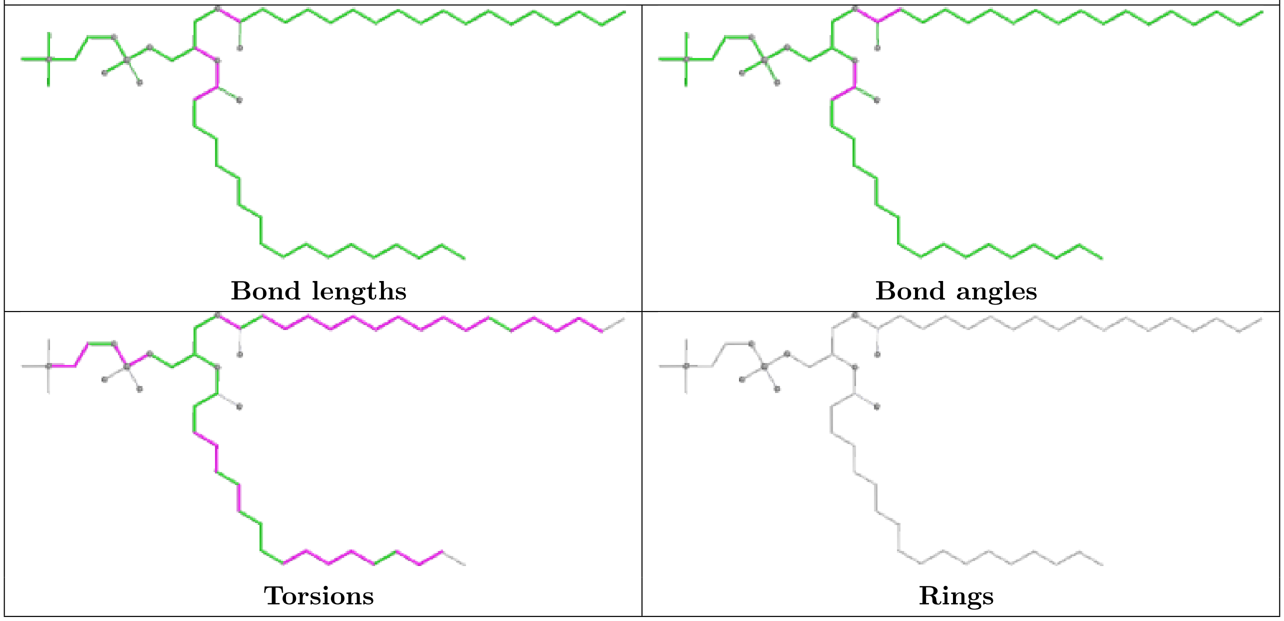
Bond lengths

Bond angles

Torsions

Rings

Ligand L9R A 5308



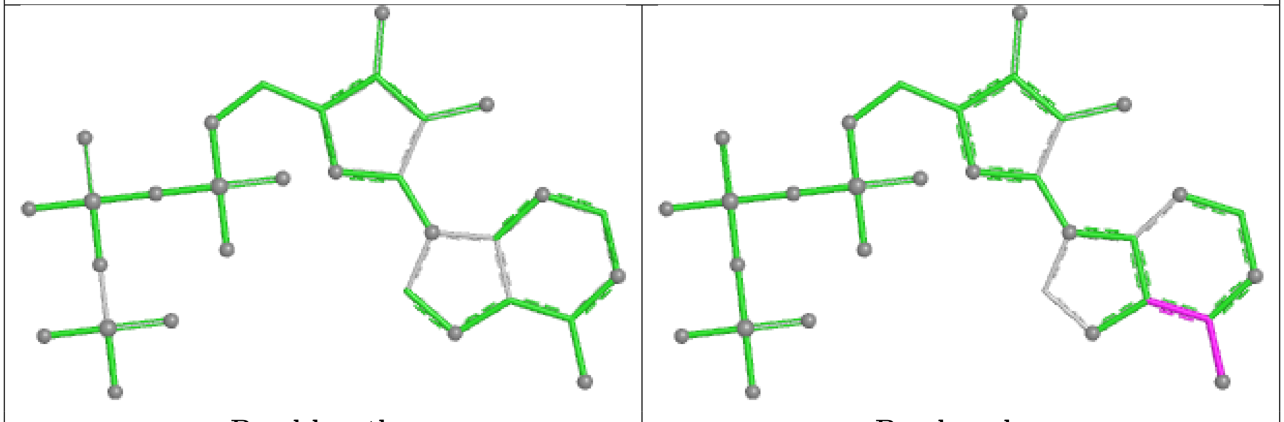
Bond lengths

Bond angles

Torsions

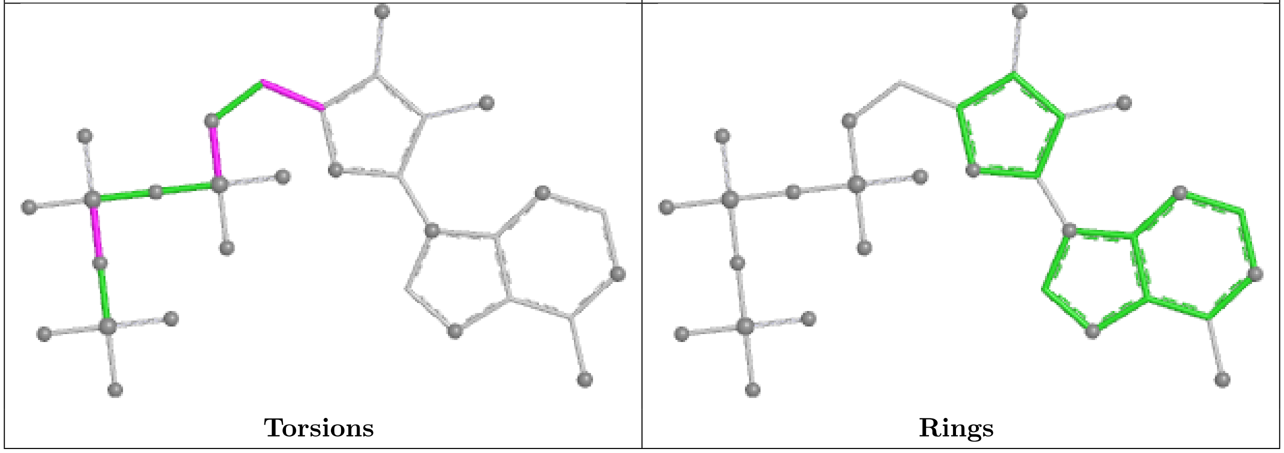
Rings

Ligand ATP I 5305



Bond lengths

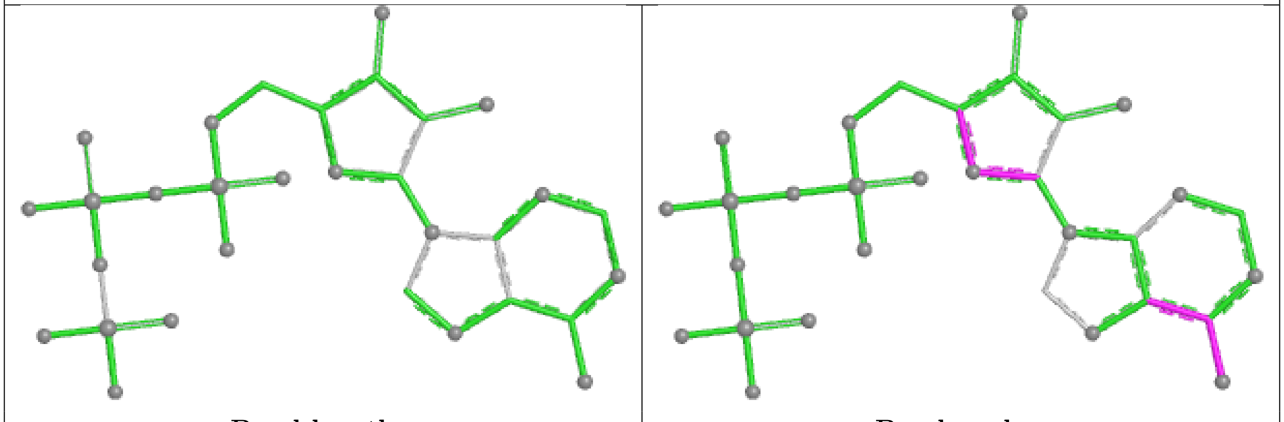
Bond angles



Torsions

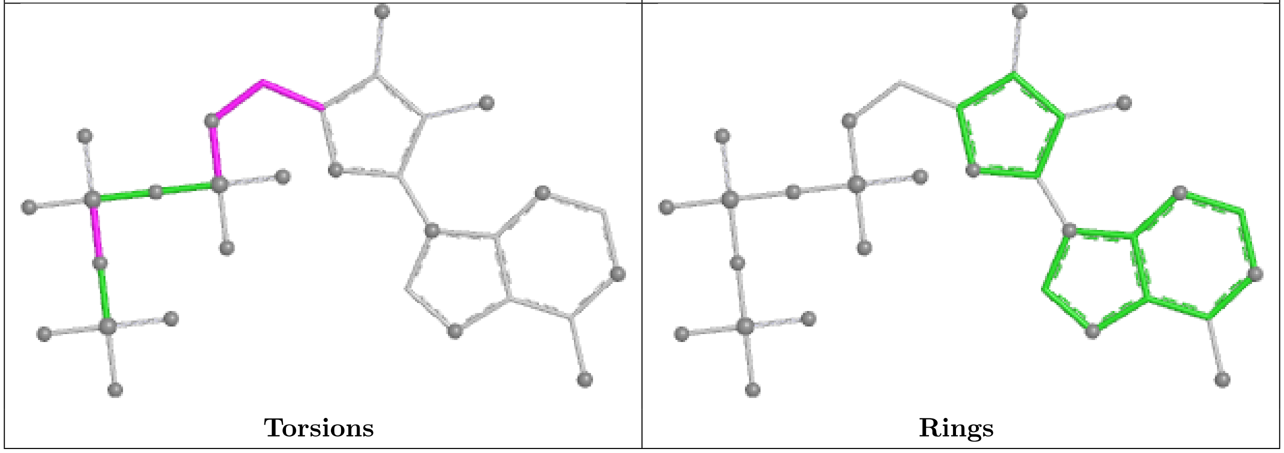
Rings

Ligand ATP I 5301



Bond lengths

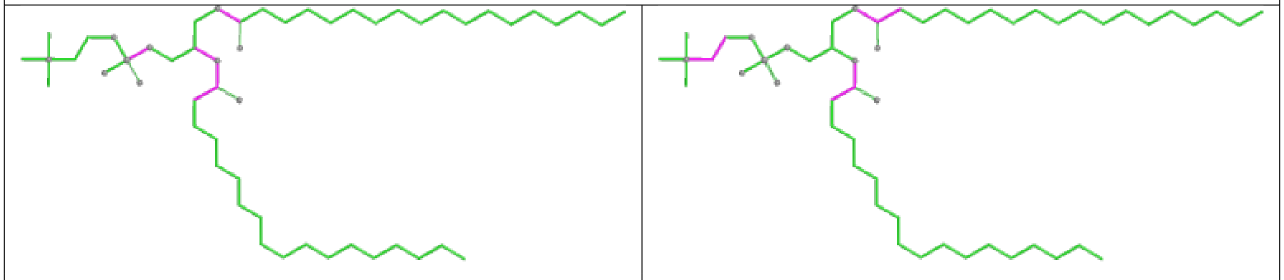
Bond angles



Torsions

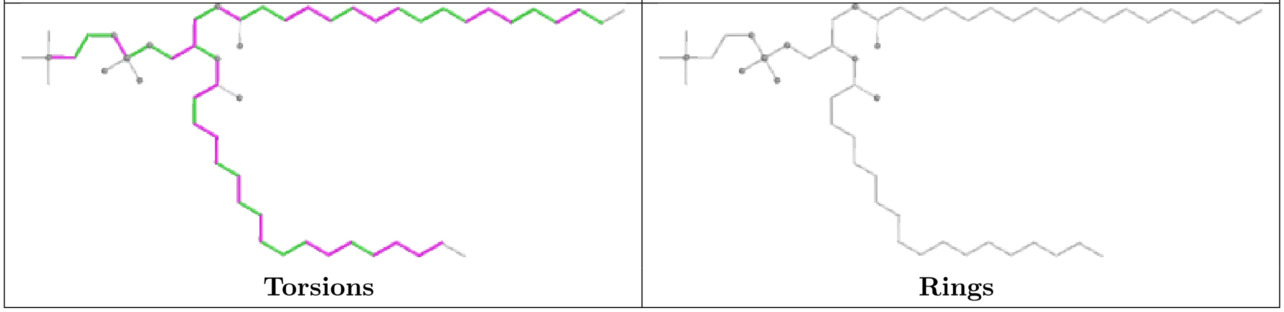
Rings

Ligand L9R I 5307



Bond lengths

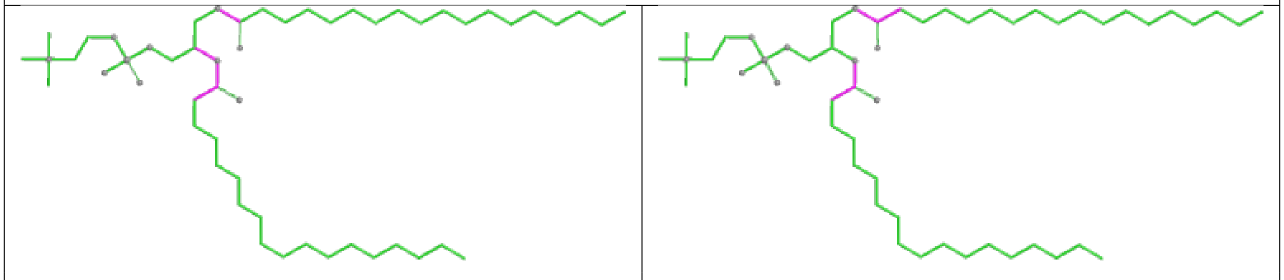
Bond angles



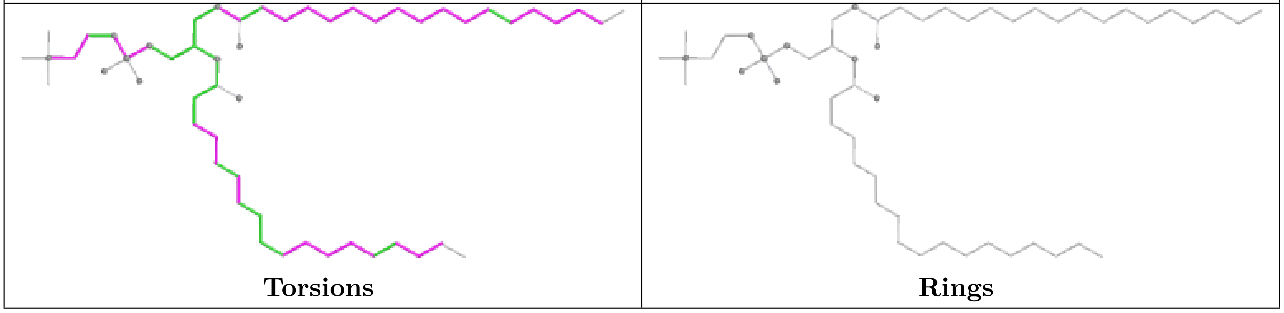
Torsions

Rings

Ligand L9R G 5308

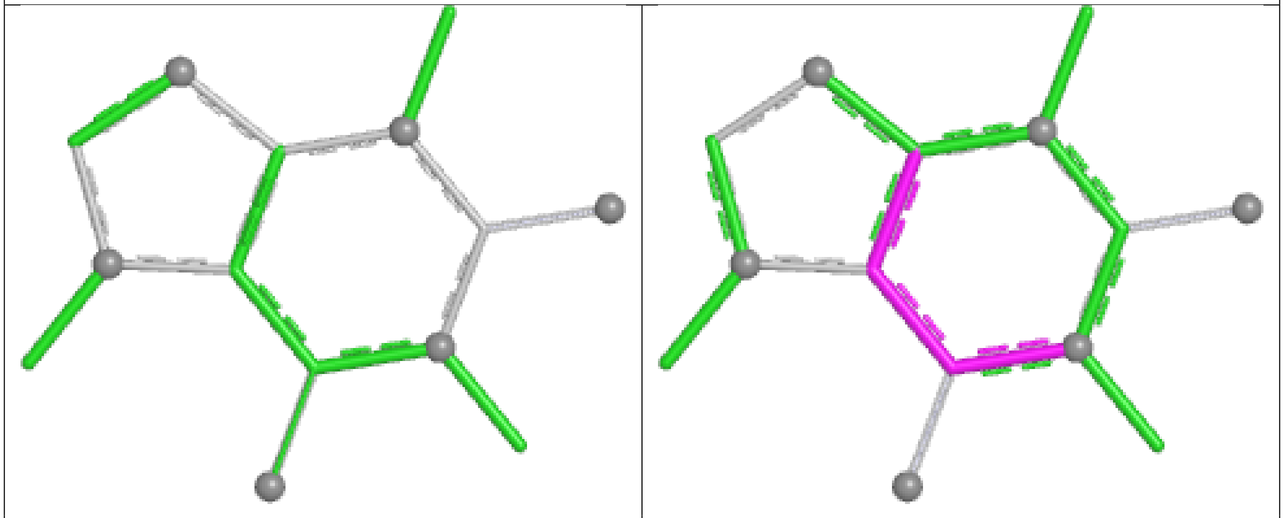


Bond lengths Bond angles

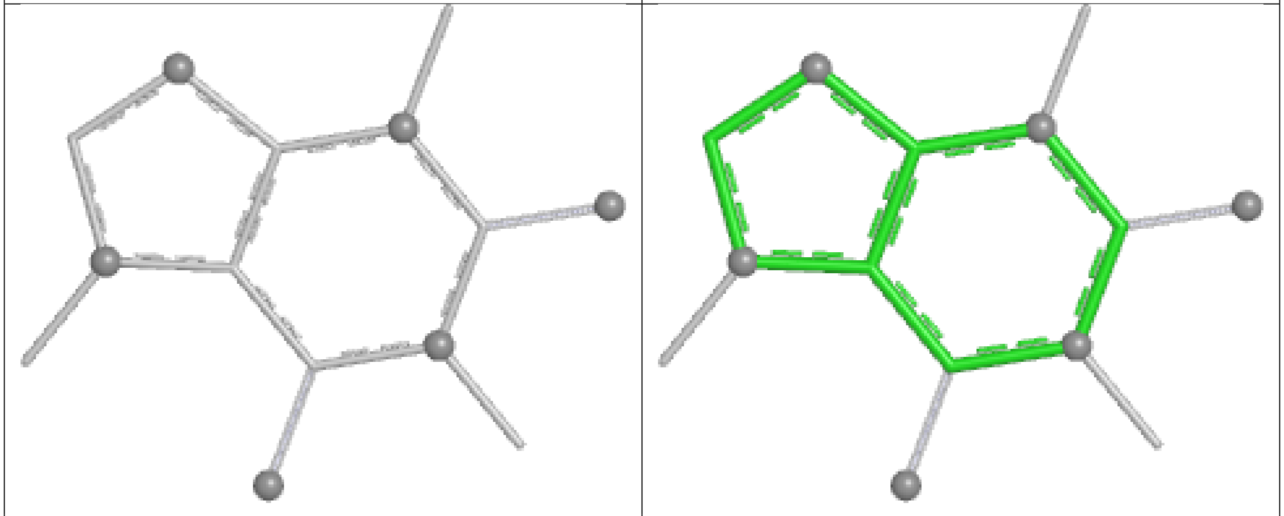


Torsions Rings

Ligand CFF B 5304

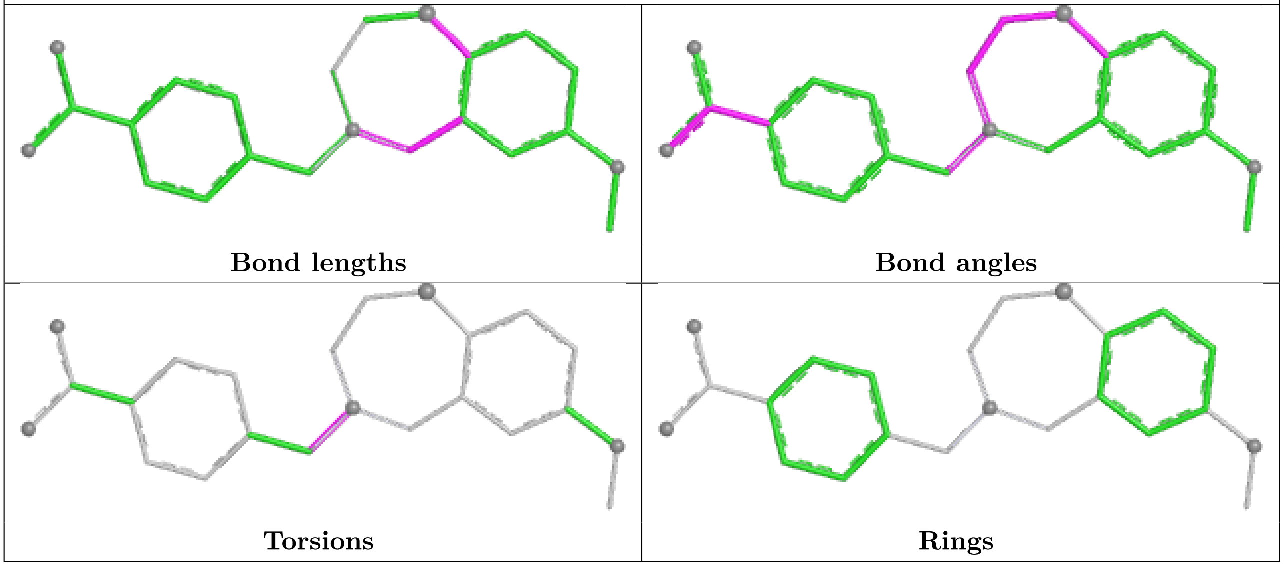


Bond lengths Bond angles

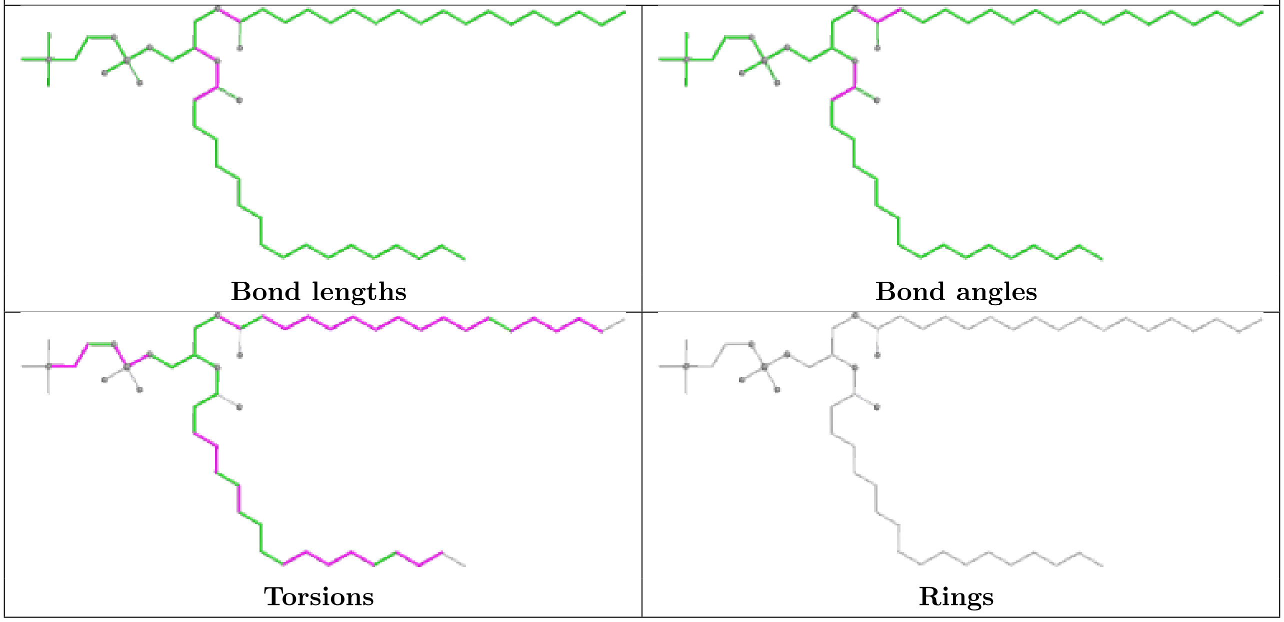


Torsions Rings

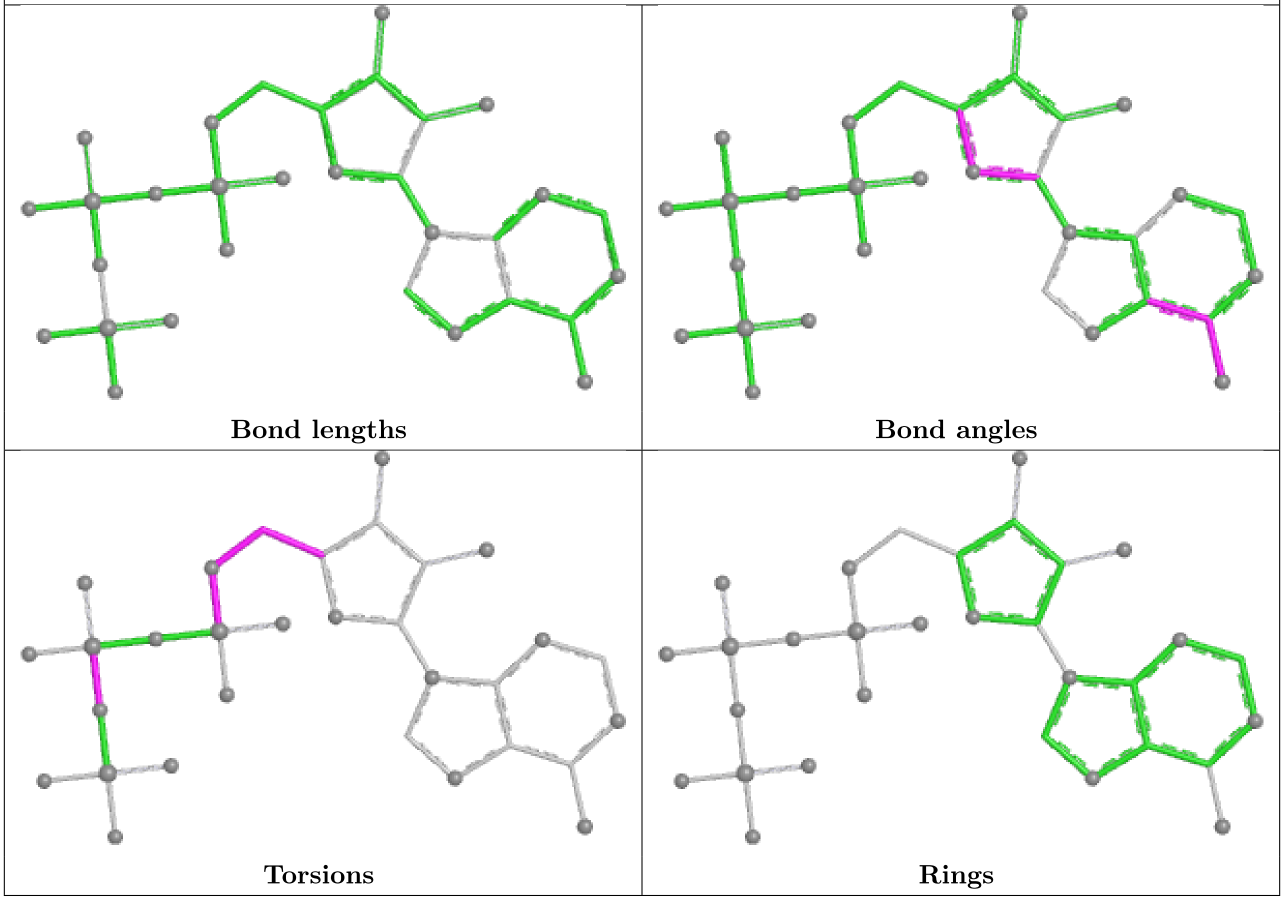
Ligand KVR G 5306



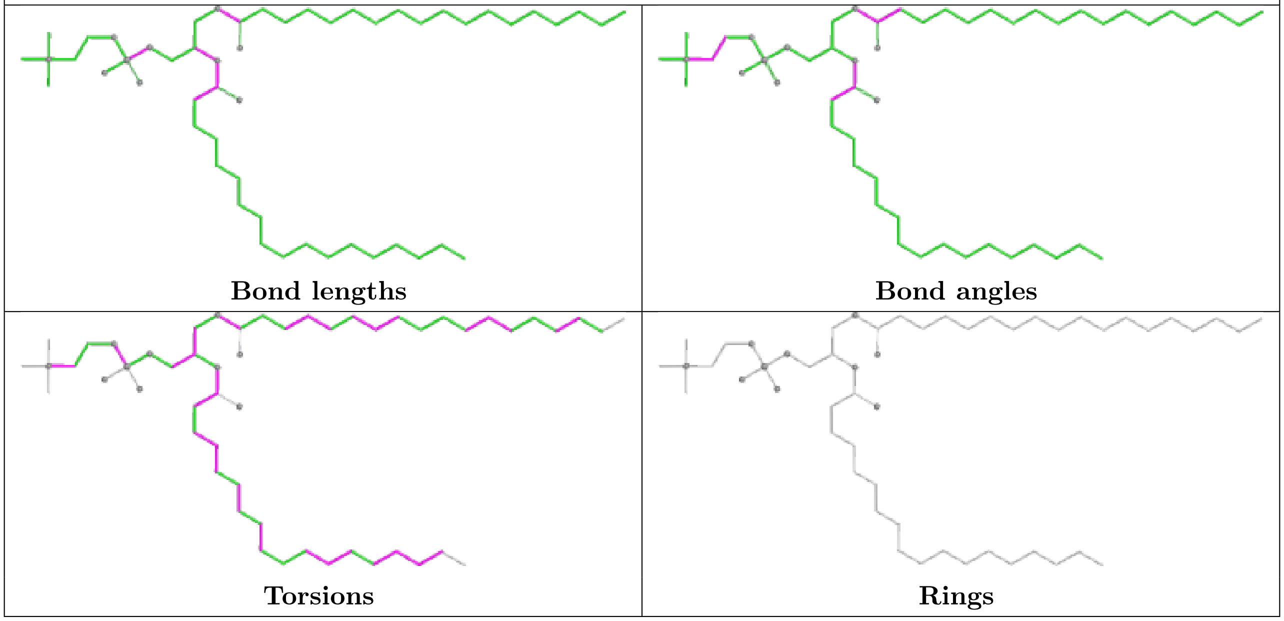
Ligand L9R B 5308



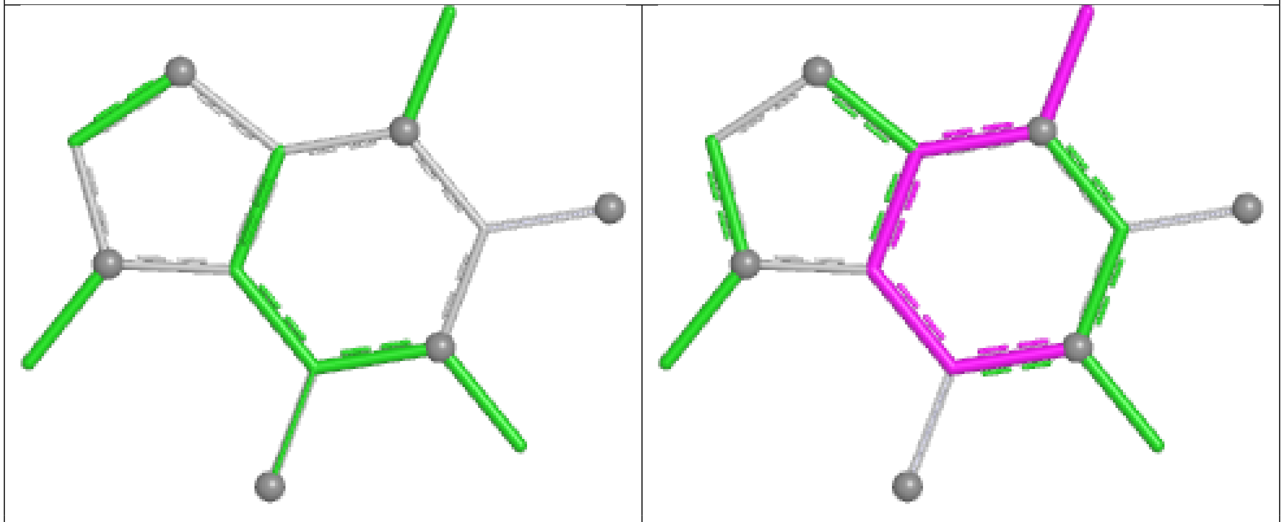
Ligand ATP A 5301



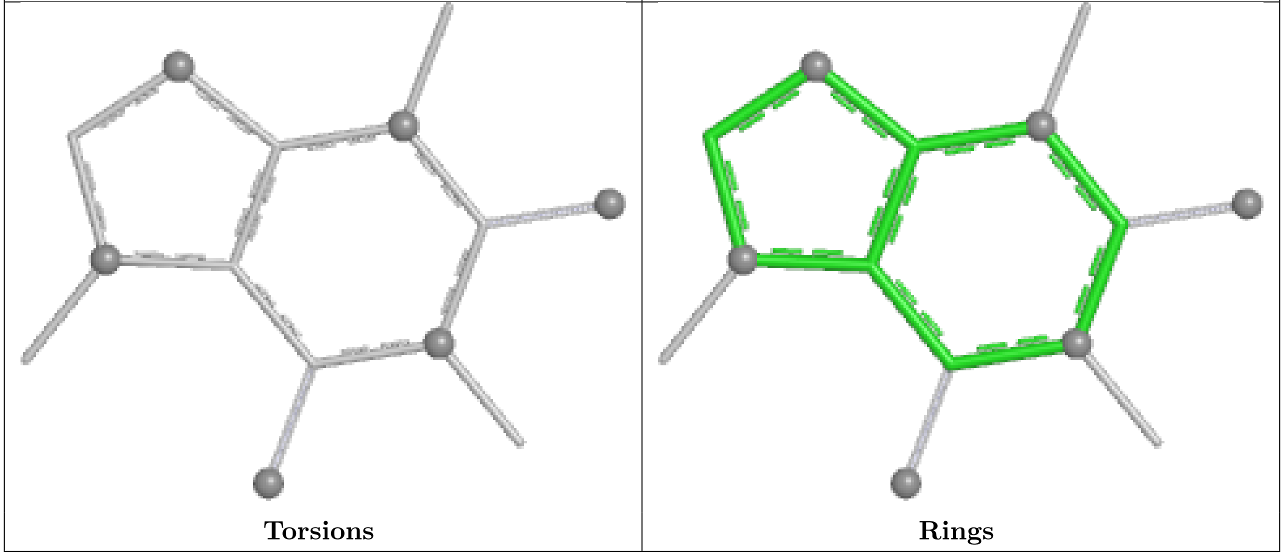
Ligand L9R A 5307



Ligand CFF I 5304

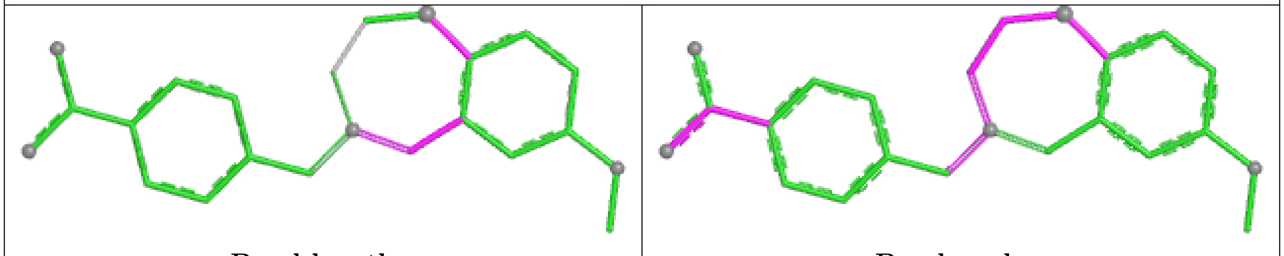


Bond lengths Bond angles

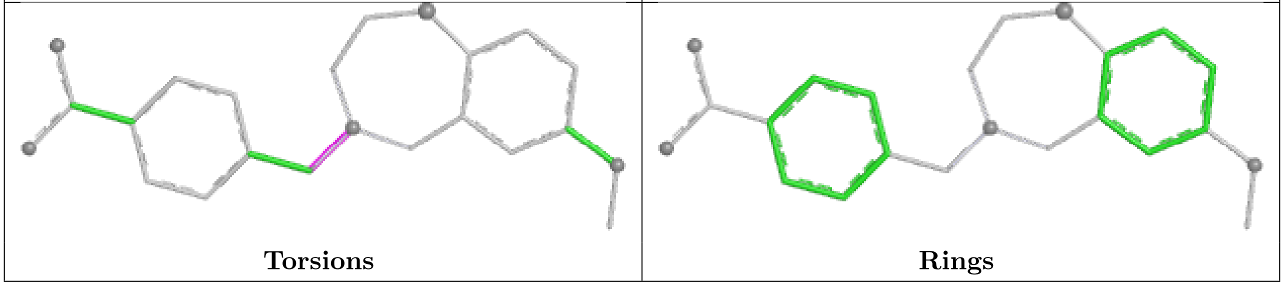


Torsions Rings

Ligand KVR A 5306

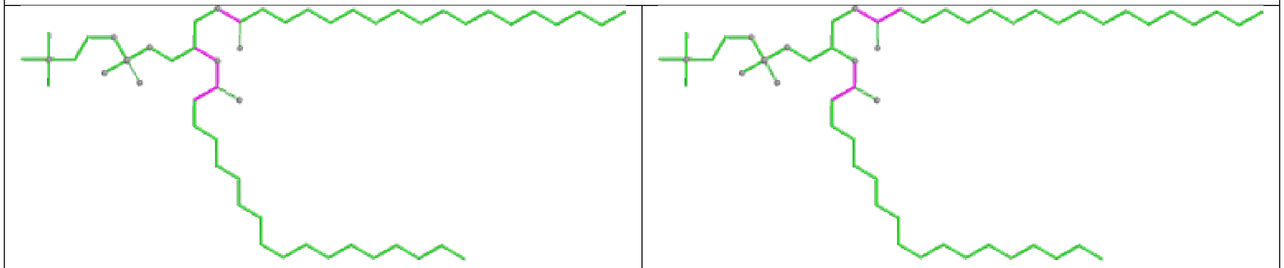


Bond lengths Bond angles



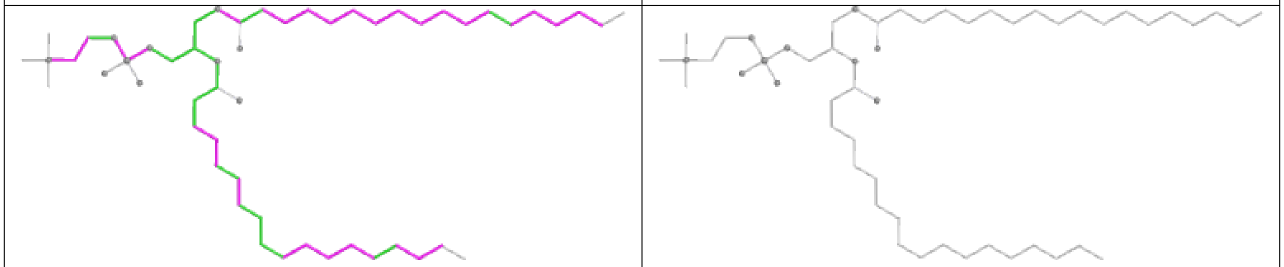
Torsions Rings

Ligand L9R I 5308



Bond lengths

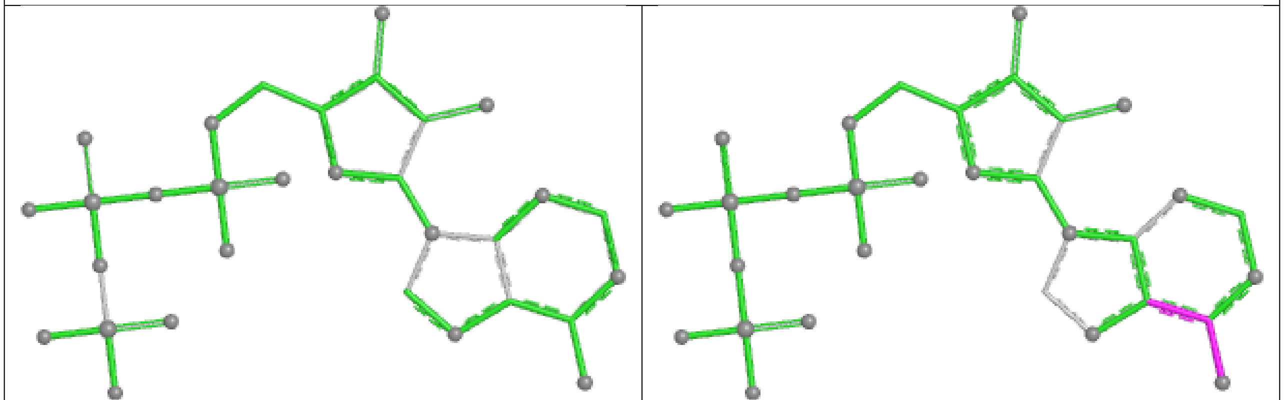
Bond angles



Torsions

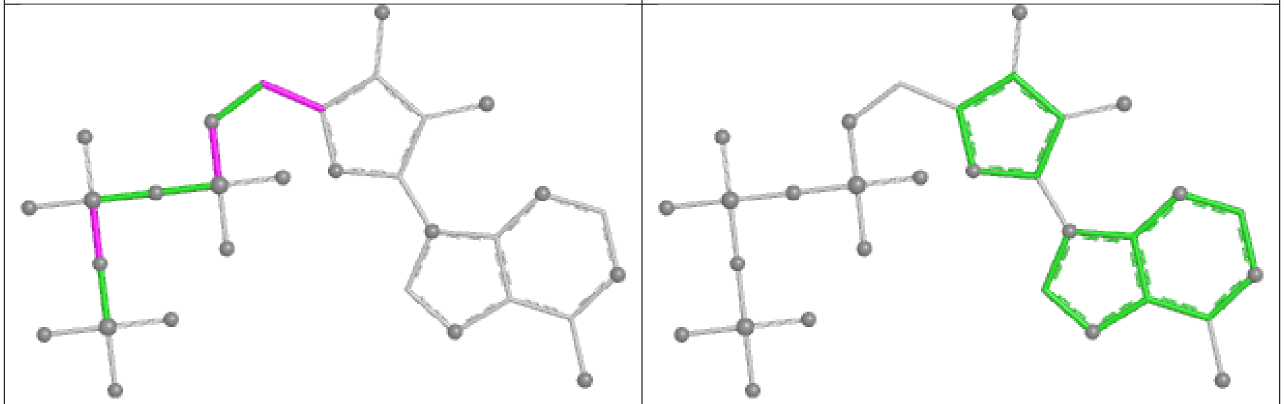
Rings

Ligand ATP A 5305



Bond lengths

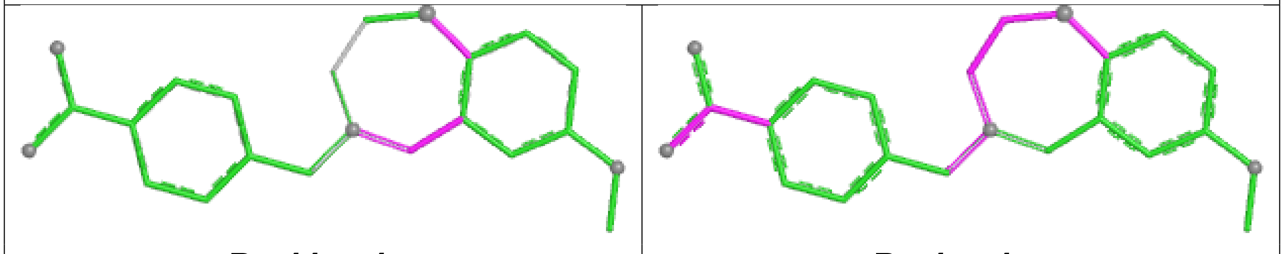
Bond angles



Torsions

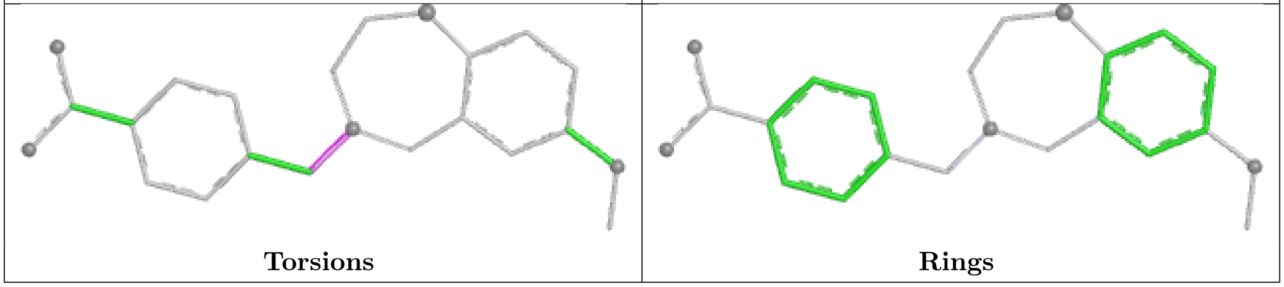
Rings

Ligand KVR B 5306



Bond lengths

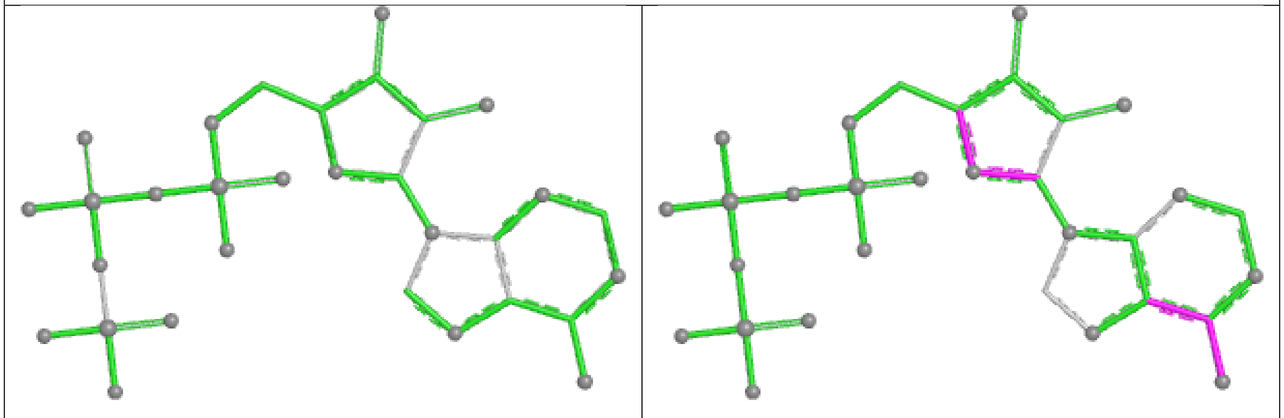
Bond angles



Torsions

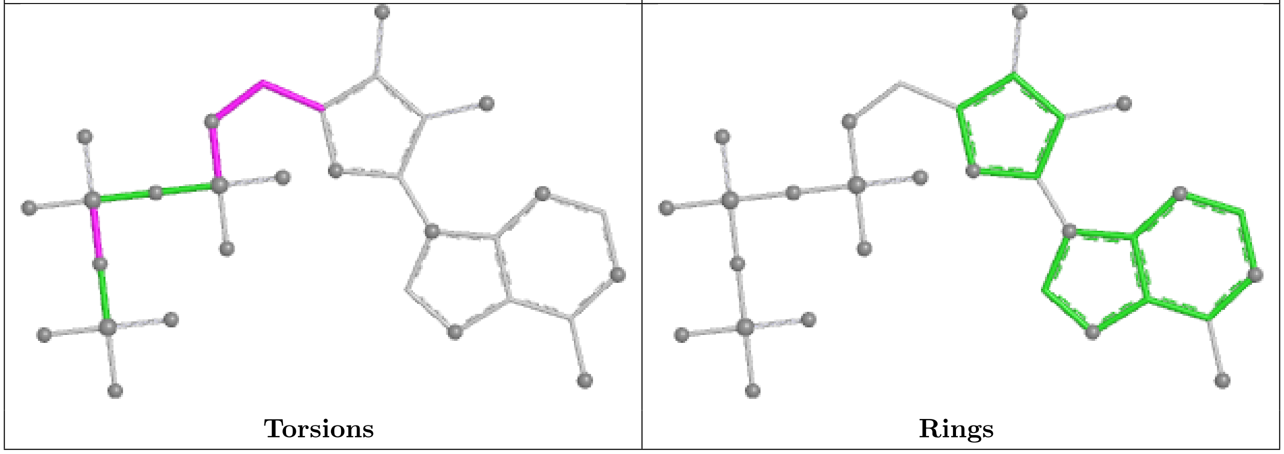
Rings

Ligand ATP G 5301



Bond lengths

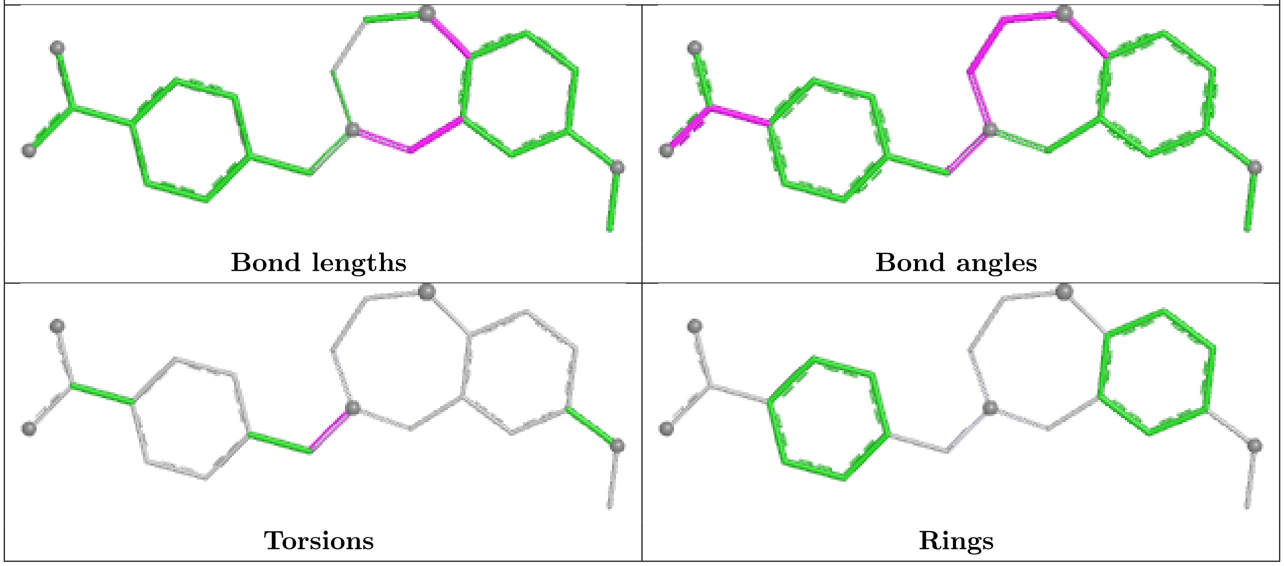
Bond angles



Torsions

Rings

Ligand KVR I 5306



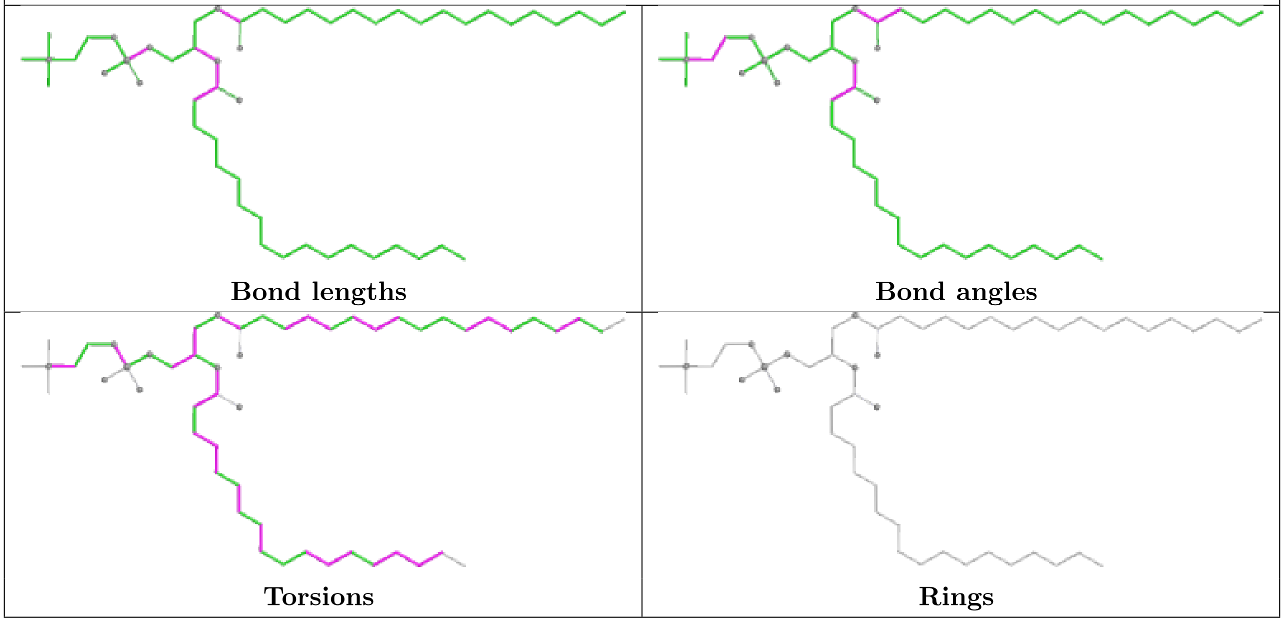
Bond lengths

Bond angles

Torsions

Rings

Ligand L9R G 5307



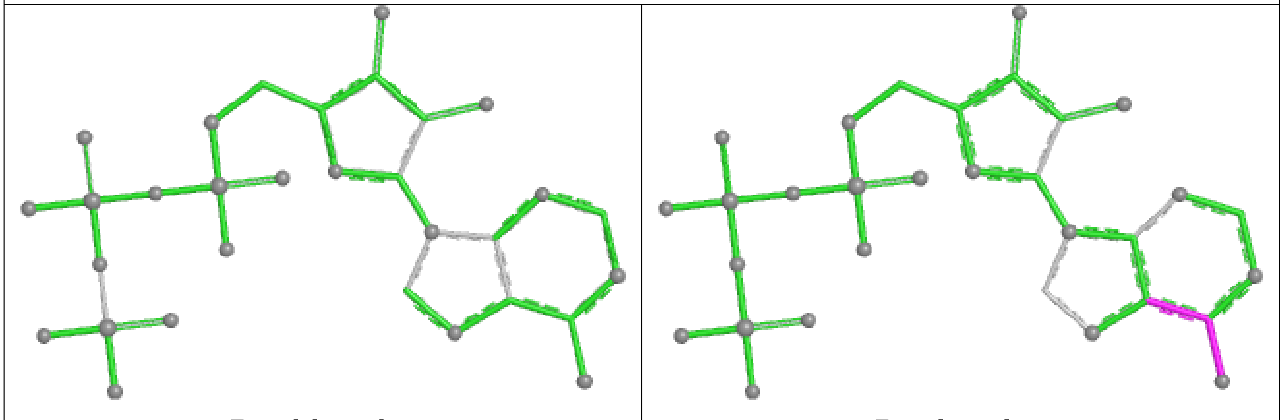
Bond lengths

Bond angles

Torsions

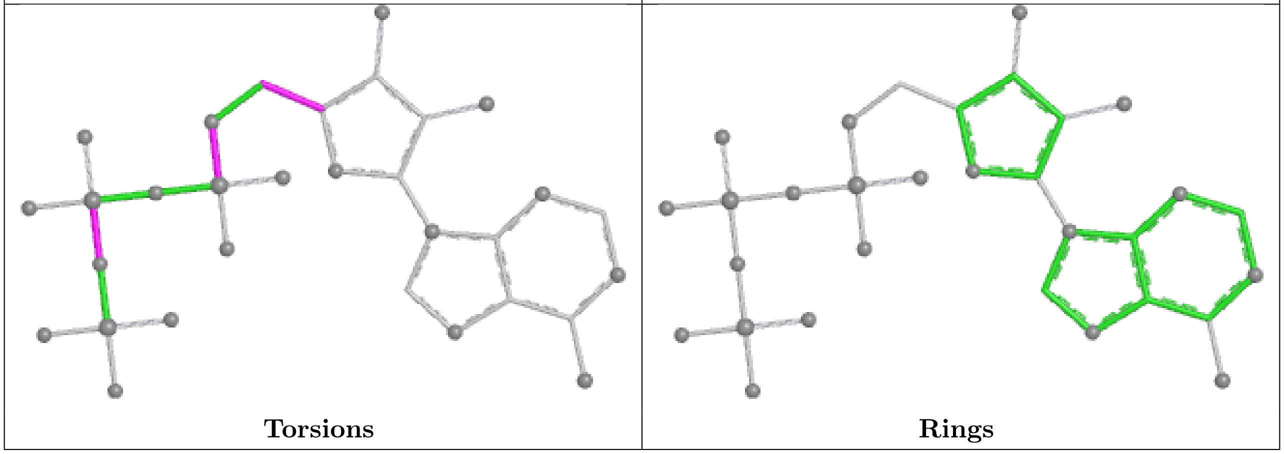
Rings

Ligand ATP G 5305



Bond lengths

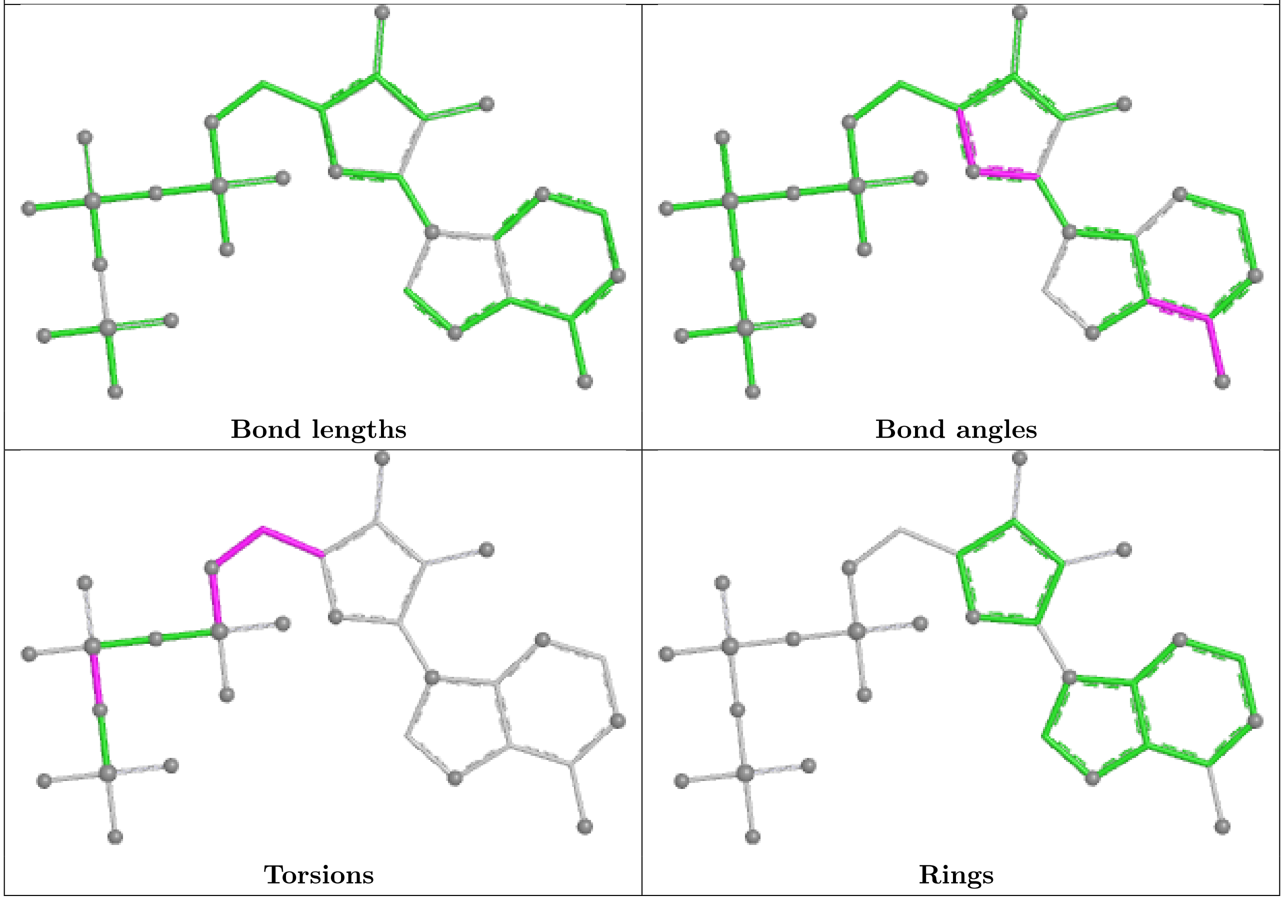
Bond angles



Torsions

Rings

Ligand ATP B 5301



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

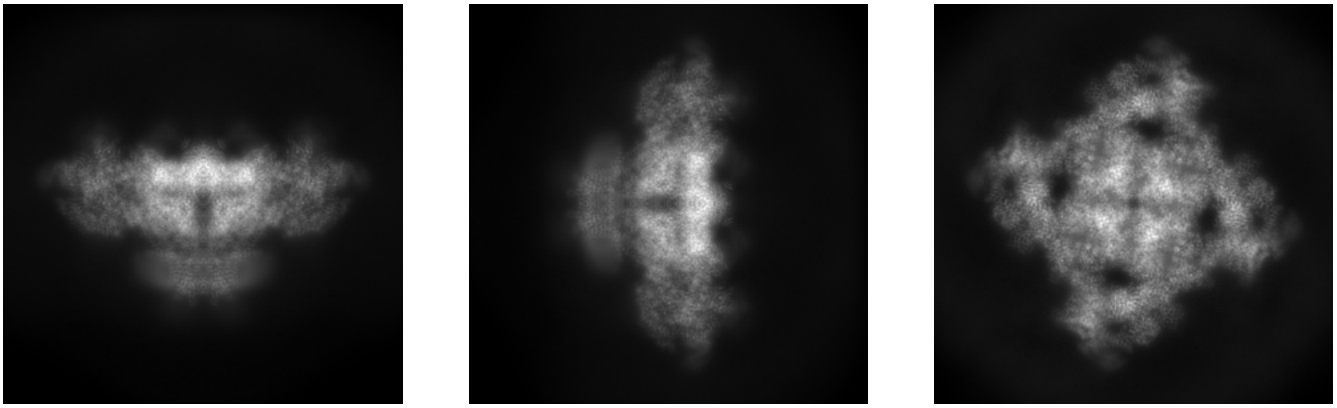
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26205. 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.

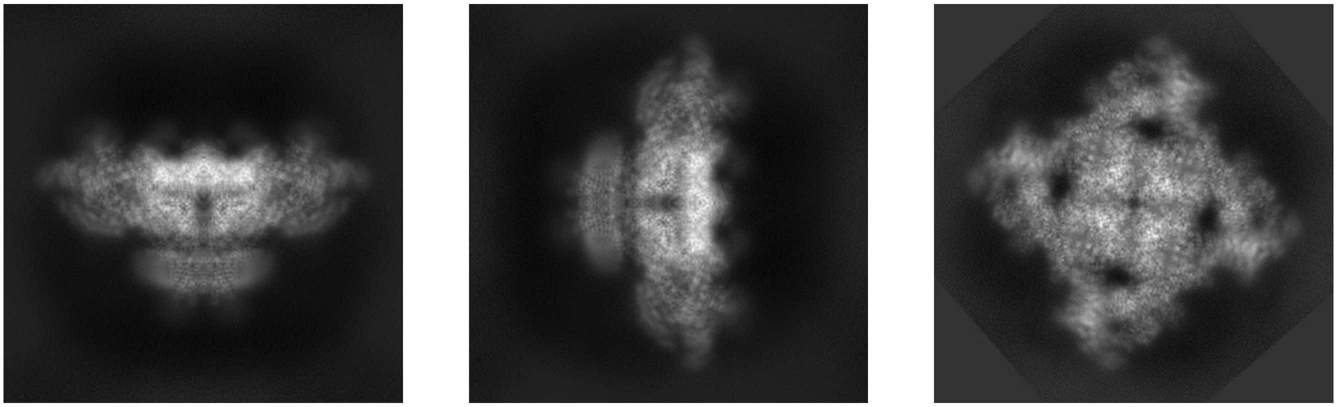
6.1 Orthogonal projections

6.1.1 Primary map



X Y Z

6.1.2 Raw map



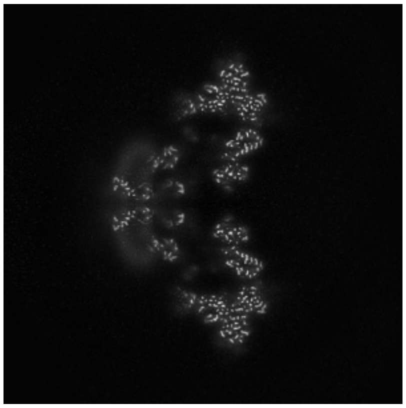
X Y Z

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

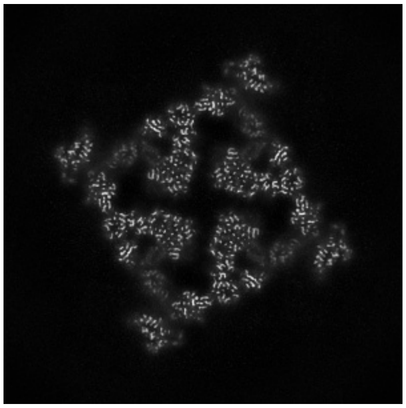
6.2 Central slices

6.2.1 Primary map

X Index: 256

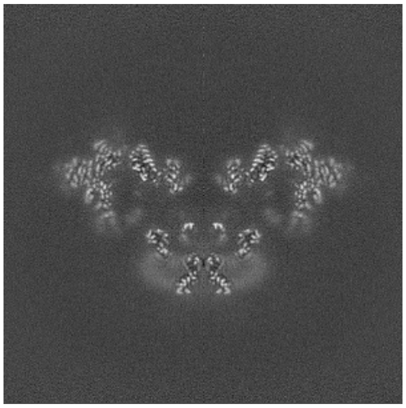


Y Index: 256

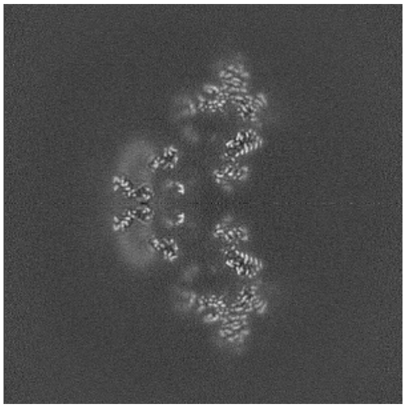


Z Index: 256

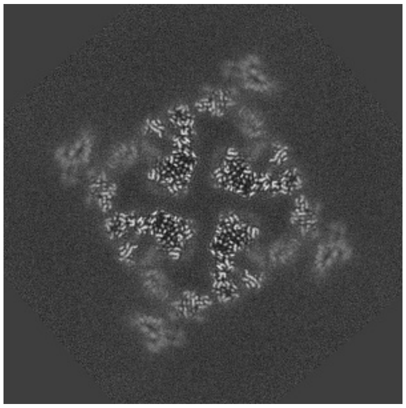
6.2.2 Raw map



X Index: 256



Y Index: 256

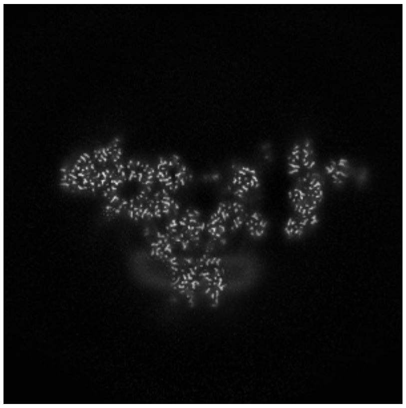


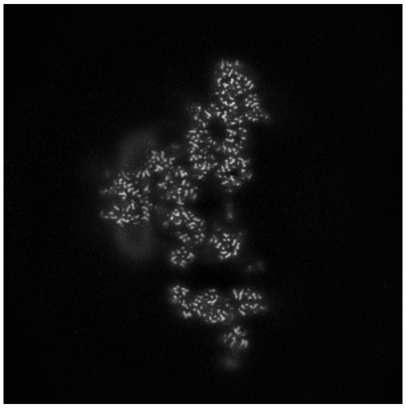
Z Index: 256

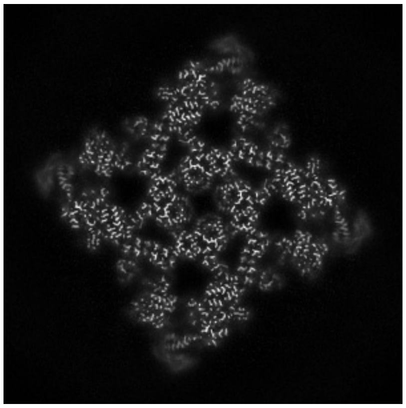
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

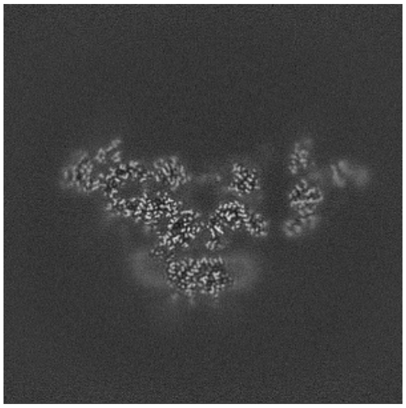
6.3.1 Primary map

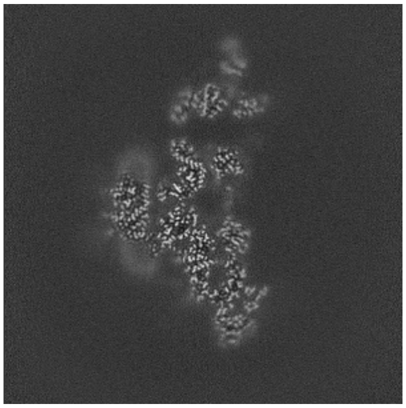

X Index: 272

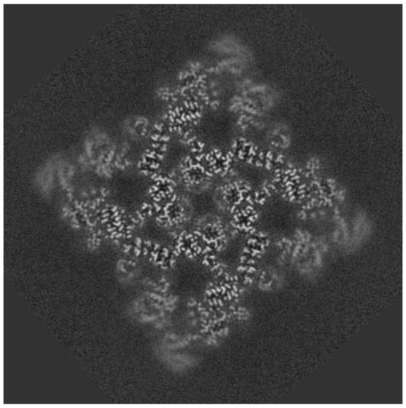

Y Index: 272


Z Index: 286

6.3.2 Raw map


X Index: 275

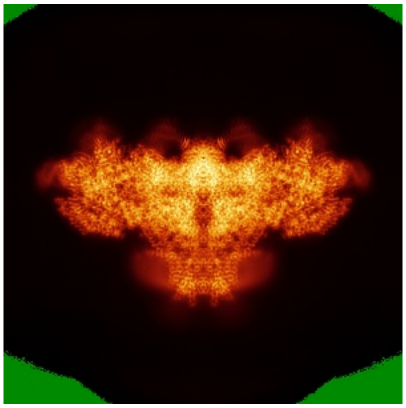

Y Index: 237


Z Index: 286

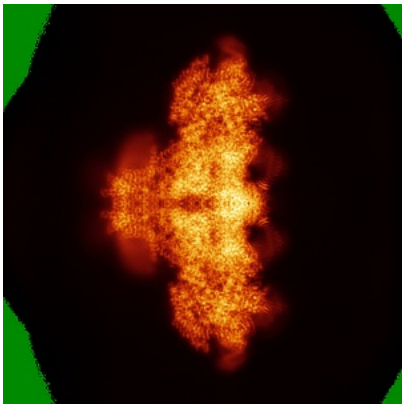
The images above show the largest variance slices of the map in three orthogonal directions.

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

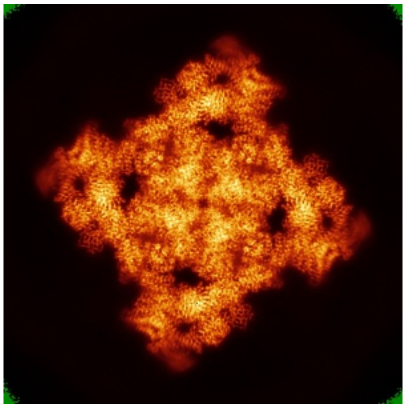
6.4.1 Primary map



X



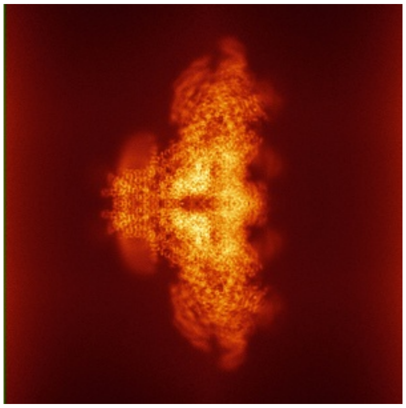
Y



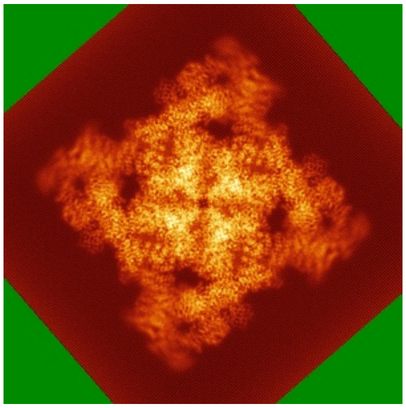
Z

6.4.2 Raw map

X



Y

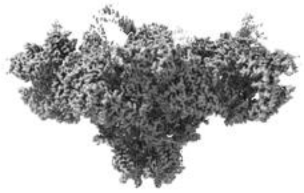


Z

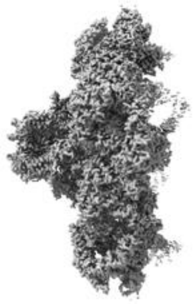
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

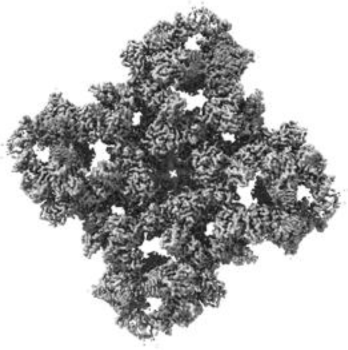
6.5.1 Primary map



X



Y

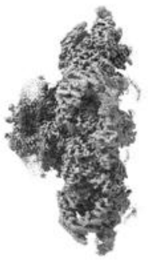


Z

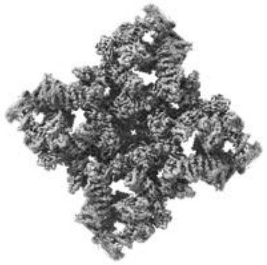
The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

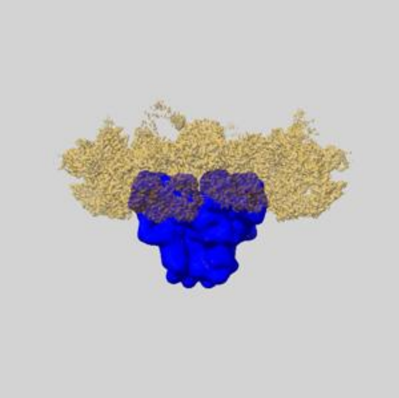
6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

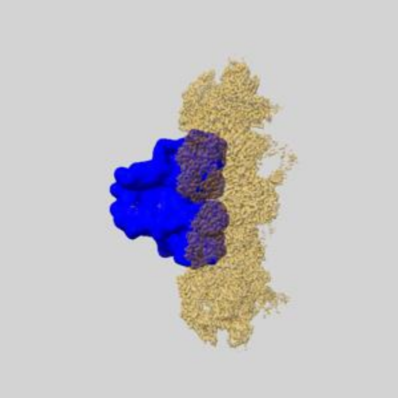
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

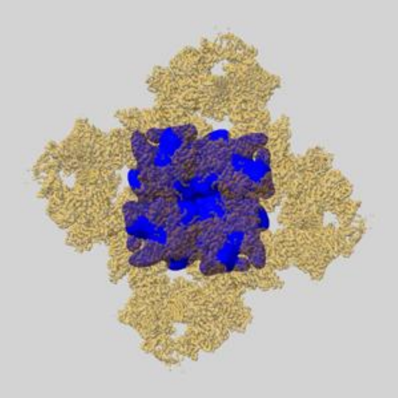
6.6.1 emd_26205_msk_1.map



X

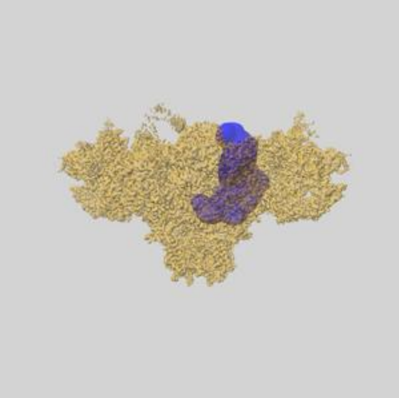


Y

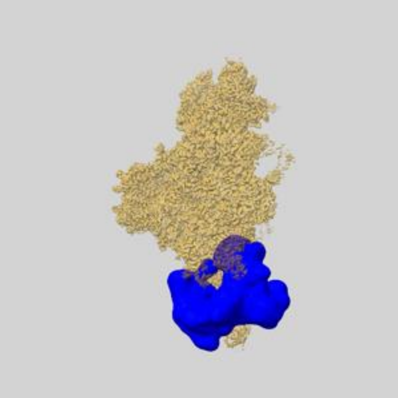


Z

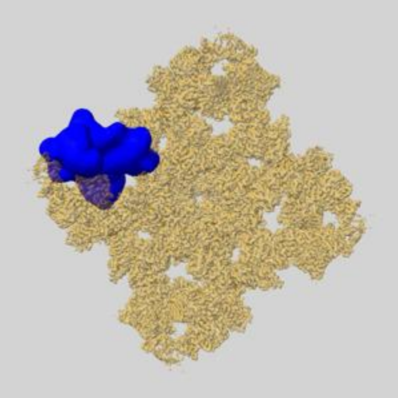
6.6.2 emd_26205_msk_2.map



X

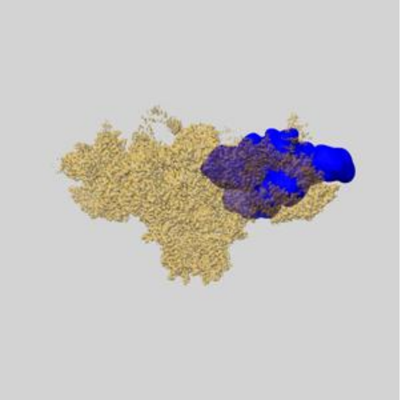


Y

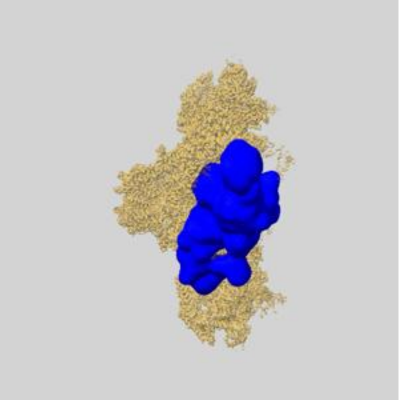


Z

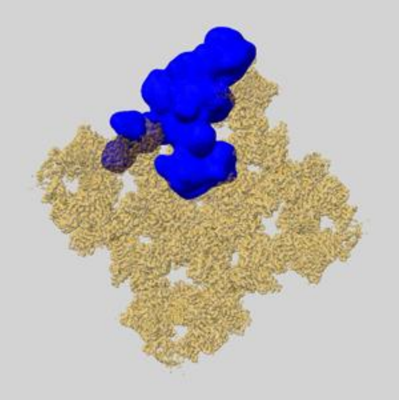
6.6.3 emd_26205_msk_3.map



X



Y

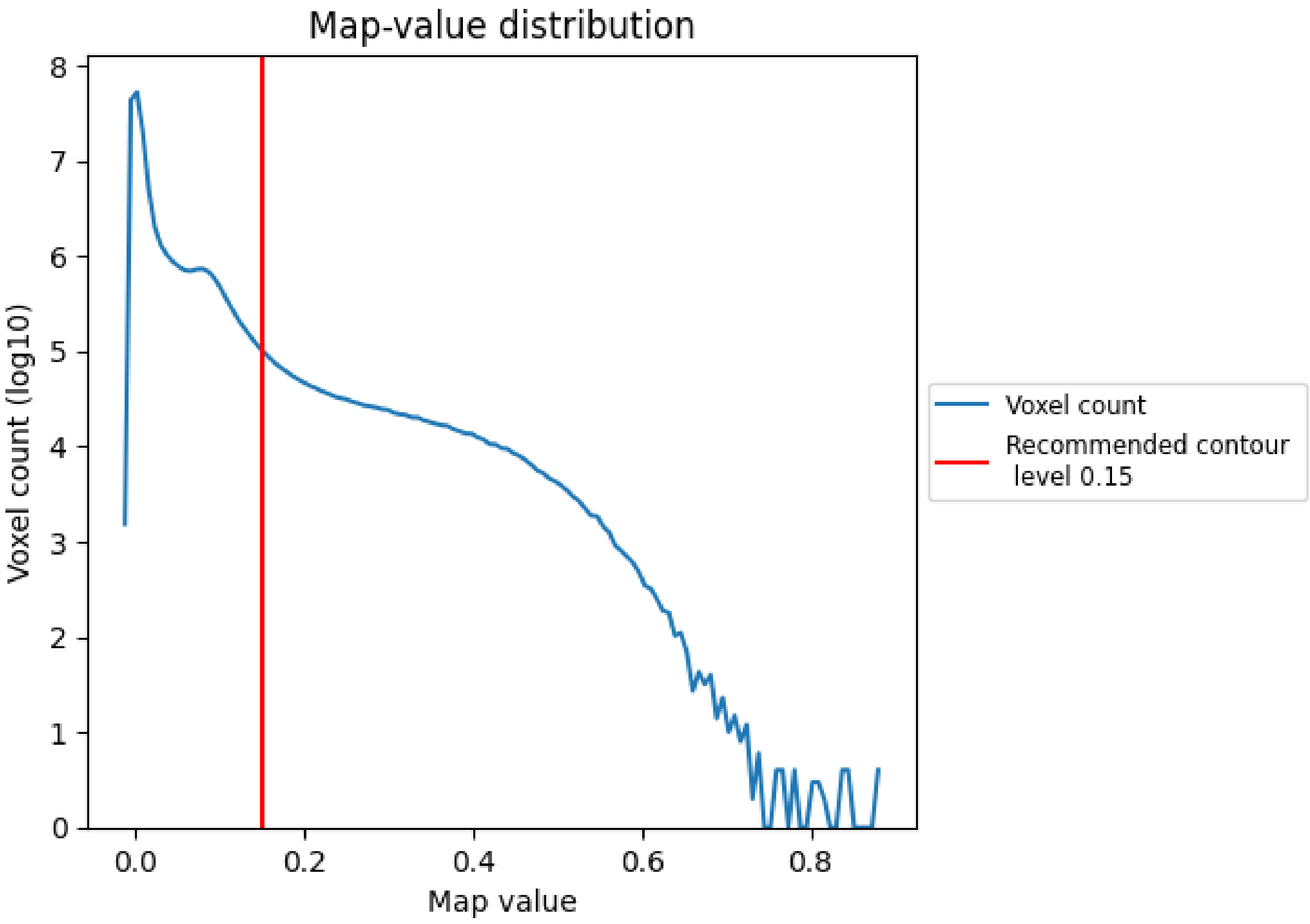


Z

7 Map analysis

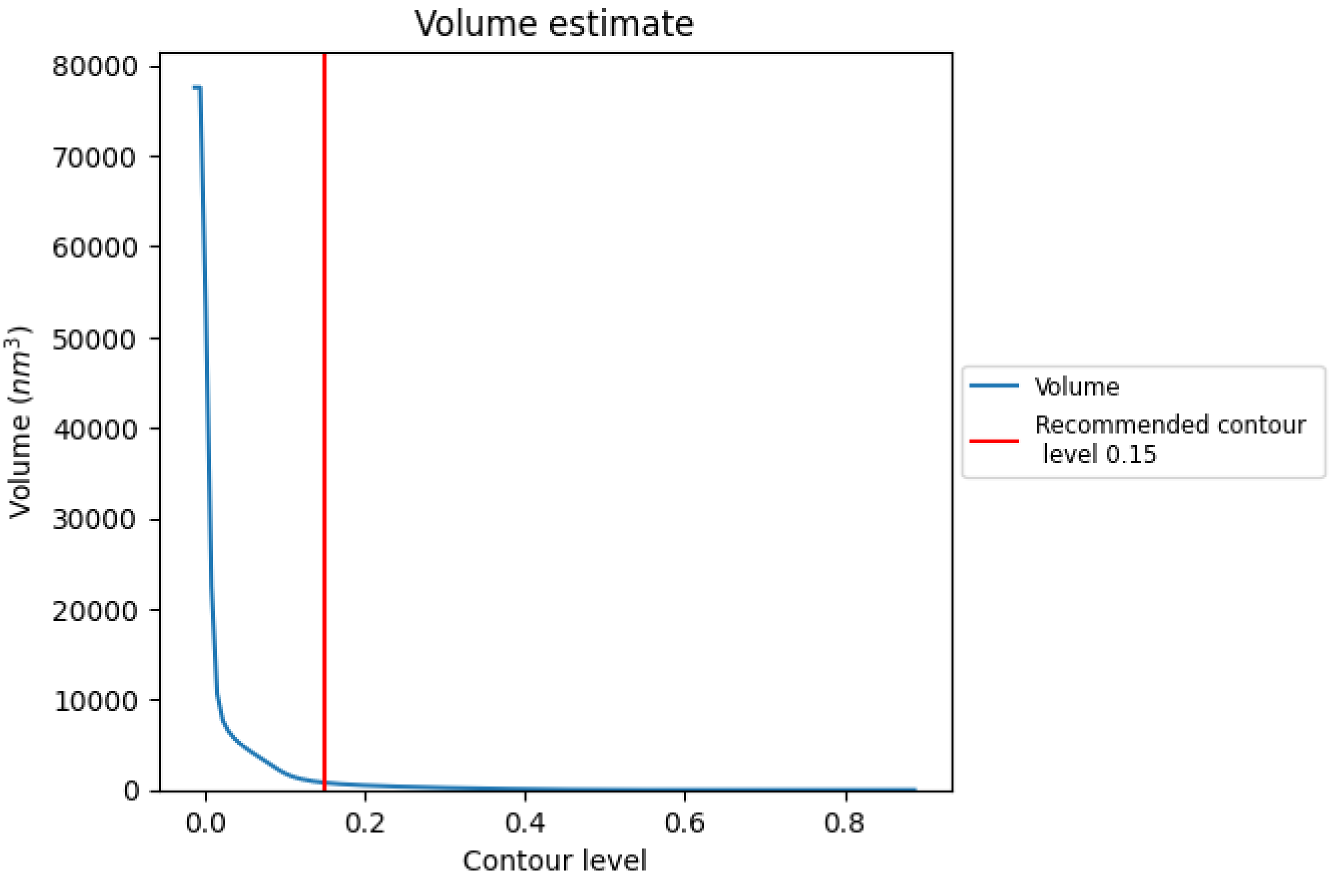
This section contains the results of statistical analysis of the map.

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.

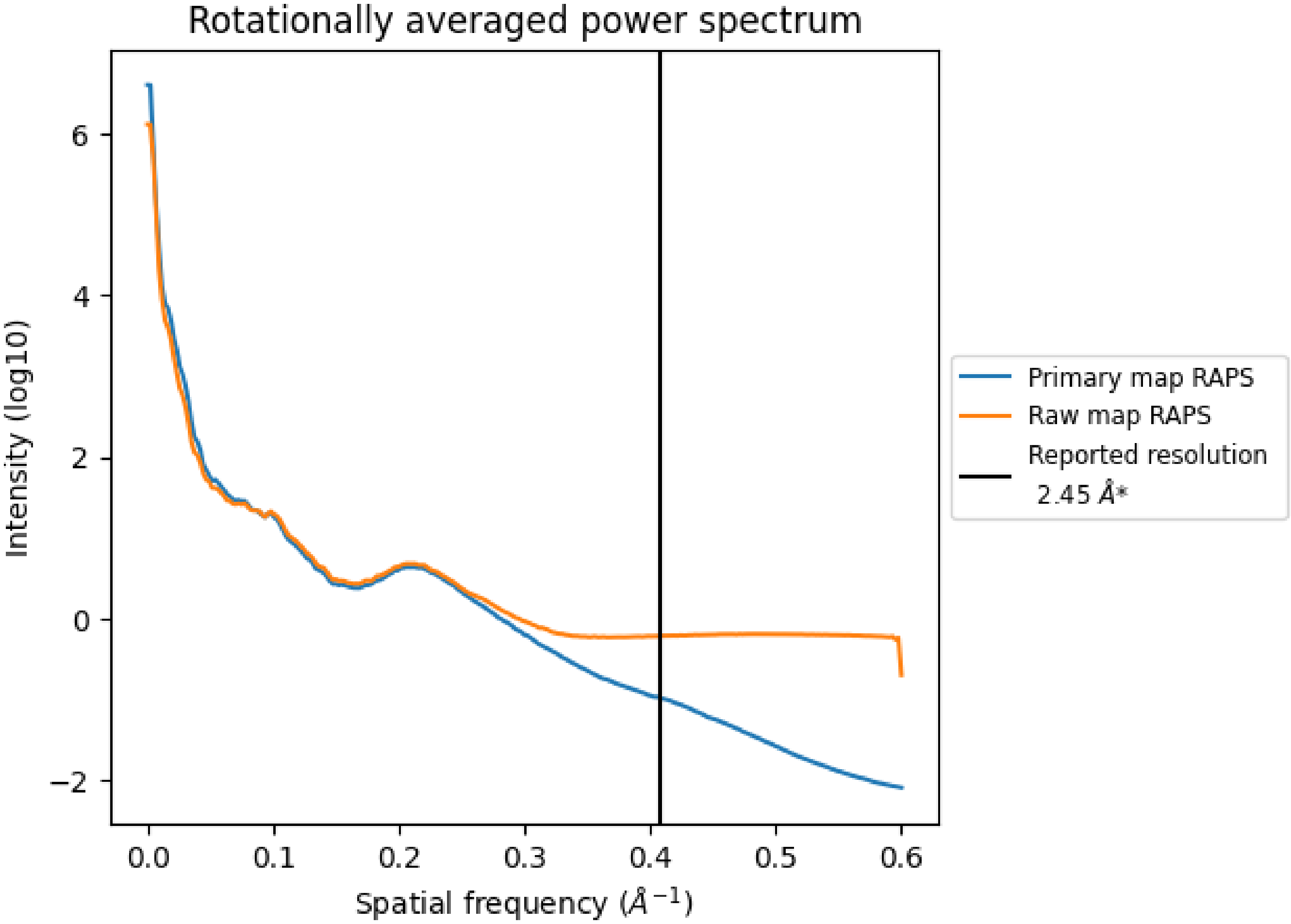
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 800 nm^3; this corresponds to an approximate mass of 723 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)

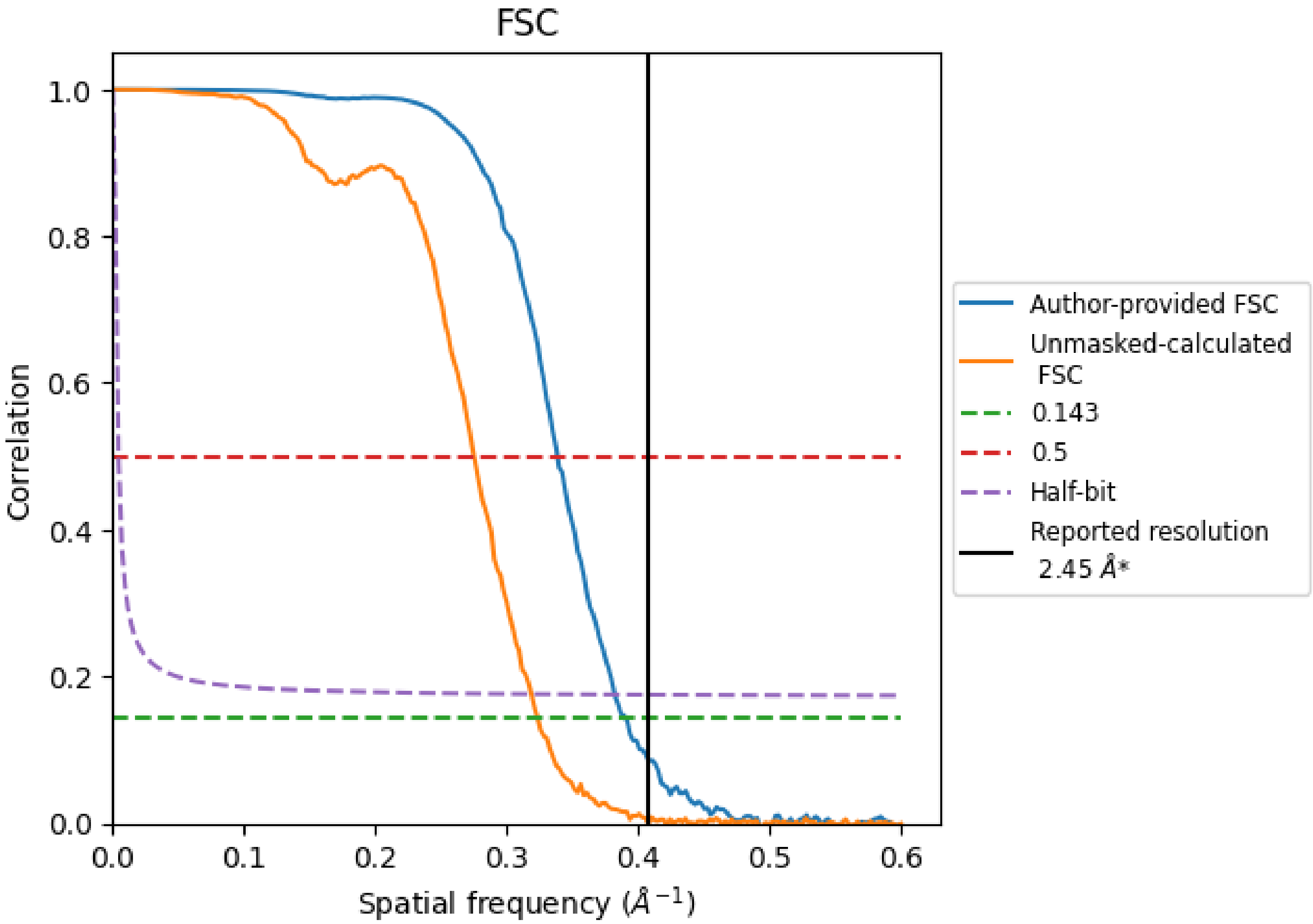


*Reported resolution corresponds to spatial frequency of 0.408 $\AA^{-1}$

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 0.408 Å^{-1}

8.2 Resolution estimates ⓘ

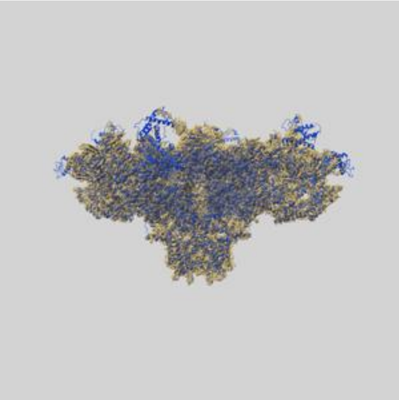
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.56	2.95	2.62
Unmasked-calculated*	3.09	3.63	3.14

*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 3.09 differs from the reported value 2.45 by more than 10 %

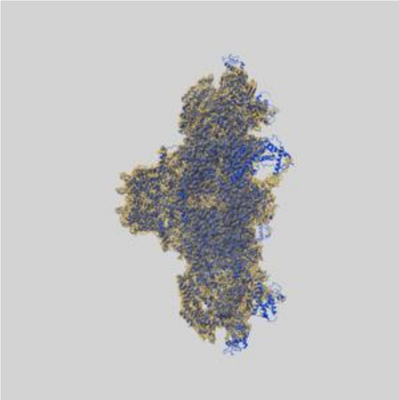
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26205 and PDB model 9E17. Per-residue inclusion information can be found in section 3 on page 10.

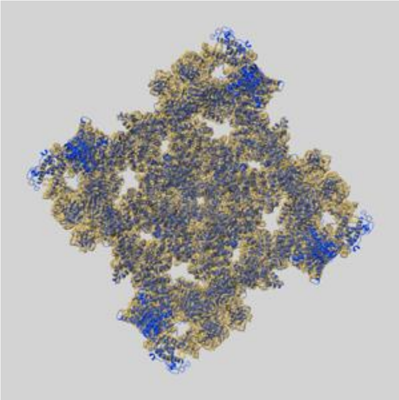
9.1 Map-model overlay



X



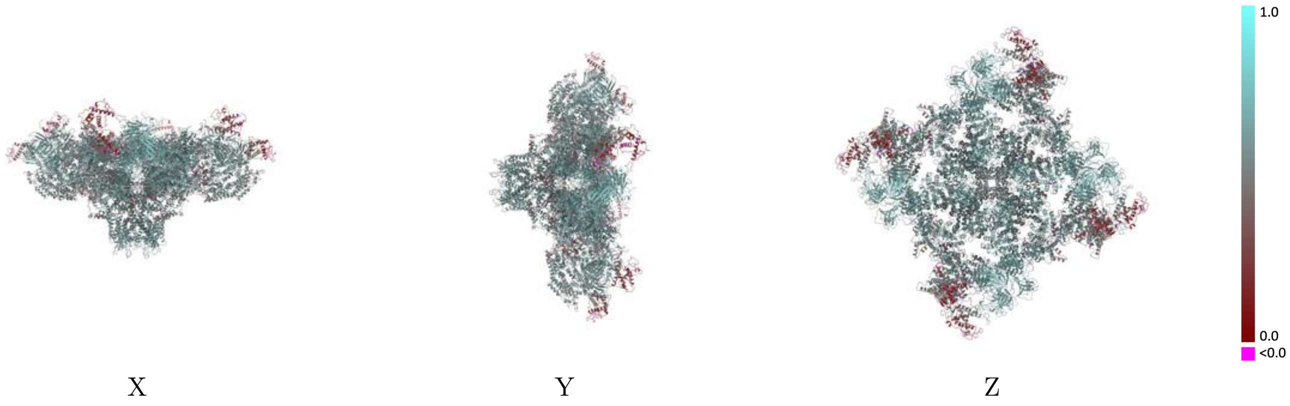
Y



Z

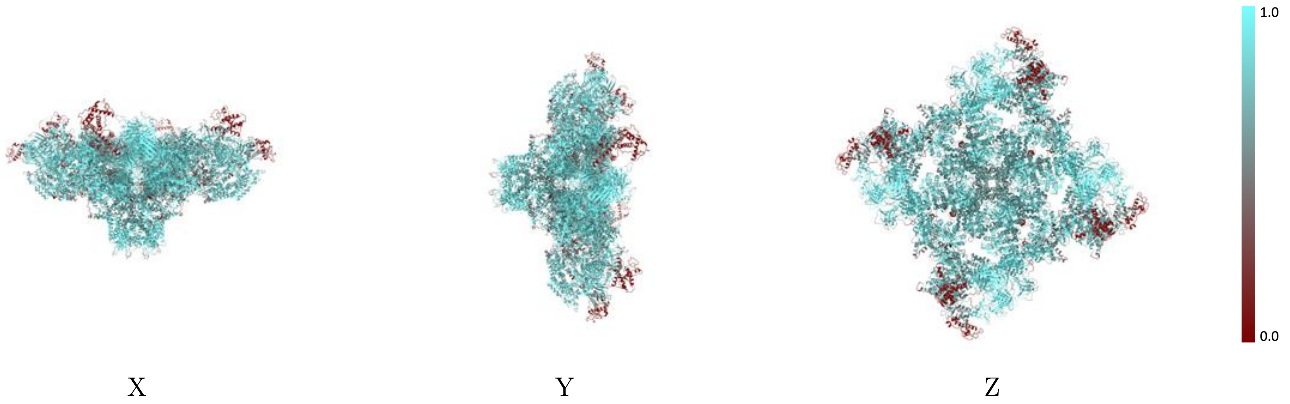
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



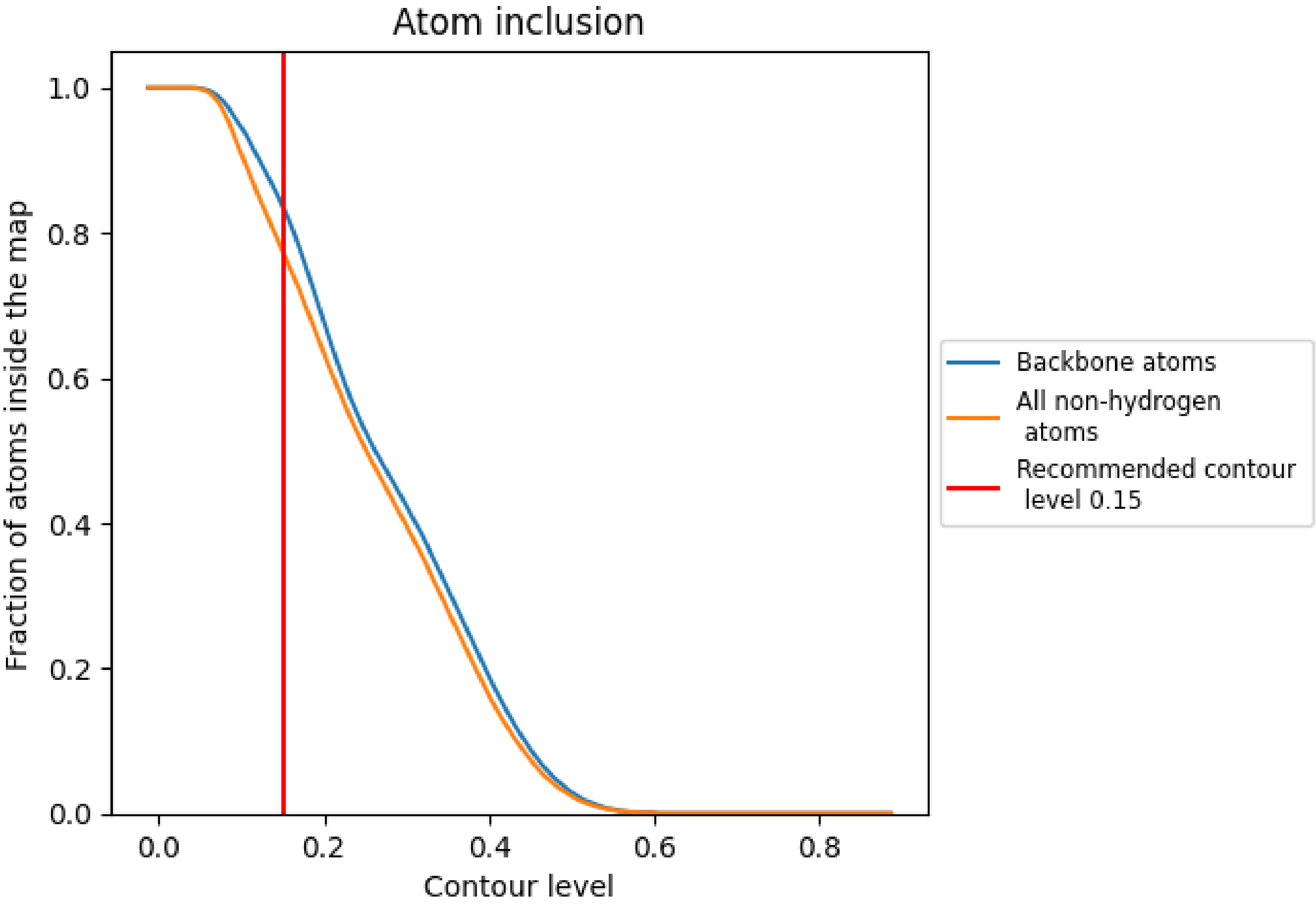
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ



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

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.5400
A	0.7900	0.5430
B	0.7890	0.5400
C	0.5240	0.4370
D	0.5310	0.4320
E	0.5310	0.4390
F	0.8040	0.6020
G	0.7890	0.5410
H	0.7930	0.6020
I	0.7890	0.5420
J	0.7890	0.6020
K	0.5280	0.4400
O	0.8020	0.6030