Full wwPDB EM Validation Report ⓘ

Mar 2, 2024 – 09:28 PM EST

PDB ID	:	5TAP
EMDB ID	:	EMD-8381
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, all particles)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.40 Å(reported)

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

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

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

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

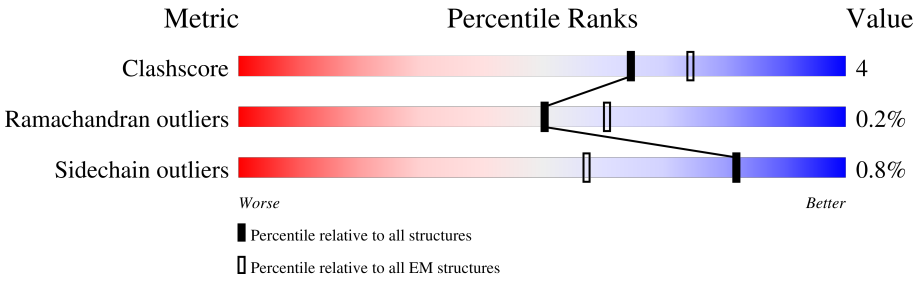
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.40 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	108	33% 85% 14%
1	F	108	32% 85% 14%
1	H	108	34% 83% 16%
1	J	108	34% 84% 15%
2	B	4416	35% 85% 9% 5%
2	E	4416	35% 85% 9% 5%
2	G	4416	35% 86% 9% 5%
2	I	4416	35% 86% 9% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121452 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.

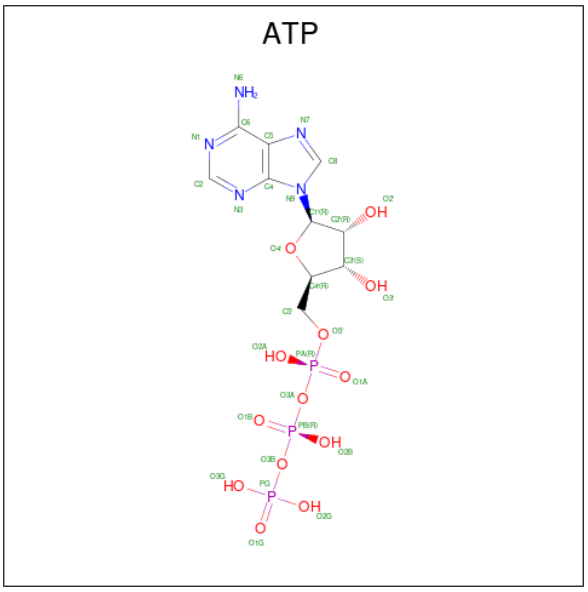
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

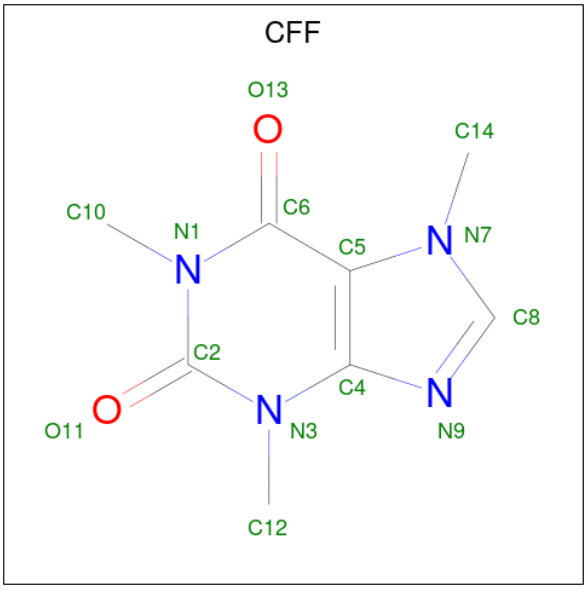
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

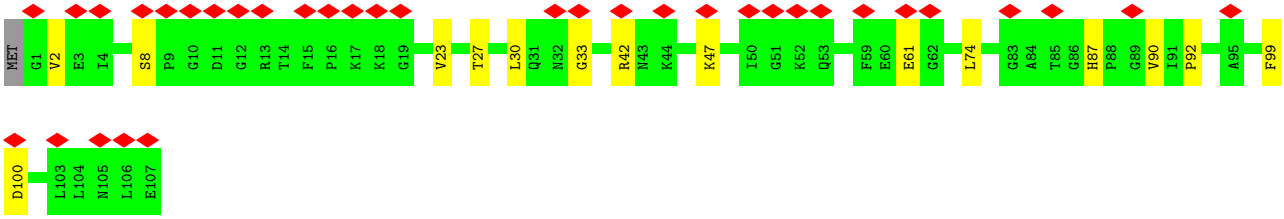
Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	
5	E	1	Total	Zn	0
			1	1	
5	I	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	

3 Residue-property plots (i)

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

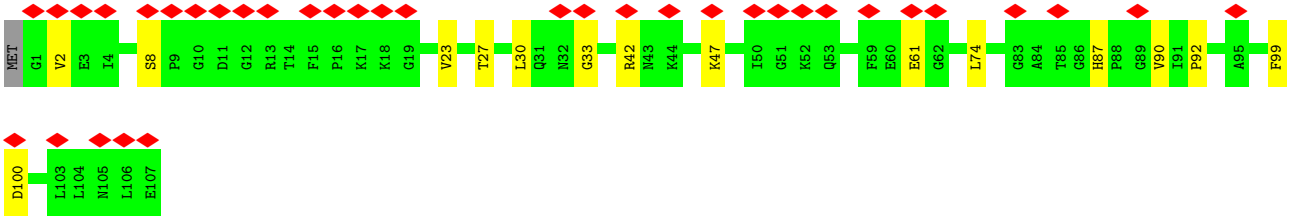
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



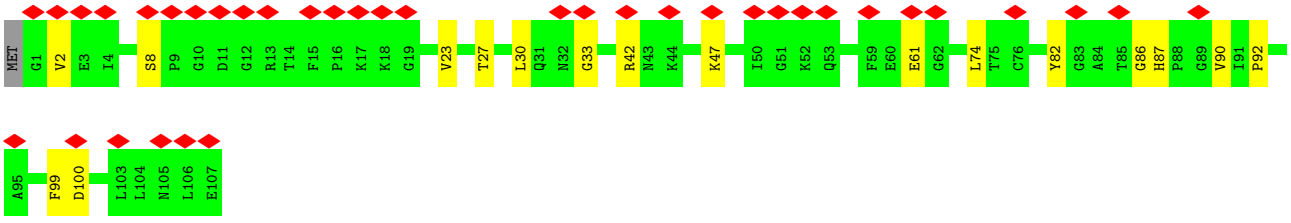
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



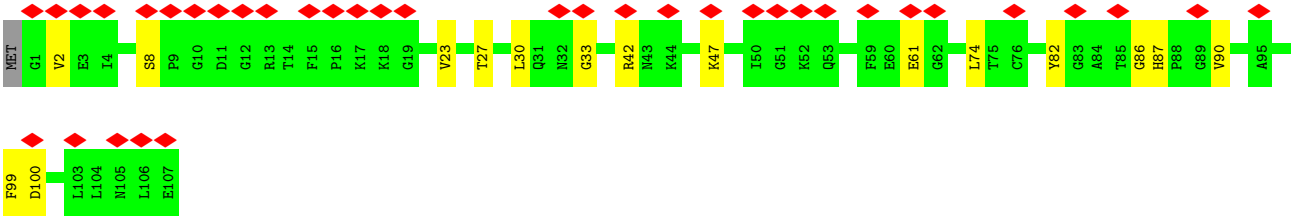
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



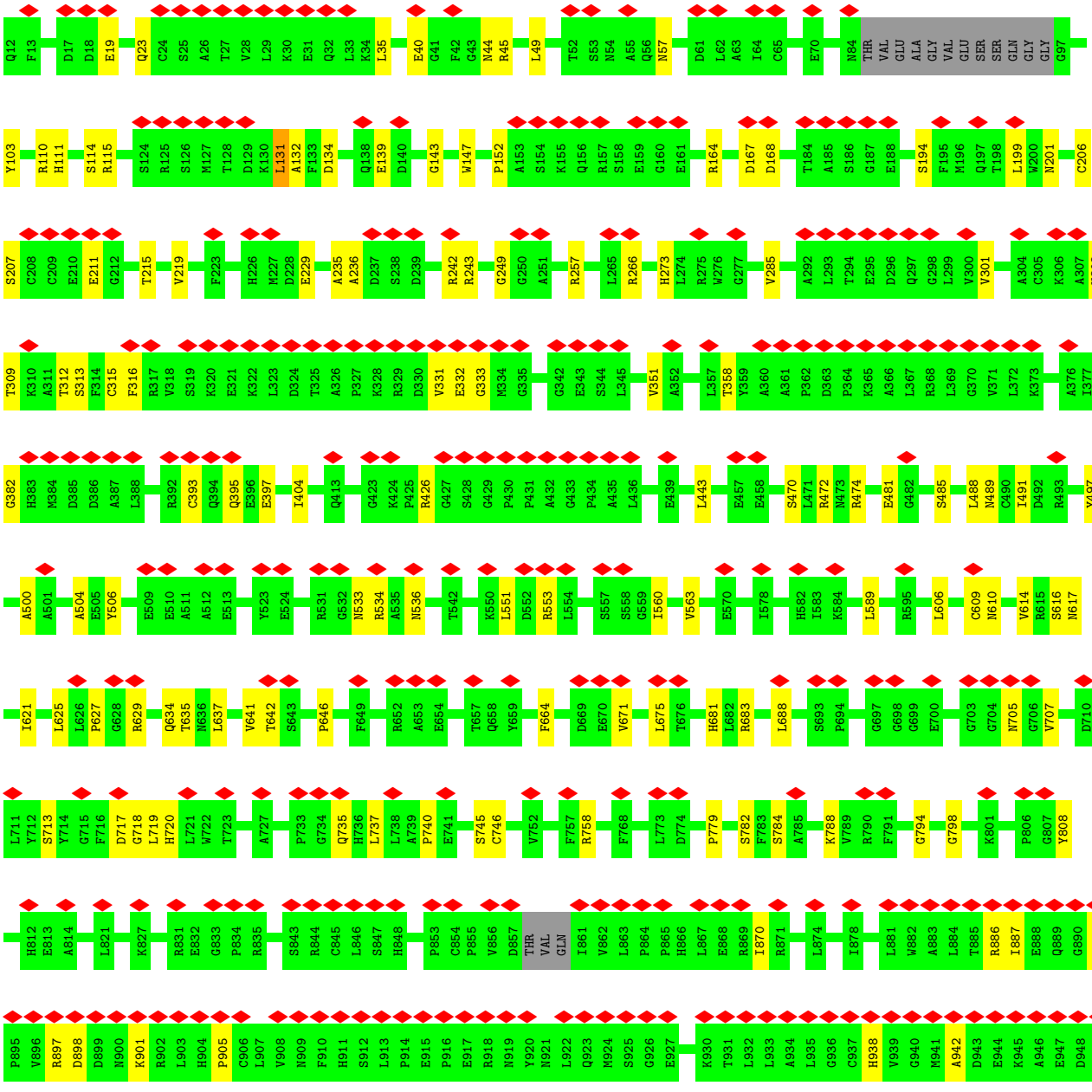
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

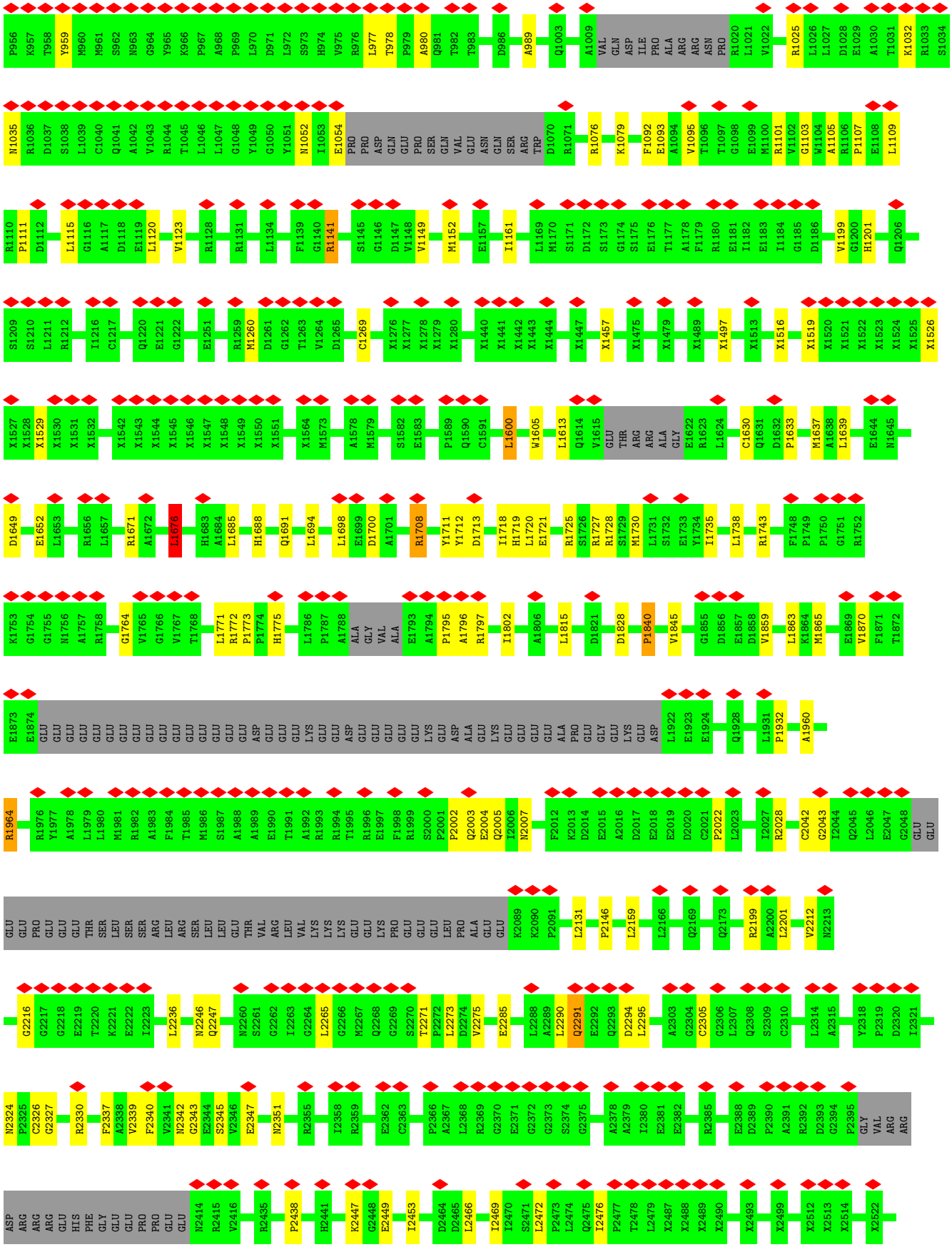
Chain J:



• Molecule 2: Ryanodine receptor 1

Chain B:

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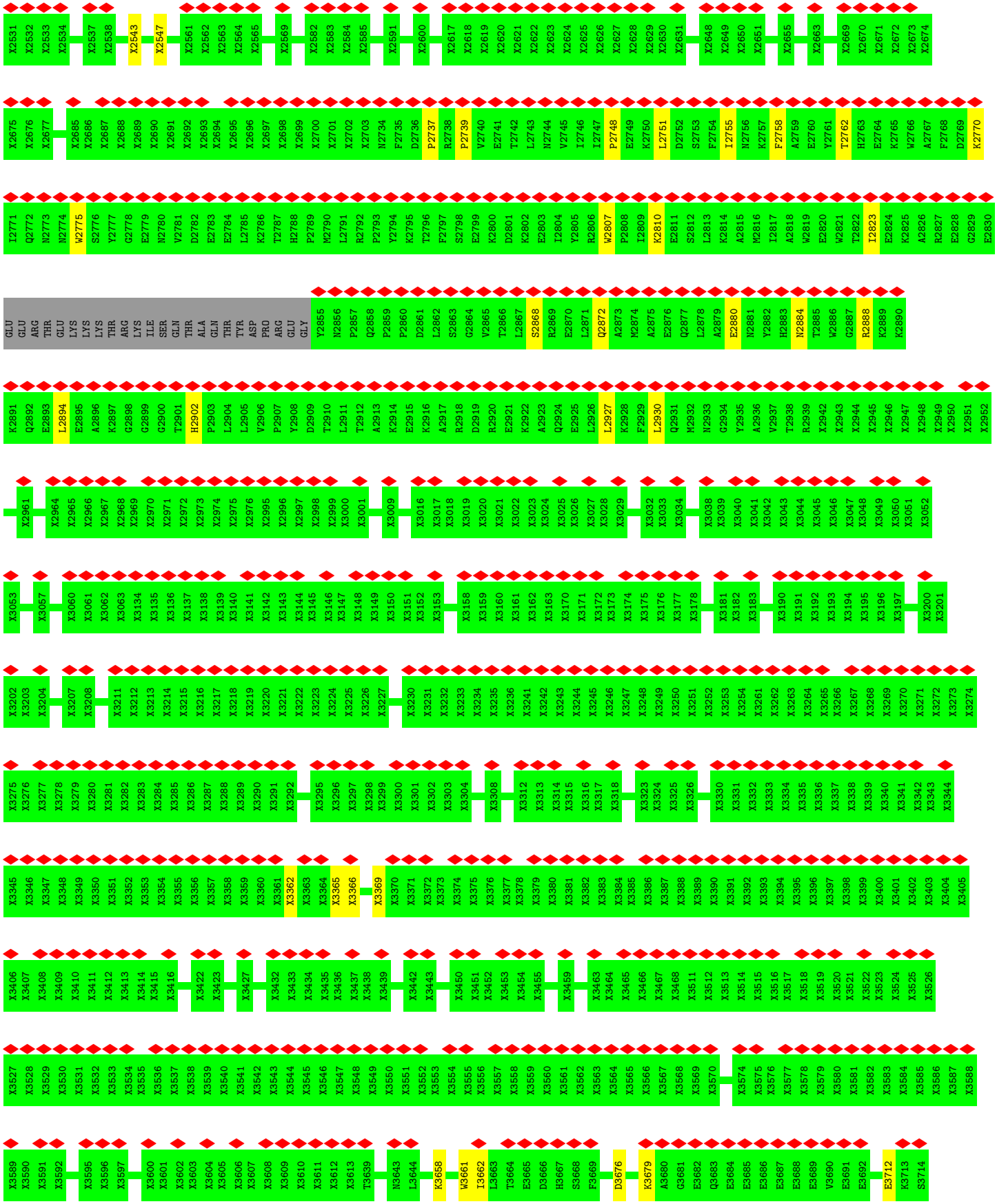
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I2771 Q2772 N2773 W2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830
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X3202 X3203 X3204 X3207 X3208 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3222 X3223 X3224 X3225 X3226 X3227 X3230 X3231 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261 X3262 X3263 X3264 X3265 X3266 X3267 X3268 X3269 X3270 X3271 X3272 X3273 X3274
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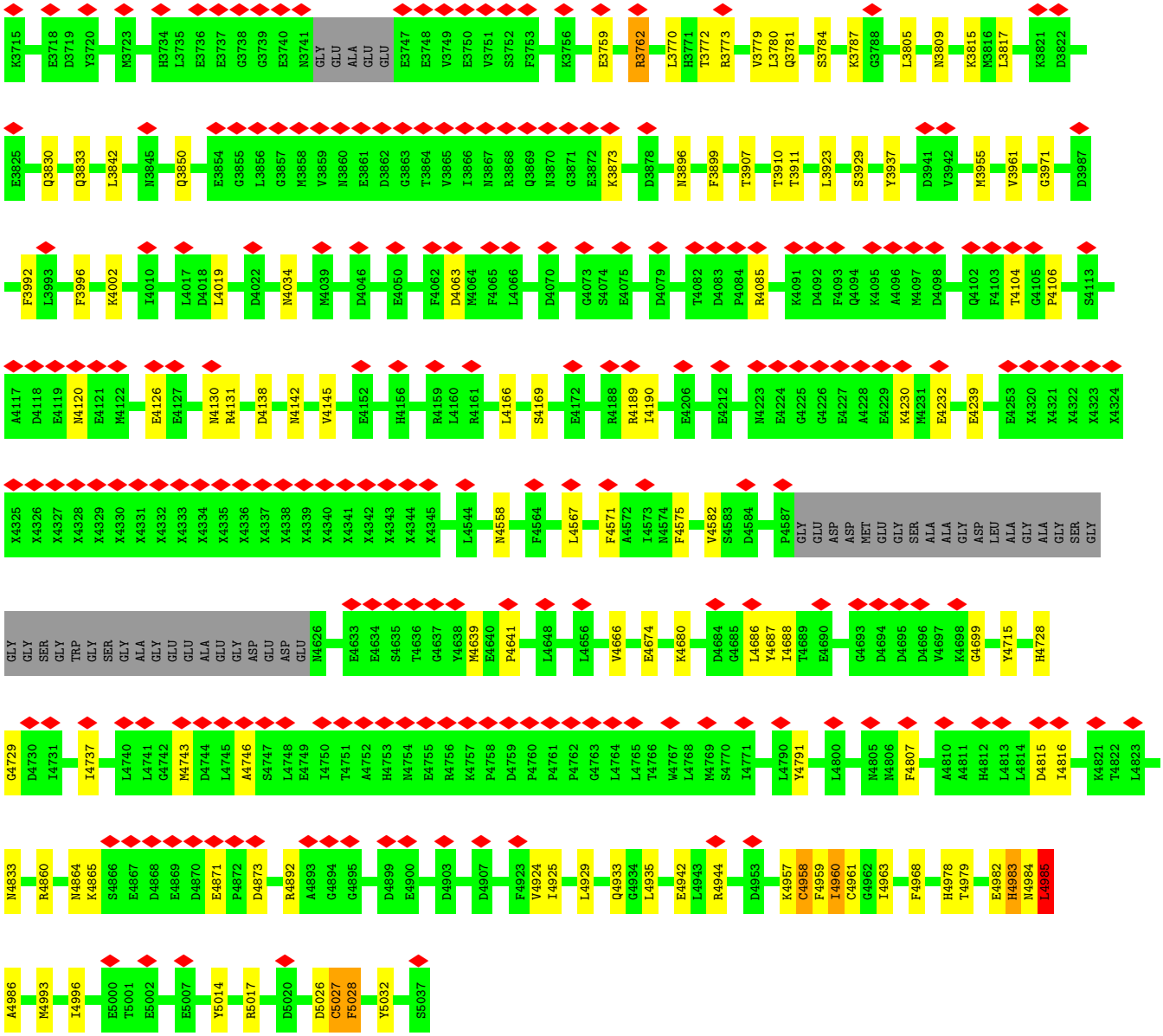
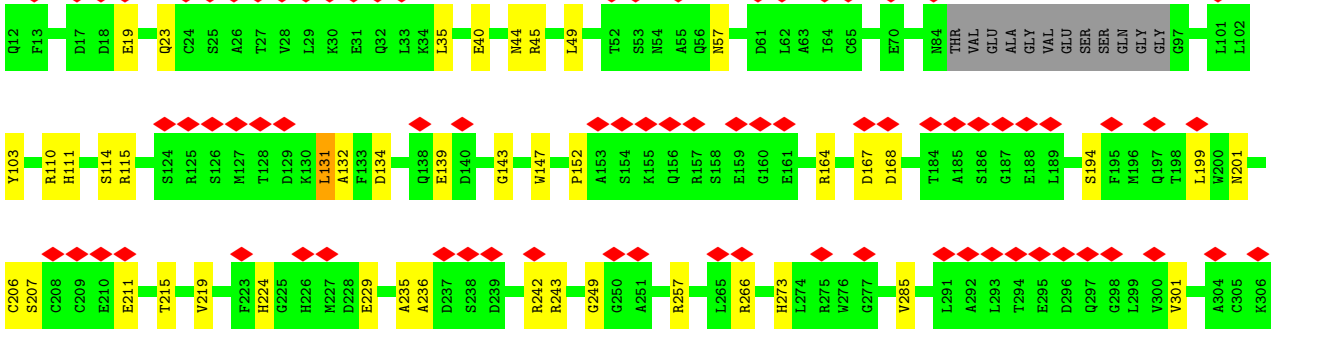
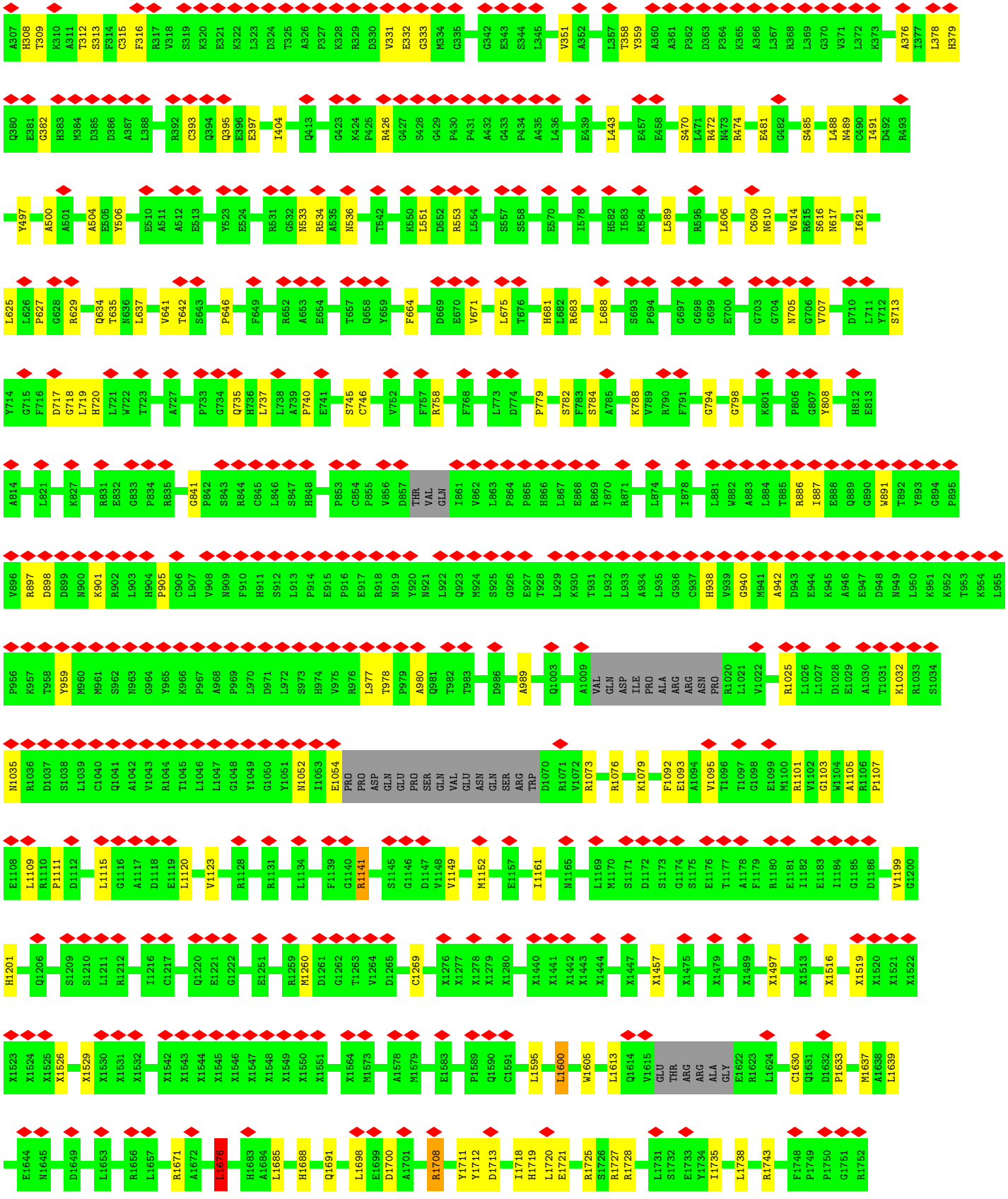


• Molecule 2: Ryanodine receptor 1

Chain E:

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Q380 E381 G382 H383 N384 D385 D386 A387 L388 R392 C393 Q394 Q395 E396 E397 I404 Q413 G423 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 E439 L443 E457 E458 S470 L471 R472 N473 R474 E481 G482 S485 L488 N489 C490 I491 D492 R493
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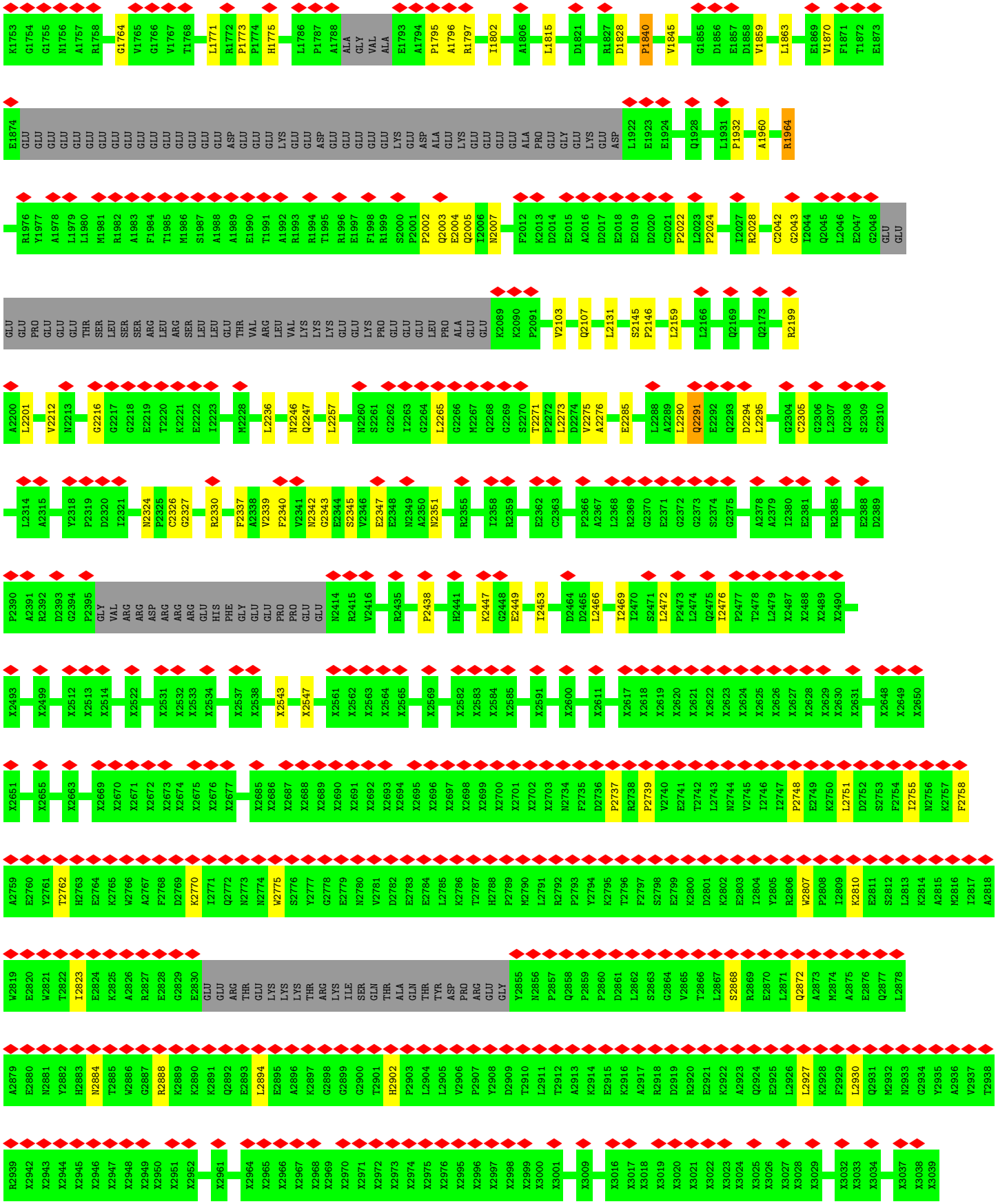

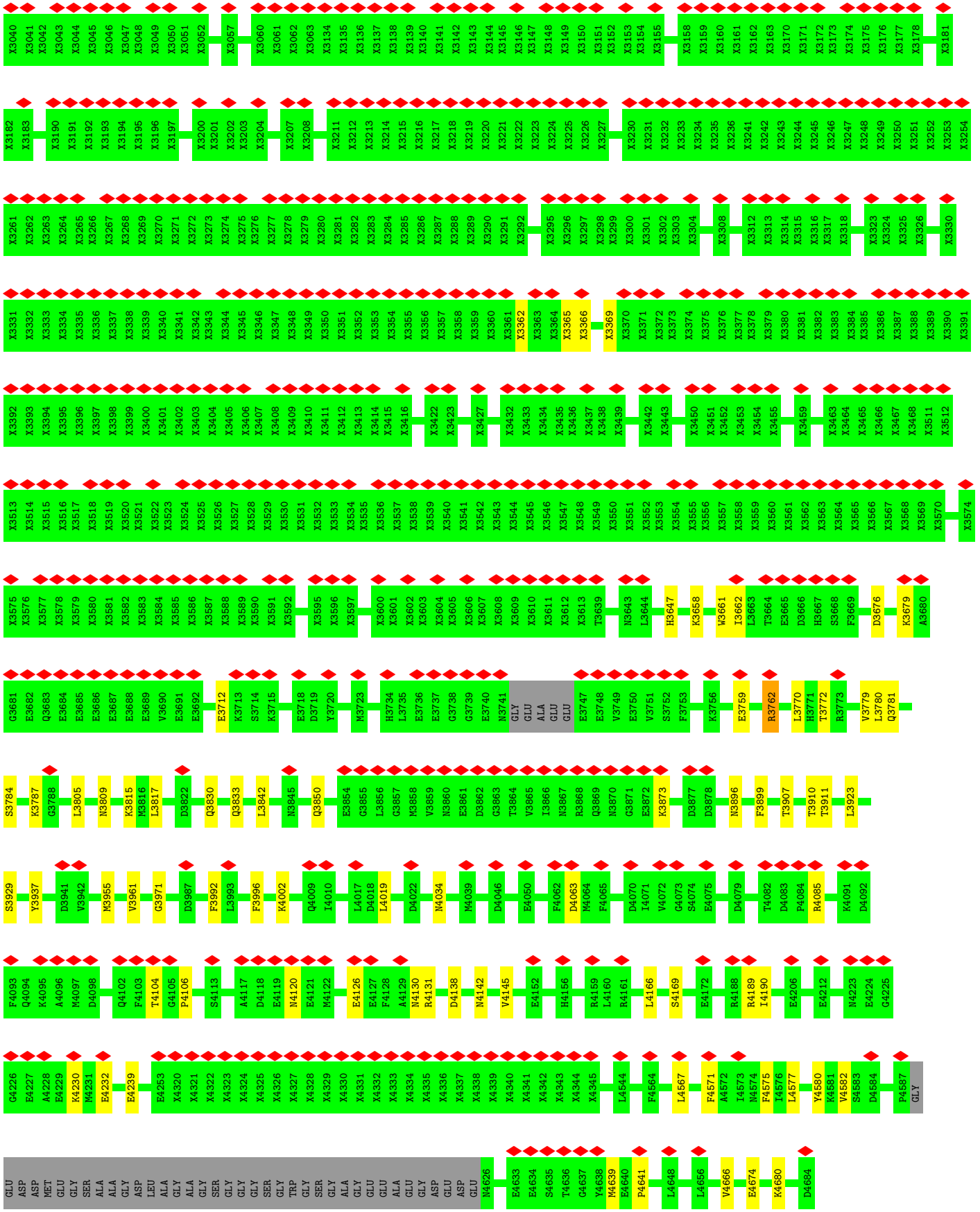
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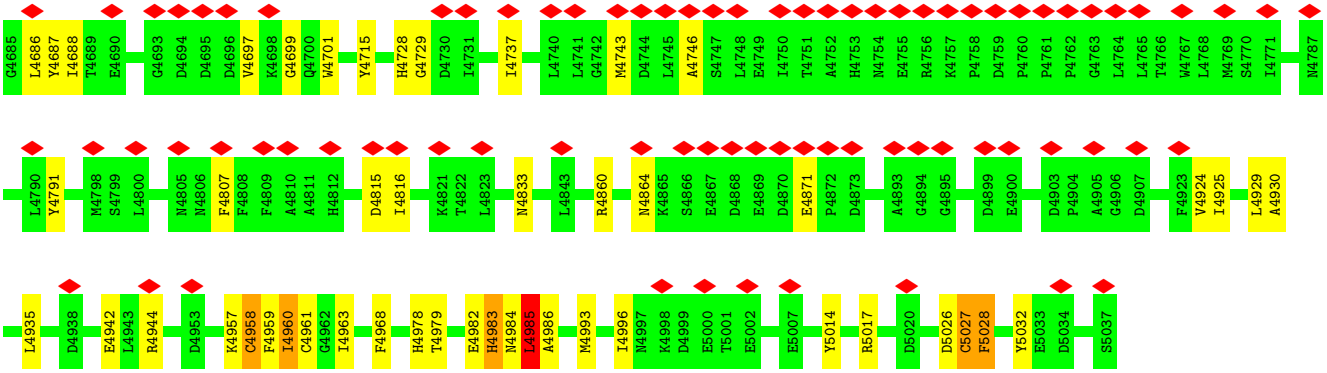
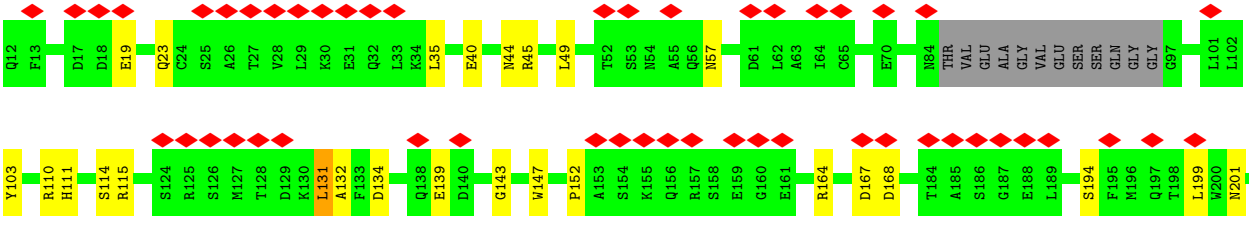
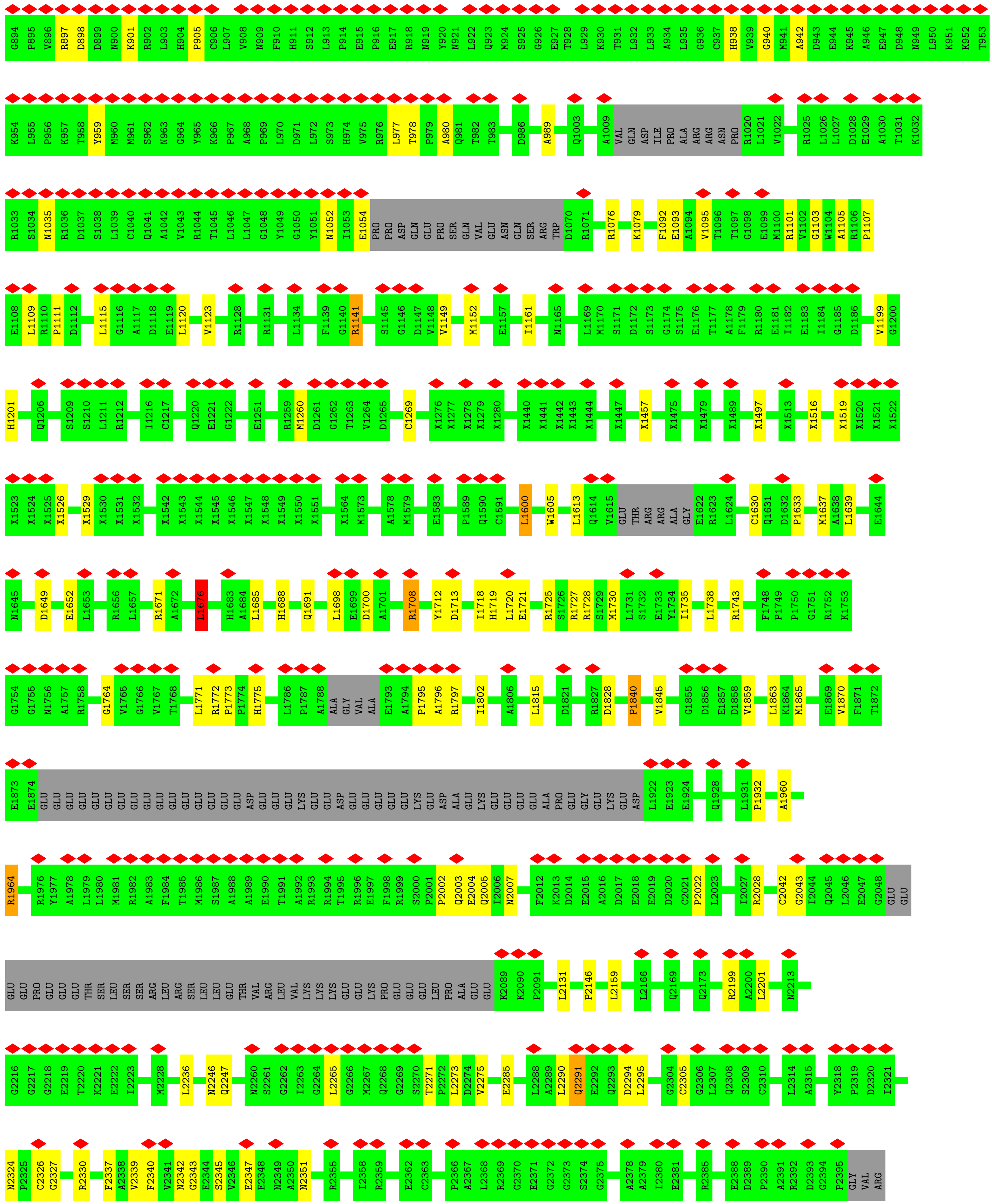


• Molecule 2: Ryanodine receptor 1

Chain I:

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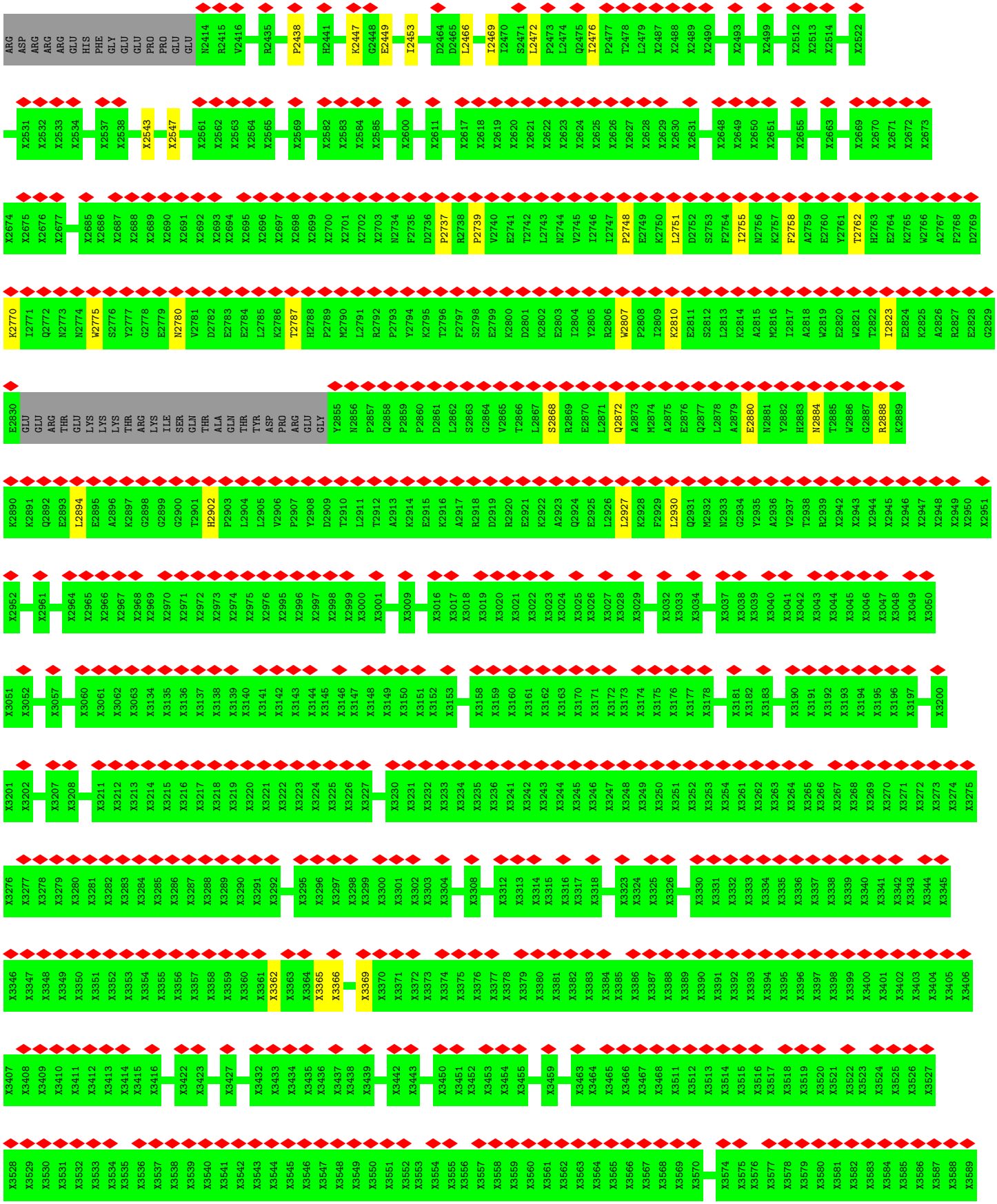
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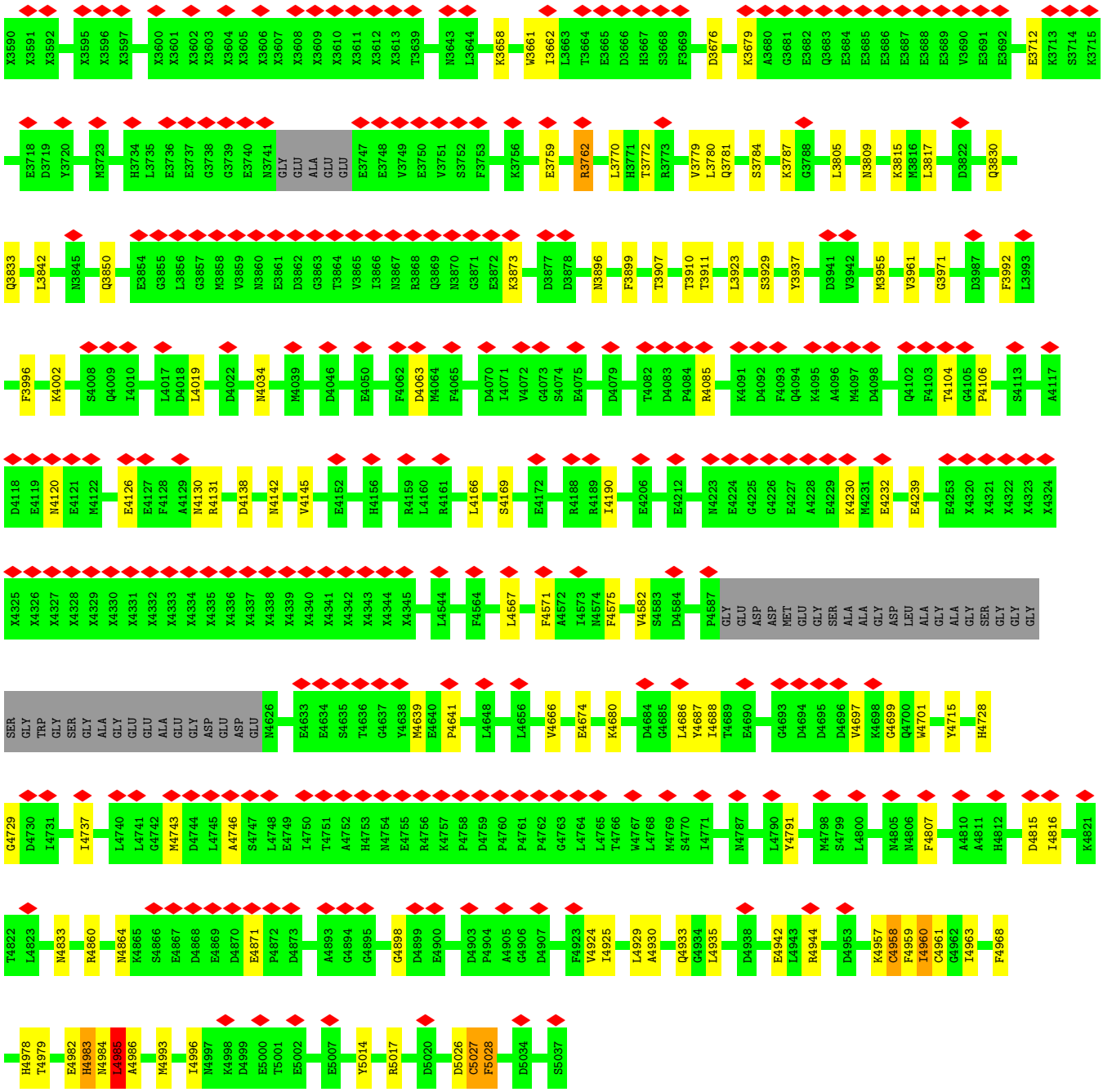
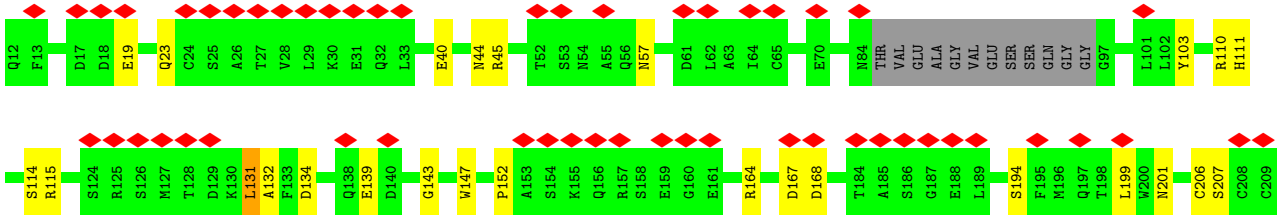
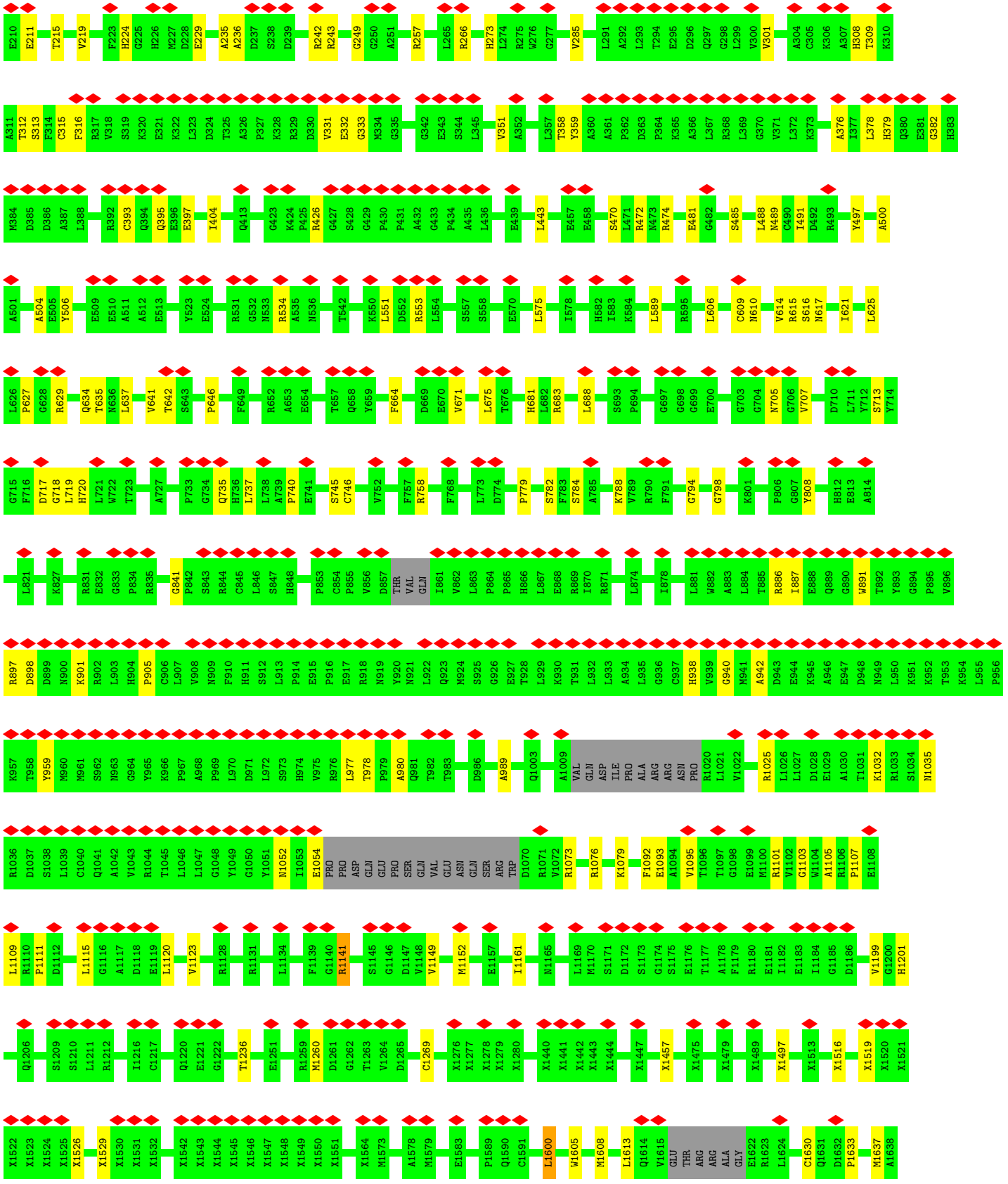


• Molecule 2: Ryanodine receptor 1

Chain G:

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M384 D385 D386 A387 L388 R392 C393 Q394 Q395 E396 E397 I404 Q413 G423 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 E439 L443 E457 E458 S470 L471 R472 N473 R474 E481 G482 S485 L488 N489 C490 I491 D492 R493 Y497 A500
A501 A504 E505 Y506 E509 E510 A511 A512 E513 Y523 E524 R531 G532 N533 R534 A535 N536 T542 K550 L551 D552 R553 L554 S557 S558 E570 L575 I578 H582 I583 K584 L589 R595 L606 C609 N610 V614 R615 S616 N617 I621 L625
L626 P627 G628 R629 Q634 T635 N636 L637 V641 T642 S643 P646 F649 R652 A653 E654 T657 Q658 Y659 F664 D669 E670 V671 L675 T676 H681 L682 R683 L688 S693 P694 G697 G698 G699 E700 G703 G704 N705 G706 V707 D710 L711 Y712 S713 Y714
G715 F716 D717 G718 L719 H720 L721 W722 T723 A727 P733 G734 Q735 H736 L737 L738 A739 P740 E741 S745 C746 V752 F757 R758 F768 L773 D774 P779 S782 F783 S784 A785 K788 V789 R790 F791 G794 G798 K801 P806 G807 Y808 H812 E813 A814
L821 K827 R831 E832 G833 P834 R835 G841 P842 S843 R844 C845 L846 S847 H848 P853 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 L874 I878 L881 W882 A883 L884 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 L933 A934 L935 G936 C937 H938 V939 G940 M941 A942 D943 E944 K945 A946 E947 D948 N949 L950 K951 K952 T953 K954 L955 P956
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R1036 D1037 S1038 L1039 C1040 Q1041 A1042 V1043 R1044 T1045 L1046 L1047 G1048 Y1049 G1050 Y1051 N1052 I1053 E1054 PRO PRO ASP GLN GLU PRO SER GLN VAL GLU ASN GLN SER ARG TRP D1070 R1071 V1072 R1073 R1076 K1079 F1092 E1093 A1094 V1095 T1096 T1097 G1098 E1099 M1100 R1101 V1102 G1103 W1104 A1105 R1106 P1107 E1108
L1109 R1110 P1111 D1112 L1115 G1116 A1117 D1118 E1119 L1120 V1123 R1128 R1131 L1134 F1139 G1140 R1141 S1145 G1146 D1147 V1148 V1149 M1152 E1157 I1161 N1165 L1169 M1170 S1171 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180 E1181 I1182 E1183 I1184 A1185 G1186 V1199 G1200 H1201
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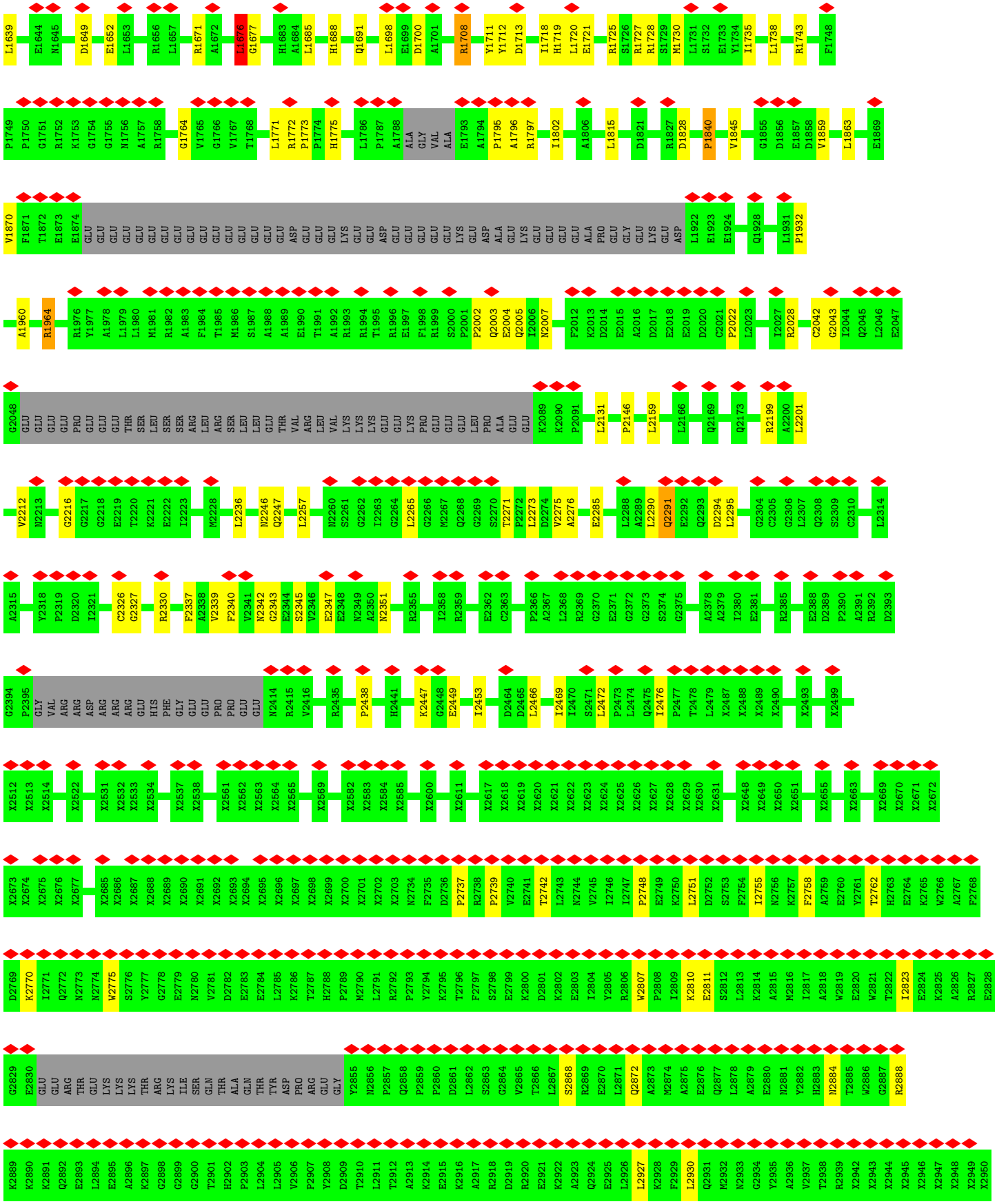
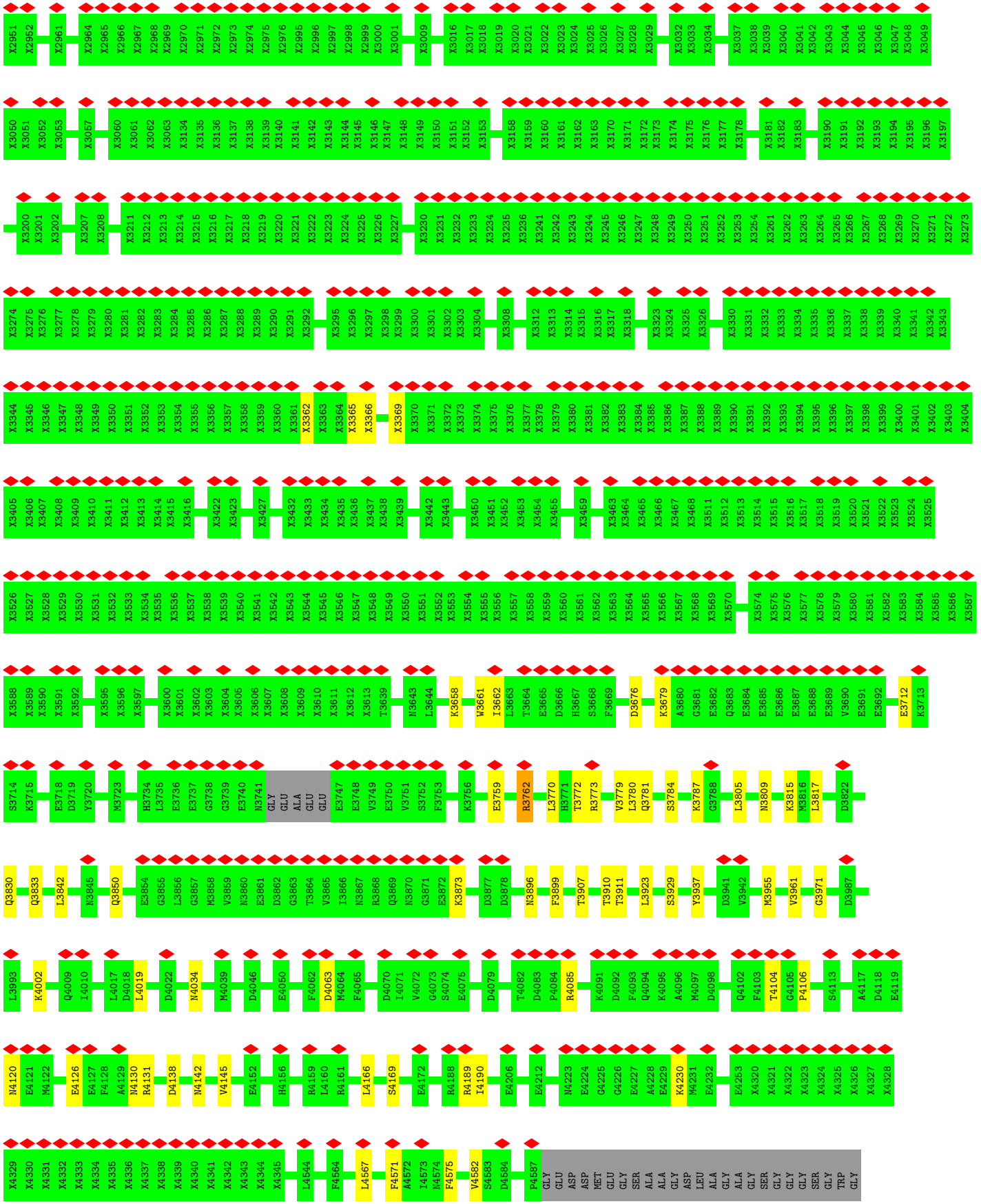
X1522 X1523 X1524 X1525 X1526 X1529 X1530 X1531 X1532 X1542 X1543 X1544 X1545 X1546 X1547 X1548 X1549 X1550 X1551 X1564 M1573 A1578 M1579 E1583 P1589 Q1590 C1591 L1600 W1605 M1608 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 C1630 Q1631 D1632 P1633 M1637 A1638

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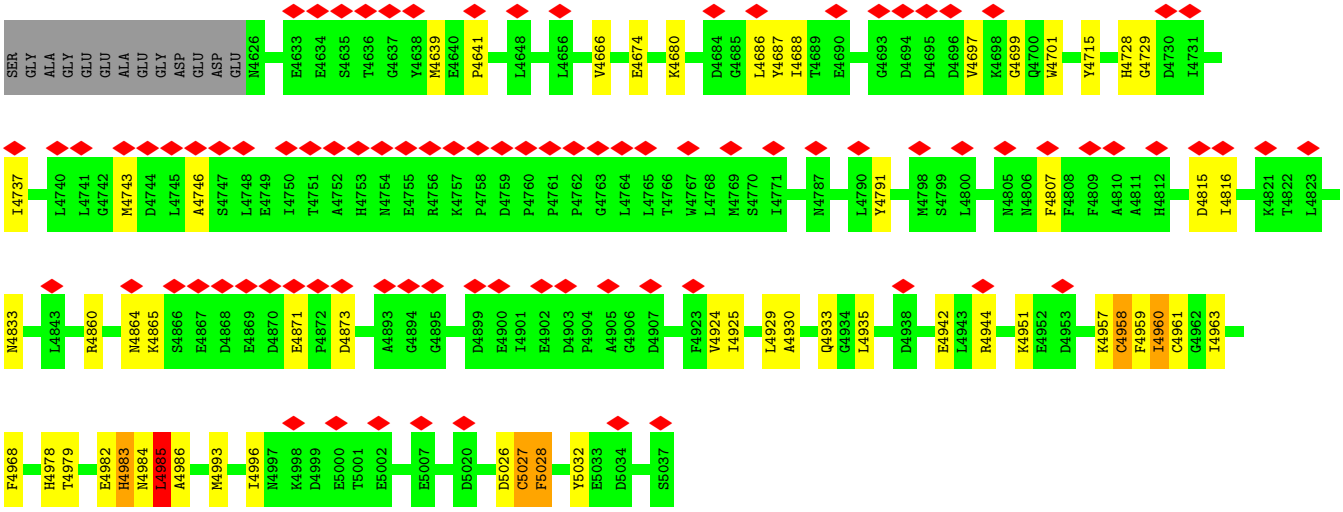
X4329 X4330 X4331 X4332 X4333 X4334 X4335 X4336 X4337 X4338 X4339 X4340 X4341 X4342 X4343 X4344 X4345 L4544 F4564 L4567 F4571 A4572 I4573 N4574 F4575 V4582 S4583 D4584 P4587 GLY GLU ASP ASP MET GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY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I4737 L4740 L4741 G4742 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 S4770 I4771 N4787 L4790 Y4791 M4798 S4799 L4800 N4805 N4806 F4807 F4808 F4809 A4810 A4811 H4812 D4815 I4816 K4821 T4822 L4823
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F4968 H4978 T4979 E4982 H4983 N4984 L4985 A4986 M4993 I4996 N4997 K4998 D4999 E5000 T5001 E5002 E5007 D5020 D5026 C5027 F5028 Y5032 E5033 D5034 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.066	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	502.0, 502.0, 502.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.255, 1.255, 1.255	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/834	0.51	0/1123
1	F	0.32	0/834	0.51	0/1123
1	H	0.32	0/834	0.51	0/1123
1	J	0.32	0/834	0.51	0/1123
2	B	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	E	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	G	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
2	I	0.31	1/25428 (0.0%)	0.54	9/34534 (0.0%)
All	All	0.31	4/105048 (0.0%)	0.54	36/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	15
2	E	0	15
2	G	0	15
2	I	0	15
All	All	0	64

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2476	ILE	C-N	5.37	1.44	1.34
2	B	2476	ILE	C-N	5.34	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2476	ILE	C-N	5.33	1.44	1.34
2	G	2476	ILE	C-N	5.30	1.44	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	131	LEU	CA-CB-CG	8.29	134.37	115.30
2	G	131	LEU	CA-CB-CG	8.28	134.35	115.30
2	B	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	E	131	LEU	CA-CB-CG	8.27	134.32	115.30
2	G	1600	LEU	CA-CB-CG	7.05	131.52	115.30
2	I	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	B	1600	LEU	CA-CB-CG	7.04	131.49	115.30
2	E	1600	LEU	CA-CB-CG	7.03	131.48	115.30
2	I	1676	LEU	CA-CB-CG	6.55	130.37	115.30
2	B	1676	LEU	CA-CB-CG	6.54	130.33	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.31	115.30
2	E	1676	LEU	CA-CB-CG	6.51	130.28	115.30
2	I	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	G	4985	LEU	CA-CB-CG	6.23	129.63	115.30
2	B	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	E	4985	LEU	CA-CB-CG	6.22	129.60	115.30
2	G	977	LEU	CA-CB-CG	5.37	127.64	115.30
2	G	688	LEU	CA-CB-CG	5.36	127.63	115.30
2	B	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	977	LEU	CA-CB-CG	5.35	127.61	115.30
2	I	688	LEU	CA-CB-CG	5.35	127.60	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	B	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	688	LEU	CA-CB-CG	5.33	127.57	115.30
2	E	3770	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	3770	LEU	CA-CB-CG	5.12	127.06	115.30
2	G	3770	LEU	CA-CB-CG	5.11	127.04	115.30
2	I	3770	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	2290	LEU	CA-CB-CG	5.08	126.97	115.30
2	E	2290	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	2290	LEU	CA-CB-CG	5.06	126.95	115.30
2	G	2290	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	4639	MET	C-N-CA	5.05	134.32	121.70
2	G	4639	MET	C-N-CA	5.03	134.27	121.70
2	E	4639	MET	C-N-CA	5.03	134.27	121.70
2	B	4639	MET	C-N-CA	5.03	134.26	121.70

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	8	0
1	F	818	0	824	8	0
1	H	818	0	824	9	0
1	J	818	0	824	8	0
2	B	29499	0	24749	236	0
2	E	29499	0	24749	235	0
2	G	29499	0	24749	231	0
2	I	29499	0	24749	233	0
3	B	31	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	31	0	12	2	0
3	G	31	0	12	2	0
3	I	31	0	12	2	0
4	B	14	0	10	0	0
4	E	14	0	10	0	0
4	G	14	0	10	0	0
4	I	14	0	10	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	G	1	0	0	0	0
5	I	1	0	0	0	0
All	All	121452	0	102380	949	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 4.

All (949) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4230:LYS:HD2	2:I:4959:PHE:HE1	1.38	0.88
2:E:4230:LYS:HD2	2:E:4959:PHE:HE1	1.38	0.88
2:B:4230:LYS:HD2	2:B:4959:PHE:HE1	1.38	0.87
2:G:4230:LYS:HD2	2:G:4959:PHE:HE1	1.38	0.87
2:B:4983:HIS:CD2	2:B:4983:HIS:H	1.94	0.86
2:G:4983:HIS:CD2	2:G:4983:HIS:H	1.94	0.86
2:I:4983:HIS:H	2:I:4983:HIS:CD2	1.94	0.84
2:B:4230:LYS:CD	2:B:4959:PHE:HE1	1.92	0.83
2:I:4230:LYS:CD	2:I:4959:PHE:HE1	1.92	0.82
2:E:4983:HIS:CD2	2:E:4983:HIS:H	1.94	0.82
2:E:4230:LYS:CD	2:E:4959:PHE:HE1	1.92	0.82
2:B:4230:LYS:HD2	2:B:4959:PHE:CE1	2.15	0.81
2:I:4230:LYS:HD2	2:I:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:HD2	2:G:4959:PHE:CE1	2.15	0.81
2:G:4230:LYS:CD	2:G:4959:PHE:HE1	1.92	0.81
2:E:4230:LYS:HD2	2:E:4959:PHE:CE1	2.15	0.80
2:G:4983:HIS:H	2:G:4983:HIS:HD2	1.29	0.79
2:B:4983:HIS:H	2:B:4983:HIS:HD2	1.29	0.77
2:I:4983:HIS:H	2:I:4983:HIS:HD2	1.29	0.77
2:E:4983:HIS:H	2:E:4983:HIS:HD2	1.29	0.77
2:B:4968:PHE:CZ	2:B:4978:HIS:CE1	2.77	0.73
2:E:4968:PHE:CZ	2:E:4978:HIS:CE1	2.77	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4968:PHE:CZ	2:G:4978:HIS:CE1	2.77	0.72
2:I:4968:PHE:CZ	2:I:4978:HIS:CE1	2.77	0.72
2:G:4960:ILE:N	2:G:4960:ILE:HD13	2.04	0.72
2:I:4960:ILE:N	2:I:4960:ILE:HD13	2.04	0.71
2:E:4960:ILE:HD13	2:E:4960:ILE:N	2.04	0.71
2:B:4960:ILE:N	2:B:4960:ILE:HD13	2.04	0.71
2:B:4968:PHE:CE2	2:B:4978:HIS:ND1	2.61	0.69
2:E:4968:PHE:CE2	2:E:4978:HIS:ND1	2.61	0.68
2:G:4968:PHE:CE2	2:G:4978:HIS:ND1	2.61	0.68
2:I:4968:PHE:CE2	2:I:4978:HIS:ND1	2.61	0.68
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.67
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.67
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.67
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.78	0.66
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.78	0.66
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.61	0.65
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.61	0.65
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.61	0.64
2:G:379:HIS:HD2	2:G:382:GLY:H	1.45	0.64
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.78	0.64
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.62	0.64
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.80	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.61	0.64
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.80	0.64
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.78	0.64
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.63	0.63
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.45	0.63
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.81	0.63
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.81	0.63
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.80	0.63
2:E:379:HIS:HD2	2:E:382:GLY:H	1.45	0.63
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.81	0.63
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.64	0.63
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.81	0.63
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.64	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.63	0.63
2:B:379:HIS:HD2	2:B:382:GLY:H	1.45	0.63
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.64	0.62
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.81	0.62
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.81	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.63	0.62
2:G:4982:GLU:HB3	2:G:4983:HIS:HD2	1.65	0.62
2:E:4982:GLU:HB3	2:E:4983:HIS:HD2	1.65	0.62
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.81	0.62
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.65	0.62
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.62
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.64	0.61
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.83	0.61
2:B:4982:GLU:HB3	2:B:4983:HIS:HD2	1.65	0.61
2:I:4982:GLU:HB3	2:I:4983:HIS:HD2	1.65	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.81	0.61
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.65	0.61
2:I:4944:ARG:HH22	2:G:4942:GLU:HA	1.65	0.61
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.82	0.61
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.83	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:4961:CYS:HB3	2:E:4983:HIS:HE1	1.66	0.61
2:I:4230:LYS:CG	2:I:4959:PHE:HE1	2.14	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.60
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.83	0.60
2:B:4230:LYS:CG	2:B:4959:PHE:HE1	2.14	0.60
2:G:4961:CYS:HB3	2:G:4983:HIS:HE1	1.66	0.60
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.34	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.82	0.60
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.83	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.82	0.60
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.65	0.60
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.65	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.60
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.34	0.60
2:B:4961:CYS:HB3	2:B:4983:HIS:HE1	1.65	0.60
2:E:4230:LYS:CG	2:E:4959:PHE:HE1	2.14	0.60
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.83	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:G:4230:LYS:CG	2:G:4959:PHE:HE1	2.14	0.60
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.83	0.59
2:B:4979:THR:HG22	3:B:5101:ATP:H2	1.67	0.59
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4979:THR:HG22	3:I:5101:ATP:H2	1.67	0.59
2:I:4961:CYS:HB3	2:I:4983:HIS:HE1	1.65	0.59
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.59
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.83	0.59
2:B:132:ALA:HA	2:B:194:SER:HB2	1.84	0.59
2:E:4942:GLU:HA	2:G:4944:ARG:HH22	1.67	0.59
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.85	0.59
2:E:132:ALA:HA	2:E:194:SER:HB2	1.84	0.59
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.85	0.59
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.59
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.36	0.59
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.85	0.59
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.85	0.59
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.36	0.59
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.59
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.36	0.58
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.86	0.58
2:I:4190:ILE:HD13	2:I:5026:ASP:CG	2.24	0.58
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.22	0.58
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.22	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.58
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.85	0.58
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.58
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.58
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.85	0.58
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.58
2:G:4979:THR:HG22	3:G:5101:ATP:H2	1.67	0.58
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.36	0.58
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.86	0.58
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.22	0.58
2:E:4979:THR:HG22	3:E:5101:ATP:H2	1.67	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.85	0.58
2:E:4190:ILE:HD13	2:E:5026:ASP:CG	2.24	0.58
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.34	0.58
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.86	0.57
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.85	0.57
2:B:4190:ILE:HD13	2:B:5026:ASP:CG	2.24	0.57
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.34	0.57
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.86	0.57
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.85	0.57
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.57
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.69	0.57
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.22	0.57
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.86	0.57
2:G:132:ALA:HA	2:G:194:SER:HB2	1.84	0.57
2:G:4190:ILE:HD13	2:G:5026:ASP:CG	2.24	0.57
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.37	0.57
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.78	0.57
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.69	0.57
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.87	0.57
2:I:132:ALA:HA	2:I:194:SER:HB2	1.84	0.57
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.87	0.57
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.87	0.57
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.87	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.69	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.78	0.57
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.87	0.57
2:E:4968:PHE:CZ	2:E:4978:HIS:ND1	2.73	0.57
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.87	0.57
2:E:4993:MET:HA	2:E:4996:ILE:HD12	1.86	0.56
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.56
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.86	0.56
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.38	0.56
2:B:4968:PHE:CZ	2:B:4978:HIS:ND1	2.73	0.56
2:I:4993:MET:HA	2:I:4996:ILE:HD12	1.86	0.56
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.38	0.56
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.88	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:E:2347:GLU:O	2:E:2351:ASN:N	2.36	0.56
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.87	0.56
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.70	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.78	0.56
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.86	0.56
2:G:4968:PHE:CZ	2:G:4978:HIS:ND1	2.73	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:4993:MET:HA	2:B:4996:ILE:HD12	1.86	0.56
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.70	0.56
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.86	0.56
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.38	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.86	0.56
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.87	0.56
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.88	0.56
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.70	0.56
2:B:4190:ILE:CD1	2:B:5026:ASP:OD2	2.54	0.56
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.88	0.56
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.69	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.86	0.56
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.88	0.56
2:G:2347:GLU:O	2:G:2351:ASN:N	2.36	0.56
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.88	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.88	0.56
2:G:4993:MET:HA	2:G:4996:ILE:HD12	1.86	0.56
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.70	0.56
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.56
2:I:4968:PHE:CZ	2:I:4978:HIS:ND1	2.73	0.56
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.38	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.55
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.55
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.88	0.55
2:E:4968:PHE:CE2	2:E:4978:HIS:CE1	2.95	0.55
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.88	0.55
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.71	0.55
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.88	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.36	0.55
2:E:4190:ILE:CD1	2:E:5026:ASP:OD2	2.54	0.55
2:G:683:ARG:NH1	2:G:707:VAL:O	2.39	0.55
2:I:2347:GLU:O	2:I:2351:ASN:N	2.36	0.55
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.88	0.55
2:B:4968:PHE:CE2	2:B:4978:HIS:CE1	2.95	0.55
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.71	0.55
2:I:4190:ILE:CD1	2:I:5026:ASP:OD2	2.54	0.55
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.55
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.88	0.55
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.71	0.55
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.71	0.55
2:G:4190:ILE:CD1	2:G:5026:ASP:OD2	2.54	0.55
2:E:229:GLU:HA	2:E:249:GLY:HA2	1.88	0.55
2:I:229:GLU:HA	2:I:249:GLY:HA2	1.88	0.55
2:I:683:ARG:NH1	2:I:707:VAL:O	2.39	0.55
2:B:229:GLU:HA	2:B:249:GLY:HA2	1.88	0.55
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.89	0.55
2:I:4968:PHE:CE2	2:I:4978:HIS:CE1	2.95	0.55
2:G:229:GLU:HA	2:G:249:GLY:HA2	1.88	0.55
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.89	0.54
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.80	0.54
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.88	0.54
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.89	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.39	0.54
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.41	0.54
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.88	0.54
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.81	0.54
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.88	0.54
2:G:4968:PHE:CE2	2:G:4978:HIS:CE1	2.95	0.54
2:E:4190:ILE:CD1	2:E:5026:ASP:CG	2.76	0.54
2:I:4190:ILE:CD1	2:I:5026:ASP:CG	2.76	0.54
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.88	0.54
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.41	0.54
2:B:4190:ILE:CD1	2:B:5026:ASP:CG	2.76	0.54
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.90	0.54
2:G:4190:ILE:CD1	2:G:5026:ASP:CG	2.76	0.54
2:E:331:VAL:HG12	2:E:333:GLY:H	1.73	0.54
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.81	0.54
2:B:111:HIS:HD2	2:B:114:SER:H	1.56	0.54
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.81	0.54
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.54
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.41	0.54
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.54
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.90	0.54
2:E:111:HIS:HD2	2:E:114:SER:H	1.56	0.54
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.70	0.54
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.41	0.54
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.39	0.54
2:G:111:HIS:HD2	2:G:114:SER:H	1.56	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.26	0.53
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.26	0.53
2:G:794:GLY:H	2:G:798:GLY:HA3	1.73	0.53
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.90	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.53
2:I:794:GLY:H	2:I:798:GLY:HA3	1.73	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.90	0.53
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.91	0.53
2:B:331:VAL:HG12	2:B:333:GLY:H	1.73	0.53
2:I:111:HIS:HD2	2:I:114:SER:H	1.56	0.53
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.41	0.53
2:B:794:GLY:H	2:B:798:GLY:HA3	1.73	0.53
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.91	0.53
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.53
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.90	0.53
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.91	0.53
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.91	0.53
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.73	0.53
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.42	0.53
2:I:313:SER:HB3	2:I:351:VAL:HB	1.91	0.53
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.26	0.53
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.42	0.53
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.74	0.53
2:E:794:GLY:H	2:E:798:GLY:HA3	1.74	0.53
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.90	0.53
2:I:331:VAL:HG12	2:I:333:GLY:H	1.73	0.53
2:G:331:VAL:HG12	2:G:333:GLY:H	1.73	0.53
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.91	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.26	0.53
1:F:2:VAL:HG21	1:F:61:GLU:HB2	1.92	0.52
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.91	0.52
2:B:2868:SER:O	2:B:2872:GLN:N	2.41	0.52
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.90	0.52
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.52
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.75	0.52
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.82	0.52
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.39	0.52
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.42	0.52
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.75	0.52
2:E:313:SER:HB3	2:E:351:VAL:HB	1.91	0.52
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.42	0.52
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.75	0.52
1:H:2:VAL:HG21	1:H:61:GLU:HB2	1.92	0.52
1:A:2:VAL:HG21	1:A:61:GLU:HB2	1.92	0.52
2:B:313:SER:HB3	2:B:351:VAL:HB	1.91	0.52
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.90	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.91	0.52
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.92	0.52
2:E:683:ARG:NH1	2:E:707:VAL:O	2.39	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.91	0.52
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.52
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.90	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.91	0.52
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.42	0.52
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.91	0.52
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.52
2:G:4979:THR:HG22	3:G:5101:ATP:C2	2.45	0.51
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.75	0.51
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.75	0.51
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.51
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.51
1:F:27:THR:HB	1:F:100:ASP:HB3	1.93	0.51
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:B:4979:THR:HG22	3:B:5101:ATP:C2	2.45	0.51
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.82	0.51
2:G:313:SER:HB3	2:G:351:VAL:HB	1.91	0.51
2:E:485:SER:O	2:E:489:ASN:N	2.39	0.51
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.41	0.51
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.82	0.51
1:J:2:VAL:HG21	1:J:61:GLU:HB2	1.92	0.51
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.41	0.51
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.39	0.51
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.46	0.51
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.43	0.51
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.75	0.51
1:A:27:THR:HB	1:A:100:ASP:HB3	1.93	0.51
1:J:27:THR:HB	1:J:100:ASP:HB3	1.93	0.51
2:G:978:THR:HB	2:G:980:ALA:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.93	0.51
2:B:614:VAL:HG22	2:B:616:SER:H	1.75	0.51
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.82	0.51
2:E:4979:THR:HG22	3:E:5101:ATP:C2	2.45	0.51
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.93	0.51
2:B:1025:ARG:O	2:B:1032:LYS:NZ	2.42	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.43	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:G:614:VAL:HG22	2:G:616:SER:H	1.75	0.51
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.46	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.45	0.50
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.45	0.50
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.93	0.50
2:E:1457:UNK:N	2:E:1497:UNK:O	2.45	0.50
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.45	0.50
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.43	0.50
2:I:4979:THR:HG22	3:I:5101:ATP:C2	2.45	0.50
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.94	0.50
1:H:27:THR:HB	1:H:100:ASP:HB3	1.93	0.50
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.50
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.94	0.50
2:I:614:VAL:HG22	2:I:616:SER:H	1.75	0.50
2:I:1457:UNK:N	2:I:1497:UNK:O	2.44	0.50
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.93	0.50
2:E:2868:SER:O	2:E:2872:GLN:N	2.41	0.50
2:B:211:GLU:OE2	2:B:3907:THR:OG1	2.30	0.50
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.93	0.50
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.50
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.93	0.50
2:G:2758:PHE:O	2:G:2762:THR:N	2.45	0.50
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.94	0.50
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.50
2:E:614:VAL:HG22	2:E:616:SER:H	1.75	0.50
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.42	0.50
2:E:2758:PHE:O	2:E:2762:THR:N	2.45	0.50
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.93	0.50
2:G:1457:UNK:N	2:G:1497:UNK:O	2.45	0.50
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
2:G:2868:SER:O	2:G:2872:GLN:N	2.41	0.50
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.93	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
2:G:211:GLU:OE2	2:G:3907:THR:OG1	2.30	0.49
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.94	0.49
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.43	0.49
2:E:4833:ASN:HB3	2:E:4935:LEU:HD23	1.94	0.49
2:B:4230:LYS:CG	2:B:4959:PHE:CE1	2.95	0.49
2:E:211:GLU:OE2	2:E:3907:THR:OG1	2.30	0.49
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.94	0.49
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.94	0.49
2:B:4833:ASN:HB3	2:B:4935:LEU:HD23	1.94	0.49
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.93	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.49
2:I:4230:LYS:CG	2:I:4959:PHE:CE1	2.95	0.49
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.94	0.49
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:4833:ASN:HB3	2:I:4935:LEU:HD23	1.94	0.49
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.95	0.49
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.94	0.49
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.95	0.49
2:B:1457:UNK:N	2:B:1497:UNK:O	2.45	0.49
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.94	0.49
2:B:2758:PHE:O	2:B:2762:THR:N	2.45	0.49
2:I:642:THR:HG23	2:I:1613:LEU:HD12	1.95	0.49
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.43	0.49
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.95	0.49
2:B:642:THR:HG23	2:B:1613:LEU:HD12	1.95	0.49
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.95	0.49
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.45	0.49
2:E:4230:LYS:CG	2:E:4959:PHE:CE1	2.95	0.49
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.46	0.49
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.49
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.41	0.49
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.45	0.49
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.95	0.49
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.95	0.49
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.94	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:G:1025:ARG:O	2:G:1032:LYS:NZ	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.45	0.49
2:B:1727:ARG:HH21	2:B:1775:HIS:CE1	2.31	0.49
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.46	0.49
2:G:4833:ASN:HB3	2:G:4935:LEU:HD23	1.94	0.49
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.94	0.48
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.95	0.48
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.78	0.48
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.48
2:G:4230:LYS:CG	2:G:4959:PHE:CE1	2.95	0.48
2:G:4924:VAL:HG23	2:G:4925:ILE:HG12	1.95	0.48
2:I:1727:ARG:HH21	2:I:1775:HIS:CE1	2.31	0.48
2:I:2868:SER:O	2:I:2872:GLN:N	2.41	0.48
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.45	0.48
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.48
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.95	0.48
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.95	0.48
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.45	0.48
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.96	0.48
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.48
2:E:4924:VAL:HG23	2:E:4925:ILE:HG12	1.95	0.48
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.93	0.48
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.46	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.32	0.48
2:B:4924:VAL:HG23	2:B:4925:ILE:HG12	1.95	0.48
2:G:642:THR:HG23	2:G:1613:LEU:HD12	1.95	0.48
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.78	0.48
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.30	0.48
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.43	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.46	0.48
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.96	0.48
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	1.96	0.48
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.48
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.95	0.48
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:B:3759:GLU:HA	2:B:3762:ARG:HE	1.78	0.48
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.45	0.48
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.94	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
2:I:3759:GLU:HA	2:I:3762:ARG:HE	1.78	0.48
2:I:4924:VAL:HG23	2:I:4925:ILE:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:111:HIS:CD2	2:G:114:SER:H	2.32	0.48
2:G:3773:ARG:HG3	2:G:3815:LYS:HZ3	1.79	0.48
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.46	0.48
2:E:1727:ARG:HH21	2:E:1775:HIS:CE1	2.31	0.48
2:I:111:HIS:CD2	2:I:114:SER:H	2.32	0.48
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.79	0.48
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.78	0.48
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.79	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.94	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:1727:ARG:HH21	2:G:1775:HIS:CE1	2.31	0.47
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.96	0.47
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.79	0.47
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.79	0.47
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.78	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.47
2:E:3759:GLU:HA	2:E:3762:ARG:HE	1.78	0.47
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.28	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.46	0.47
2:E:642:THR:HG23	2:E:1613:LEU:HD12	1.95	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:G:485:SER:O	2:G:489:ASN:N	2.39	0.47
2:G:3759:GLU:HA	2:G:3762:ARG:HE	1.78	0.47
2:B:3773:ARG:HG3	2:B:3815:LYS:HZ3	1.80	0.47
2:E:111:HIS:CD2	2:E:114:SER:H	2.32	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.79	0.47
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.79	0.47
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.79	0.47
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.79	0.47
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.96	0.47
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.96	0.47
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.96	0.47
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.96	0.47
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.97	0.47
2:E:898:ASP:HB3	2:E:901:LYS:HB2	1.97	0.47
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.97	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.79	0.47
2:G:898:ASP:HB3	2:G:901:LYS:HB2	1.97	0.47
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.47	0.47
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.97	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:3676:ASP:HA	2:B:3679:LYS:HB3	1.97	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.96	0.47
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.96	0.47
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.96	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.79	0.47
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.96	0.47
2:I:3676:ASP:HA	2:I:3679:LYS:HB3	1.97	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.79	0.47
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.79	0.46
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.79	0.46
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.79	0.46
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.28	0.46
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.46
2:B:1738:LEU:HB3	2:B:2146:PRO:HG3	1.97	0.46
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.46
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.46
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.46
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.97	0.46
2:I:898:ASP:HB3	2:I:901:LYS:HB2	1.97	0.46
2:G:3676:ASP:HA	2:G:3679:LYS:HB3	1.97	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.79	0.46
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.96	0.46
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.97	0.46
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.98	0.46
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.97	0.46
2:G:2327:GLY:HA2	2:G:2330:ARG:HD3	1.97	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.98	0.46
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.46
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.49	0.46
2:G:1738:LEU:HB3	2:G:2146:PRO:HG3	1.97	0.46
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.98	0.46
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.98	0.46
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.46
2:B:243:ARG:NH1	2:B:301:VAL:O	2.46	0.46
2:B:898:ASP:HB3	2:B:901:LYS:HB2	1.97	0.46
2:I:2327:GLY:HA2	2:I:2330:ARG:HD3	1.97	0.46
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.96	0.46
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.97	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.39	0.46
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.97	0.46
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.98	0.46
2:E:1738:LEU:HB3	2:E:2146:PRO:HG3	1.97	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:I:1738:LEU:HB3	2:I:2146:PRO:HG3	1.97	0.46
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.46
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.98	0.46
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.47	0.46
2:G:4063:ASP:OD1	2:G:4169:SER:OG	2.34	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.45
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.79	0.45
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.97	0.45
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	1.98	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.45
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.43	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:B:621:ILE:O	2:B:625:LEU:N	2.48	0.45
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.45
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.98	0.45
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.98	0.45
2:B:2327:GLY:HA2	2:B:2330:ARG:HD3	1.97	0.45
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1694:LEU:O	2:B:1712:TYR:OH	2.27	0.45
2:E:3676:ASP:HA	2:E:3679:LYS:HB3	1.97	0.45
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.39	0.45
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.45
2:E:2327:GLY:HA2	2:E:2330:ARG:HD3	1.97	0.45
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	1.98	0.45
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.45
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.45
2:E:940:GLY:O	2:E:1052:ASN:N	2.49	0.45
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.98	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.70	0.45
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.45
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.45
1:F:92:PRO:HD3	2:E:627:PRO:HB2	1.99	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4571:PHE:O	2:B:4575:PHE:N	2.50	0.45
2:B:4729:GLY:HA2	2:B:4737:ILE:HG13	1.99	0.45
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.99	0.45
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.45
2:E:4571:PHE:O	2:E:4575:PHE:N	2.50	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.52	0.45
2:B:1516:UNK:N	2:B:1529:UNK:O	2.50	0.45
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.45
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.45
2:E:309:THR:O	2:E:313:SER:OG	2.35	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:4063:ASP:OD1	2:I:4169:SER:OG	2.34	0.45
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.99	0.44
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.28	0.44
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.99	0.44
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.44
2:G:1516:UNK:N	2:G:1529:UNK:O	2.50	0.44
2:G:4729:GLY:HA2	2:G:4737:ILE:HG13	1.99	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.51	0.44
2:B:3910:THR:HG23	2:B:3911:THR:HG23	2.00	0.44
2:B:500:ALA:HB1	2:B:504:ALA:HB2	2.00	0.44
2:B:1093:GLU:OE1	2:B:1201:HIS:NE2	2.49	0.44
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4063:ASP:OD1	2:E:4169:SER:OG	2.34	0.44
2:I:1093:GLU:OE1	2:I:1201:HIS:NE2	2.49	0.44
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	2.00	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.51	0.44
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	2.00	0.44
2:G:3365:UNK:O	2:G:3369:UNK:N	2.51	0.44
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.99	0.44
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.44
2:E:500:ALA:HB1	2:E:504:ALA:HB2	2.00	0.44
2:E:3910:THR:HG23	2:E:3911:THR:HG23	2.00	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:G:309:THR:O	2:G:313:SER:OG	2.35	0.44
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	2.00	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	2.00	0.44
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.52	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.44
2:I:266:ARG:NH1	2:I:332:GLU:OE2	2.51	0.44
2:I:309:THR:O	2:I:313:SER:OG	2.35	0.44
2:I:1516:UNK:N	2:I:1529:UNK:O	2.50	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.44
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.99	0.44
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.44
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.44
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.99	0.44
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.44
2:E:2159:LEU:HD22	2:E:2201:LEU:HD23	1.99	0.44
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.44
2:B:897:ARG:HB2	2:B:905:PRO:HG3	2.00	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	2.00	0.44
2:E:621:ILE:O	2:E:625:LEU:N	2.48	0.44
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.00	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.00	0.44
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	2.00	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:2159:LEU:HD22	2:B:2201:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3365:UNK:O	2:E:3369:UNK:N	2.51	0.44
2:I:224:HIS:N	2:I:229:GLU:O	2.46	0.44
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.00	0.44
2:I:2159:LEU:HD22	2:I:2201:LEU:HD23	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.51	0.44
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.44
2:G:897:ARG:HB2	2:G:905:PRO:HG3	2.00	0.44
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.83	0.43
2:E:4729:GLY:HA2	2:E:4737:ILE:HG13	1.99	0.43
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.70	0.43
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.99	0.43
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.50	0.43
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.43
2:G:497:TYR:HB3	2:G:500:ALA:HB2	2.00	0.43
2:G:500:ALA:HB1	2:G:504:ALA:HB2	2.00	0.43
2:G:887:ILE:HG21	2:G:959:TYR:HA	2.00	0.43
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.99	0.43
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	1.98	0.43
2:E:887:ILE:HG21	2:E:959:TYR:HA	2.00	0.43
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.84	0.43
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	2.00	0.43
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	2.00	0.43
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.00	0.43
2:G:266:ARG:NH1	2:G:332:GLU:OE2	2.51	0.43
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.84	0.43
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.52	0.43
2:B:3365:UNK:O	2:B:3369:UNK:N	2.51	0.43
2:B:4063:ASP:OD1	2:B:4169:SER:OG	2.34	0.43
2:E:497:TYR:HB3	2:E:500:ALA:HB2	2.00	0.43
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.00	0.43
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	1.98	0.43
2:E:4697:VAL:O	2:E:4701:TRP:N	2.50	0.43
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.99	0.43
2:G:621:ILE:O	2:G:625:LEU:N	2.48	0.43
2:G:4571:PHE:O	2:G:4575:PHE:N	2.50	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.35	0.43
2:B:4933:GLN:HG2	2:I:4930:ALA:HB2	2.00	0.43
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.43
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:266:ARG:NH1	2:E:332:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:897:ARG:HB2	2:E:905:PRO:HG3	2.00	0.43
2:I:897:ARG:HB2	2:I:905:PRO:HG3	2.00	0.43
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.99	0.43
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.52	0.43
1:J:23:VAL:HG22	1:J:47:LYS:HG2	2.01	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	2.00	0.43
2:E:5028:PHE:O	2:E:5028:PHE:CG	2.70	0.43
2:I:887:ILE:HG21	2:I:959:TYR:HA	2.00	0.43
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.84	0.43
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.00	0.43
1:A:23:VAL:HG22	1:A:47:LYS:HG2	2.01	0.43
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	2.00	0.43
2:B:4984:ASN:C	2:B:4986:ALA:H	2.22	0.43
2:I:4960:ILE:N	2:I:4960:ILE:CD1	2.73	0.43
2:I:4984:ASN:C	2:I:4986:ALA:H	2.22	0.43
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.50	0.43
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.00	0.43
2:B:4892:ARG:NH2	2:I:4898:GLY:O	2.52	0.43
2:G:4982:GLU:HB3	2:G:4983:HIS:H	1.67	0.43
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.41	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:4571:PHE:O	2:I:4575:PHE:N	2.50	0.43
2:B:887:ILE:HG21	2:B:959:TYR:HA	2.00	0.43
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	2.00	0.43
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.00	0.43
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.52	0.43
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	2.01	0.43
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.01	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	2.00	0.43
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.00	0.42
2:E:2103:VAL:O	2:E:2107:GLN:N	2.46	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.51	0.42
1:F:23:VAL:HG22	1:F:47:LYS:HG2	2.01	0.42
1:F:30:LEU:HD23	1:F:33:GLY:HA3	2.01	0.42
2:B:266:ARG:NH1	2:B:332:GLU:OE2	2.51	0.42
2:I:4729:GLY:HA2	2:I:4737:ILE:HG13	1.99	0.42
1:H:30:LEU:HD23	1:H:33:GLY:HA3	2.01	0.42
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.52	0.42
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	2.02	0.42
2:E:4982:GLU:HB3	2:E:4983:HIS:H	1.67	0.42
2:E:4984:ASN:C	2:E:4986:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.52	0.42
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	2.00	0.42
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	2.01	0.42
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.42
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.00	0.42
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.50	0.42
2:I:485:SER:O	2:I:489:ASN:N	2.39	0.42
2:G:224:HIS:N	2:G:229:GLU:O	2.46	0.42
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.42
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.50	0.42
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.52	0.42
2:G:2159:LEU:HD22	2:G:2201:LEU:HD23	1.99	0.42
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.52	0.42
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.47	0.42
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	2.02	0.42
2:G:235:ALA:HA	2:G:257:ARG:HD3	2.01	0.42
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	2.01	0.42
2:G:4984:ASN:C	2:G:4986:ALA:H	2.22	0.42
2:B:4558:ASN:OD1	2:B:4558:ASN:N	2.51	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.53	0.42
2:I:4190:ILE:HD13	2:I:5026:ASP:OD2	2.19	0.42
1:A:30:LEU:HD23	1:A:33:GLY:HA3	2.01	0.42
1:H:23:VAL:HG22	1:H:47:LYS:HG2	2.01	0.42
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.53	0.42
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.51	0.42
1:J:30:LEU:HD23	1:J:33:GLY:HA3	2.01	0.42
2:B:3992:PHE:O	2:B:3996:PHE:N	2.42	0.42
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	2.01	0.42
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	2.01	0.42
2:G:3781:GLN:HA	2:G:3784:SER:HB3	2.02	0.42
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.53	0.42
2:I:621:ILE:O	2:I:625:LEU:N	2.48	0.42
2:B:206:CYS:SG	2:B:207:SER:N	2.93	0.41
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	2.02	0.41
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.02	0.41
2:B:4230:LYS:CD	2:B:4959:PHE:CE1	2.83	0.41
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.41
2:E:3781:GLN:HA	2:E:3784:SER:HB3	2.02	0.41
2:E:4189:ARG:NH1	2:E:5032:TYR:OH	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:940:GLY:O	2:I:1052:ASN:N	2.49	0.41
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.53	0.41
2:G:358:THR:HG21	2:G:382:GLY:HA2	2.02	0.41
2:G:1093:GLU:OE1	2:G:1201:HIS:NE2	2.49	0.41
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.53	0.41
2:G:2212:VAL:O	2:G:2216:GLY:N	2.45	0.41
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.02	0.41
2:B:4958:CYS:O	2:B:4958:CYS:SG	2.79	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.94	0.41
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.41
2:E:215:THR:HG22	2:E:273:HIS:HA	2.03	0.41
2:E:359:TYR:HA	2:E:376:ALA:HA	2.02	0.41
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.41	0.41
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.41
2:E:4958:CYS:O	2:E:4958:CYS:SG	2.79	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.03	0.41
2:B:215:THR:HG22	2:B:273:HIS:HA	2.03	0.41
2:E:206:CYS:SG	2:E:207:SER:N	2.93	0.41
2:E:1101:ARG:HH21	2:E:1115:LEU:HB3	1.86	0.41
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.92	0.41
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.03	0.41
2:G:615:ARG:NH2	2:G:1677:GLY:O	2.47	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.41
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:B:4189:ARG:NH1	2:B:5032:TYR:OH	2.53	0.41
2:E:1595:LEU:HD23	2:E:1595:LEU:HA	1.96	0.41
2:I:358:THR:HG21	2:I:382:GLY:HA2	2.02	0.41
2:I:707:VAL:HG23	2:I:713:SER:HB2	2.03	0.41
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.52	0.41
2:G:206:CYS:SG	2:G:207:SER:N	2.93	0.41
2:G:2265:LEU:O	2:G:2330:ARG:NH1	2.54	0.41
2:G:2339:VAL:HG12	2:G:2345:SER:H	1.86	0.41
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.03	0.41
2:E:358:THR:HG21	2:E:382:GLY:HA2	2.02	0.41
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	2.02	0.41
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.03	0.41
2:I:215:THR:HG22	2:I:273:HIS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.70	0.41
2:G:378:LEU:HD23	2:G:378:LEU:HA	1.88	0.41
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.94	0.41
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.41
2:B:168:ASP:HB3	2:B:199:LEU:HD22	2.02	0.41
2:B:2339:VAL:HG12	2:B:2345:SER:H	1.85	0.41
2:B:4865:LYS:HB2	2:B:4873:ASP:HB3	2.03	0.41
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.53	0.41
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.53	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:G:359:TYR:HA	2:G:376:ALA:HA	2.02	0.41
2:G:938:HIS:HB2	2:G:1054:GLU:HB2	2.03	0.41
2:G:940:GLY:O	2:G:1052:ASN:N	2.49	0.41
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.41
1:J:82:TYR:O	1:J:86:GLY:N	2.54	0.41
2:B:235:ALA:HA	2:B:257:ARG:HD3	2.01	0.41
2:B:938:HIS:HB2	2:B:1054:GLU:HB2	2.03	0.41
2:B:1708:ARG:HG2	2:B:1711:TYR:CE2	2.56	0.41
2:B:3781:GLN:HA	2:B:3784:SER:HB3	2.02	0.41
2:E:224:HIS:N	2:E:229:GLU:O	2.46	0.41
2:E:235:ALA:HA	2:E:257:ARG:HD3	2.01	0.41
2:E:2265:LEU:O	2:E:2330:ARG:NH1	2.54	0.41
2:E:2339:VAL:HG12	2:E:2345:SER:H	1.86	0.41
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.41
2:I:359:TYR:HA	2:I:376:ALA:HA	2.02	0.41
2:I:1101:ARG:HH21	2:I:1115:LEU:HB3	1.86	0.41
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.41
2:I:2543:UNK:O	2:I:2547:UNK:N	2.54	0.41
2:I:4958:CYS:O	2:I:4958:CYS:SG	2.79	0.41
2:I:4982:GLU:N	2:I:4982:GLU:OE1	2.54	0.41
2:G:707:VAL:HG23	2:G:713:SER:HB2	2.03	0.41
2:G:1708:ARG:HG2	2:G:1711:TYR:CE2	2.56	0.41
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	2.02	0.41
2:G:2742:THR:OG1	2:G:2811:GLU:OE1	2.35	0.41
2:G:4951:LYS:HE2	2:G:4951:LYS:HB3	1.96	0.41
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.88	0.41
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.94	0.41
2:B:2305:CYS:O	2:B:2324:ASN:ND2	2.54	0.41
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.03	0.41
2:E:1093:GLU:OE1	2:E:1201:HIS:NE2	2.49	0.41
2:E:2543:UNK:O	2:E:2547:UNK:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.86	0.41
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.41	0.41
2:I:2880:GLU:O	2:I:2884:ASN:N	2.53	0.41
2:G:1101:ARG:HH21	2:G:1115:LEU:HB3	1.86	0.41
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	2.03	0.41
2:G:4697:VAL:O	2:G:4701:TRP:N	2.50	0.41
2:G:4958:CYS:O	2:G:4958:CYS:SG	2.79	0.41
2:B:358:THR:HG21	2:B:382:GLY:HA2	2.02	0.40
2:B:707:VAL:HG23	2:B:713:SER:HB2	2.03	0.40
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	2.03	0.40
2:B:4968:PHE:CZ	2:B:4978:HIS:HE1	2.37	0.40
2:B:4982:GLU:OE1	2:B:4982:GLU:N	2.54	0.40
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	2.04	0.40
2:I:206:CYS:SG	2:I:207:SER:N	2.93	0.40
2:I:938:HIS:HB2	2:I:1054:GLU:HB2	2.03	0.40
2:I:4933:GLN:HG2	2:G:4930:ALA:HB2	2.03	0.40
2:I:4982:GLU:HB3	2:I:4983:HIS:H	1.67	0.40
2:G:215:THR:HG22	2:G:273:HIS:HA	2.03	0.40
2:G:575:LEU:HD22	2:G:609:CYS:HB3	2.03	0.40
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.03	0.40
1:H:82:TYR:O	1:H:86:GLY:N	2.54	0.40
1:H:92:PRO:HD3	2:G:627:PRO:HB2	2.02	0.40
2:B:1101:ARG:HH21	2:B:1115:LEU:HB3	1.86	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.95	0.40
2:B:4138:ASP:N	2:B:4138:ASP:OD1	2.52	0.40
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.02	0.40
2:E:4930:ALA:HB2	2:G:4933:GLN:HG2	2.03	0.40
2:I:1865:MET:N	2:I:1865:MET:SD	2.94	0.40
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	2.04	0.40
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	2.03	0.40
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.40
2:B:870:ILE:HD12	2:B:870:ILE:HA	1.92	0.40
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.86	0.40
2:E:378:LEU:HD23	2:E:378:LEU:HA	1.88	0.40
2:E:938:HIS:HB2	2:E:1054:GLU:HB2	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:1708:ARG:HG2	2:E:1711:TYR:CE2	2.56	0.40
2:E:3992:PHE:O	2:E:3996:PHE:N	2.42	0.40
2:E:4982:GLU:OE1	2:E:4982:GLU:N	2.54	0.40
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.94	0.40
2:I:560:ILE:HA	2:I:563:VAL:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2265:LEU:O	2:I:2330:ARG:NH1	2.54	0.40
2:I:2339:VAL:HG12	2:I:2345:SER:H	1.86	0.40
2:I:3781:GLN:HA	2:I:3784:SER:HB3	2.02	0.40
2:I:4697:VAL:O	2:I:4701:TRP:N	2.50	0.40
2:G:841:GLY:HA2	2:G:1073:ARG:HD2	2.04	0.40
2:G:1236:THR:OG1	2:G:1608:MET:SD	2.79	0.40
2:G:4865:LYS:HB2	2:G:4873:ASP:HB3	2.03	0.40
2:B:560:ILE:HA	2:B:563:VAL:HG12	2.04	0.40
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.03	0.40
2:B:2543:UNK:O	2:B:2547:UNK:N	2.54	0.40
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.02	0.40
2:E:841:GLY:HA2	2:E:1073:ARG:HD2	2.04	0.40
2:E:2212:VAL:O	2:E:2216:GLY:N	2.45	0.40
2:I:3992:PHE:O	2:I:3996:PHE:N	2.42	0.40
2:G:4189:ARG:NH1	2:G:5032:TYR:OH	2.53	0.40
2:B:2212:VAL:O	2:B:2216:GLY:N	2.45	0.40
2:B:2265:LEU:O	2:B:2330:ARG:NH1	2.54	0.40
2:B:2880:GLU:O	2:B:2884:ASN:N	2.53	0.40
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	2.04	0.40
2:E:707:VAL:HG23	2:E:713:SER:HB2	2.03	0.40
2:E:2145:SER:HB2	2:E:3647:HIS:CE1	2.57	0.40
2:E:2305:CYS:O	2:E:2324:ASN:ND2	2.55	0.40
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	2.03	0.40
2:I:2305:CYS:O	2:I:2324:ASN:ND2	2.54	0.40
2:I:2780:ASN:O	2:I:2787:THR:OG1	2.31	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	105/108 (97%)	96 (91%)	9 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	H	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
1	J	105/108 (97%)	96 (91%)	9 (9%)	0	100	100
2	B	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
2	E	3235/4416 (73%)	2908 (90%)	321 (10%)	6 (0%)	47	81
2	G	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
2	I	3235/4416 (73%)	2906 (90%)	323 (10%)	6 (0%)	47	81
All	All	13360/18096 (74%)	12010 (90%)	1326 (10%)	24 (0%)	50	81

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	5028	PHE
2	E	5028	PHE
2	I	5028	PHE
2	G	5028	PHE
2	B	1708	ARG
2	B	4985	LEU
2	E	1708	ARG
2	E	4985	LEU
2	I	1708	ARG
2	I	4985	LEU
2	G	1708	ARG
2	G	4985	LEU
2	B	1840	PRO
2	E	1840	PRO
2	I	1840	PRO
2	G	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	I	4641	PRO
2	G	4641	PRO
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO

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	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3022 (82%)	2472 (99%)	21 (1%)	81 89
2	E	2493/3022 (82%)	2472 (99%)	21 (1%)	81 89
2	G	2493/3022 (82%)	2472 (99%)	21 (1%)	81 89
2	I	2493/3022 (82%)	2472 (99%)	21 (1%)	81 89
All	All	10324/12444 (83%)	10240 (99%)	84 (1%)	82 89

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	534	ARG
2	B	553	ARG
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4131	ARG
2	B	4166	LEU
2	B	4957	LYS
2	B	4958	CYS
2	B	4960	ILE

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Mol	Chain	Res	Type
2	B	4983	HIS
2	B	5027	CYS
2	E	131	LEU
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4131	ARG
2	E	4166	LEU
2	E	4957	LYS
2	E	4958	CYS
2	E	4960	ILE
2	E	4983	HIS
2	E	5027	CYS
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4131	ARG
2	I	4166	LEU
2	I	4957	LYS
2	I	4958	CYS
2	I	4960	ILE

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Mol	Chain	Res	Type
2	I	4983	HIS
2	I	5027	CYS
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4131	ARG
2	G	4166	LEU
2	G	4957	LYS
2	G	4958	CYS
2	G	4960	ILE
2	G	4983	HIS
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	43	ASN
1	F	87	HIS
1	A	43	ASN
1	A	87	HIS
1	H	43	ASN
1	H	87	HIS
1	J	43	ASN
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	224	HIS
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	582	HIS

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Mol	Chain	Res	Type
2	B	1041	GLN
2	B	1598	GLN
2	B	1688	HIS
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2041	HIS
2	B	3809	ASN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	4034	ASN
2	B	4120	ASN
2	B	4806	ASN
2	B	4973	HIS
2	B	4983	HIS
2	E	57	ASN
2	E	111	HIS
2	E	224	HIS
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	582	HIS
2	E	1041	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2041	HIS
2	E	3781	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN

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Mol	Chain	Res	Type
2	E	4034	ASN
2	E	4120	ASN
2	E	4806	ASN
2	E	4973	HIS
2	E	4983	HIS
2	I	57	ASN
2	I	111	HIS
2	I	224	HIS
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	582	HIS
2	I	1041	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2041	HIS
2	I	2884	ASN
2	I	3809	ASN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4120	ASN
2	I	4806	ASN
2	I	4973	HIS
2	I	4983	HIS
2	G	57	ASN
2	G	111	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	582	HIS
2	G	1041	GLN

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Mol	Chain	Res	Type
2	G	1598	GLN
2	G	1688	HIS
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2041	HIS
2	G	3781	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4120	ASN
2	G	4806	ASN
2	G	4973	HIS
2	G	4983	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CFF	I	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.41	2 (25%)
3	ATP	G	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
4	CFF	E	5102	-	8,15,15	2.57	3 (37%)	8,23,23	1.43	2 (25%)
3	ATP	I	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.34	5 (16%)
4	CFF	G	5102	-	8,15,15	2.59	3 (37%)	8,23,23	1.43	2 (25%)
4	CFF	B	5102	-	8,15,15	2.58	3 (37%)	8,23,23	1.42	2 (25%)
3	ATP	B	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)
3	ATP	E	5101	-	26,33,33	0.89	1 (3%)	31,52,52	1.35	5 (16%)

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
4	CFF	I	5102	-	-	-	0/2/2/2
3	ATP	G	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	E	5102	-	-	-	0/2/2/2
3	ATP	I	5101	-	-	5/18/38/38	0/3/3/3
4	CFF	G	5102	-	-	-	0/2/2/2
4	CFF	B	5102	-	-	-	0/2/2/2
3	ATP	B	5101	-	-	5/18/38/38	0/3/3/3
3	ATP	E	5101	-	-	5/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C5-C4	-4.82	1.33	1.39
4	I	5102	CFF	C5-C4	-4.82	1.33	1.39
4	E	5102	CFF	C5-C4	-4.81	1.33	1.39
4	B	5102	CFF	C5-C4	-4.81	1.33	1.39
4	I	5102	CFF	C6-N1	-4.19	1.32	1.38
4	B	5102	CFF	C6-N1	-4.13	1.32	1.38
4	G	5102	CFF	C6-N1	-4.13	1.32	1.38
4	E	5102	CFF	C6-N1	-4.12	1.32	1.38
4	G	5102	CFF	O13-C6	-2.42	1.18	1.24
4	B	5102	CFF	O13-C6	-2.41	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	5102	CFF	O13-C6	-2.41	1.18	1.24
4	E	5102	CFF	O13-C6	-2.38	1.18	1.24
3	E	5101	ATP	C5-C4	2.07	1.46	1.40
3	B	5101	ATP	C5-C4	2.04	1.46	1.40
3	G	5101	ATP	C5-C4	2.04	1.46	1.40
3	I	5101	ATP	C5-C4	2.02	1.46	1.40

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5101	ATP	N3-C2-N1	-3.25	123.60	128.68
3	E	5101	ATP	N3-C2-N1	-3.23	123.62	128.68
3	B	5101	ATP	N3-C2-N1	-3.22	123.64	128.68
3	I	5101	ATP	N3-C2-N1	-3.19	123.69	128.68
3	I	5101	ATP	PB-O3B-PG	-2.90	122.87	132.83
3	B	5101	ATP	PB-O3B-PG	-2.89	122.89	132.83
3	E	5101	ATP	PB-O3B-PG	-2.89	122.92	132.83
3	G	5101	ATP	PB-O3B-PG	-2.88	122.93	132.83
4	B	5102	CFF	C14-N7-C8	-2.77	112.09	125.43
4	I	5102	CFF	C14-N7-C8	-2.77	112.09	125.43
4	E	5102	CFF	C14-N7-C8	-2.77	112.11	125.43
4	G	5102	CFF	C14-N7-C8	-2.76	112.14	125.43
3	G	5101	ATP	PA-O3A-PB	-2.60	123.92	132.83
3	E	5101	ATP	PA-O3A-PB	-2.59	123.94	132.83
3	B	5101	ATP	PA-O3A-PB	-2.59	123.95	132.83
3	I	5101	ATP	PA-O3A-PB	-2.58	123.98	132.83
3	G	5101	ATP	C3'-C2'-C1'	2.44	104.65	100.98
3	B	5101	ATP	C3'-C2'-C1'	2.41	104.61	100.98
3	E	5101	ATP	C3'-C2'-C1'	2.40	104.60	100.98
3	I	5101	ATP	C3'-C2'-C1'	2.39	104.58	100.98
4	E	5102	CFF	C5-C6-N1	2.29	120.64	118.20
4	G	5102	CFF	C5-C6-N1	2.29	120.64	118.20
4	B	5102	CFF	C5-C6-N1	2.25	120.60	118.20
4	I	5102	CFF	C5-C6-N1	2.24	120.59	118.20
3	G	5101	ATP	C4-C5-N7	-2.21	107.10	109.40
3	E	5101	ATP	C4-C5-N7	-2.19	107.11	109.40
3	B	5101	ATP	C4-C5-N7	-2.17	107.14	109.40
3	I	5101	ATP	C4-C5-N7	-2.13	107.18	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	C5'-O5'-PA-O3A
3	E	5101	ATP	C5'-O5'-PA-O3A
3	I	5101	ATP	C5'-O5'-PA-O3A
3	G	5101	ATP	C5'-O5'-PA-O3A
3	B	5101	ATP	O4'-C4'-C5'-O5'
3	E	5101	ATP	O4'-C4'-C5'-O5'
3	I	5101	ATP	O4'-C4'-C5'-O5'
3	G	5101	ATP	O4'-C4'-C5'-O5'
3	B	5101	ATP	C3'-C4'-C5'-O5'
3	E	5101	ATP	C3'-C4'-C5'-O5'
3	I	5101	ATP	C3'-C4'-C5'-O5'
3	G	5101	ATP	C3'-C4'-C5'-O5'
3	B	5101	ATP	C4'-C5'-O5'-PA
3	E	5101	ATP	C4'-C5'-O5'-PA
3	I	5101	ATP	C4'-C5'-O5'-PA
3	G	5101	ATP	C4'-C5'-O5'-PA
3	B	5101	ATP	C5'-O5'-PA-O1A
3	E	5101	ATP	C5'-O5'-PA-O1A
3	I	5101	ATP	C5'-O5'-PA-O1A
3	G	5101	ATP	C5'-O5'-PA-O1A

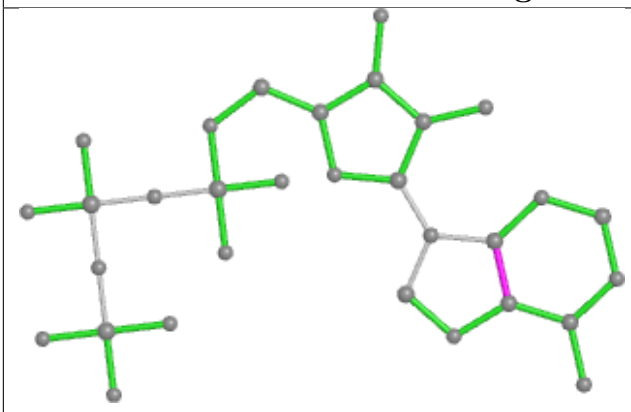
There are no ring outliers.

4 monomers are involved in 8 short contacts:

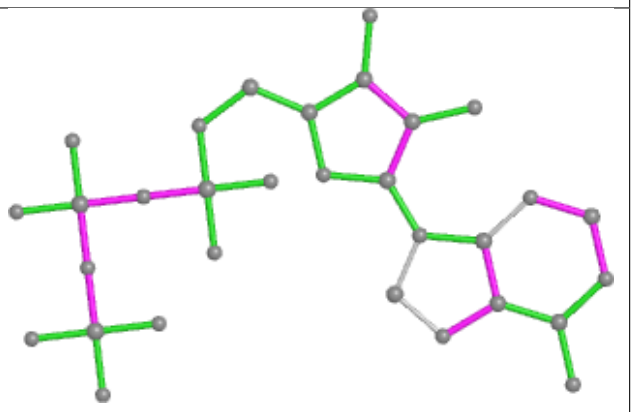
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	5101	ATP	2	0
3	I	5101	ATP	2	0
3	B	5101	ATP	2	0
3	E	5101	ATP	2	0

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

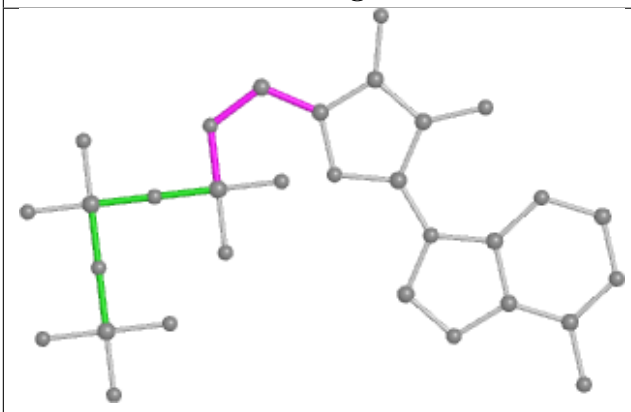
Ligand ATP G 5101



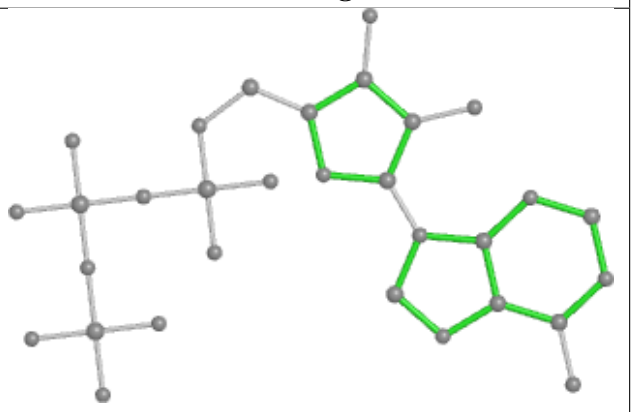
Bond lengths



Bond angles

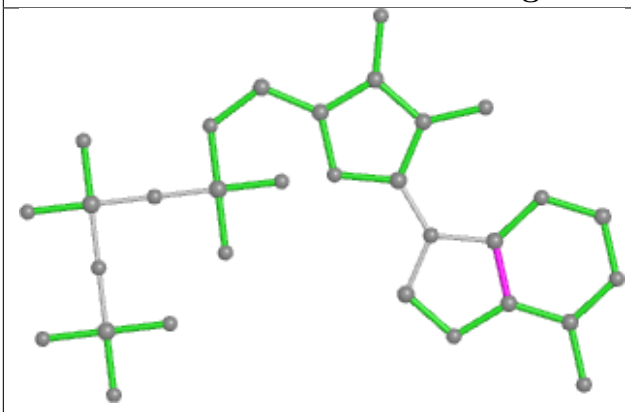


Torsions

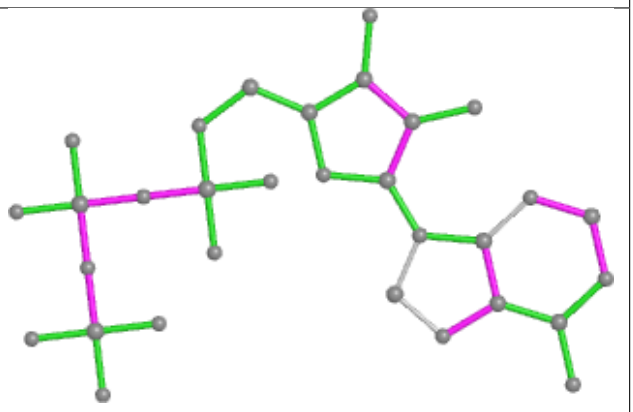


Rings

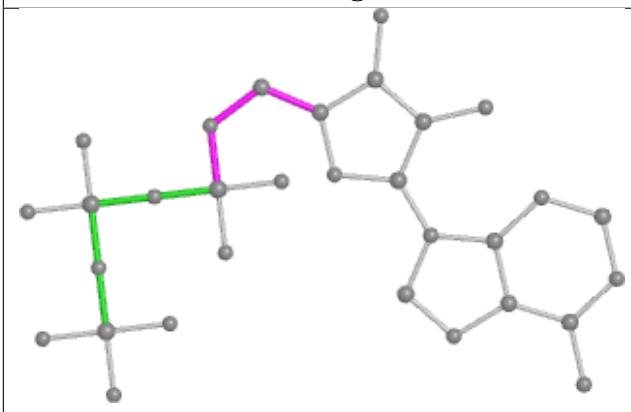
Ligand ATP I 5101



Bond lengths



Bond angles



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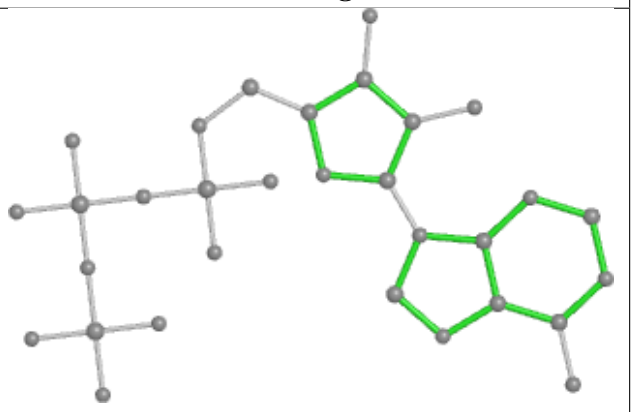
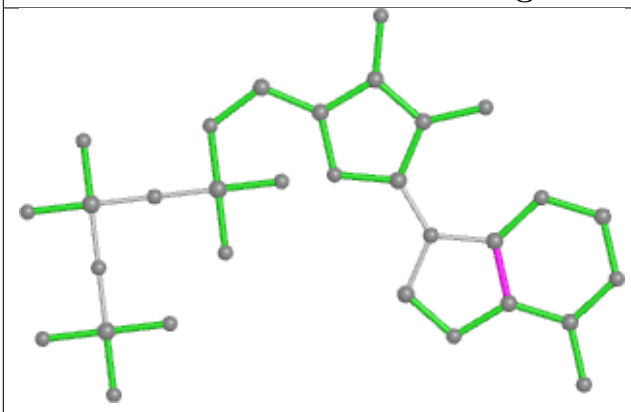
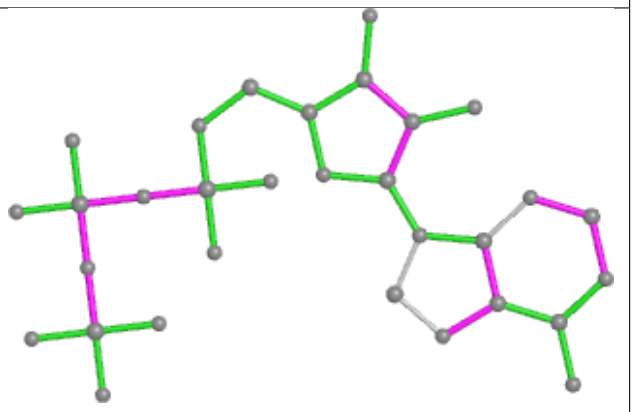


Rings

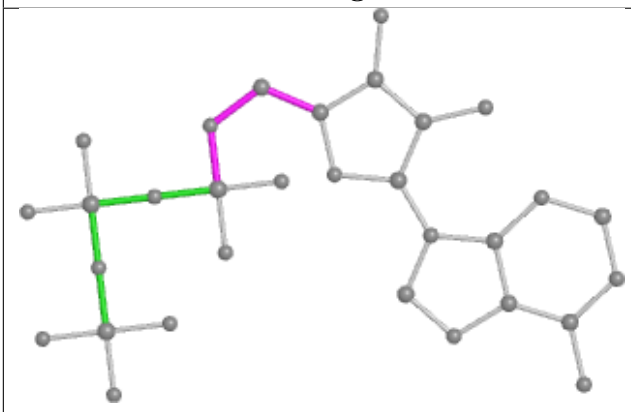
Ligand ATP B 5101



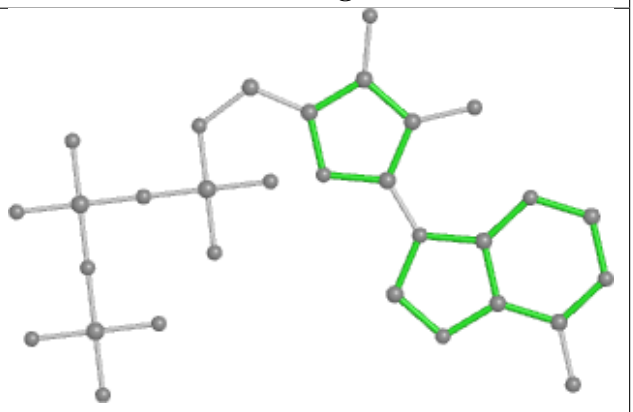
Bond lengths



Bond angles

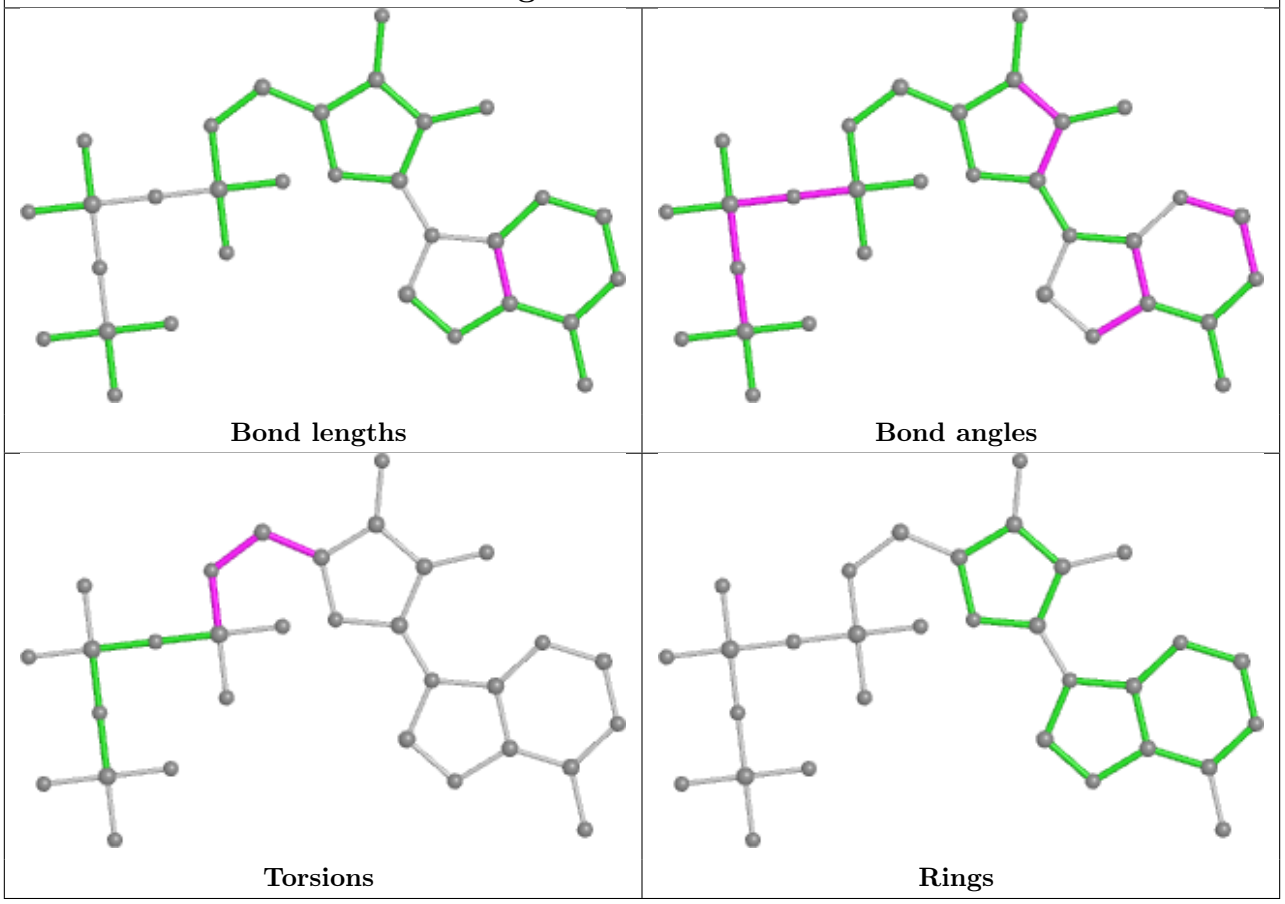


Torsions



Rings

Ligand ATP E 5101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	14
2	E	14
2	I	14
2	G	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	74.00
1	E	4345:UNK	C	4540:PHE	N	74.00

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	74.00
1	G	4345:UNK	C	4540:PHE	N	74.00
1	B	3613:UNK	C	3639:THR	N	43.80
1	E	3613:UNK	C	3639:THR	N	43.80
1	I	3613:UNK	C	3639:THR	N	43.80
1	G	3613:UNK	C	3639:THR	N	43.80
1	B	4253:GLU	C	4320:UNK	N	26.28
1	E	4253:GLU	C	4320:UNK	N	26.28
1	I	4253:GLU	C	4320:UNK	N	26.28
1	G	4253:GLU	C	4320:UNK	N	26.28
1	G	3163:UNK	C	3170:UNK	N	16.13
1	B	3163:UNK	C	3170:UNK	N	16.12
1	E	3163:UNK	C	3170:UNK	N	16.12
1	I	3163:UNK	C	3170:UNK	N	16.12
1	B	3063:UNK	C	3134:UNK	N	15.30
1	E	3063:UNK	C	3134:UNK	N	15.30
1	I	3063:UNK	C	3134:UNK	N	15.30
1	G	3063:UNK	C	3134:UNK	N	15.30
1	B	3468:UNK	C	3511:UNK	N	14.89
1	E	3468:UNK	C	3511:UNK	N	14.89
1	I	3468:UNK	C	3511:UNK	N	14.89
1	G	3468:UNK	C	3511:UNK	N	14.89
1	B	2703:UNK	C	2734:ASN	N	13.90
1	E	2703:UNK	C	2734:ASN	N	13.90
1	I	2703:UNK	C	2734:ASN	N	13.90
1	G	2703:UNK	C	2734:ASN	N	13.90
1	B	3236:UNK	C	3241:UNK	N	13.63
1	E	3236:UNK	C	3241:UNK	N	13.63
1	I	3236:UNK	C	3241:UNK	N	13.63
1	G	3236:UNK	C	3241:UNK	N	13.63
1	B	2976:UNK	C	2995:UNK	N	12.77
1	E	2976:UNK	C	2995:UNK	N	12.77
1	I	2976:UNK	C	2995:UNK	N	12.77
1	G	2976:UNK	C	2995:UNK	N	12.77
1	B	1564:UNK	C	1573:MET	N	12.33
1	E	1564:UNK	C	1573:MET	N	12.33
1	I	1564:UNK	C	1573:MET	N	12.33
1	G	1564:UNK	C	1573:MET	N	12.33
1	B	3254:UNK	C	3261:UNK	N	8.26
1	E	3254:UNK	C	3261:UNK	N	8.26
1	I	3254:UNK	C	3261:UNK	N	8.26
1	G	3254:UNK	C	3261:UNK	N	8.26

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	1297:UNK	C	1430:UNK	N	6.06
1	G	1297:UNK	C	1430:UNK	N	6.06
1	B	1297:UNK	C	1430:UNK	N	6.05
1	I	1297:UNK	C	1430:UNK	N	6.05
1	B	2939:ARG	C	2942:UNK	N	3.63
1	E	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.63
1	G	2939:ARG	C	2942:UNK	N	3.63
1	B	2479:LEU	C	2487:UNK	N	3.24
1	E	2479:LEU	C	2487:UNK	N	3.24
1	I	2479:LEU	C	2487:UNK	N	3.24
1	G	2479:LEU	C	2487:UNK	N	3.24

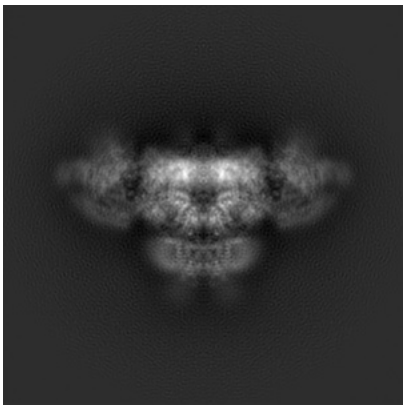
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8381. These allow visual inspection of the internal detail of the map and identification of artifacts.

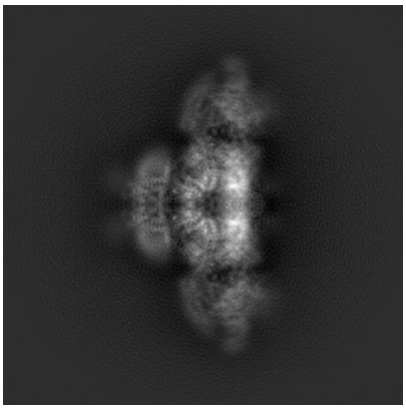
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

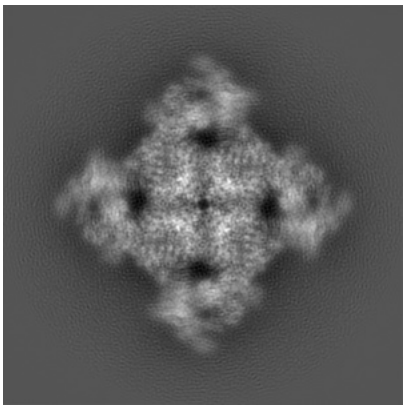
6.1.1 Primary map



X

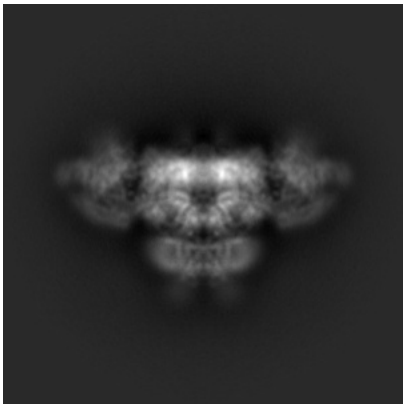


Y

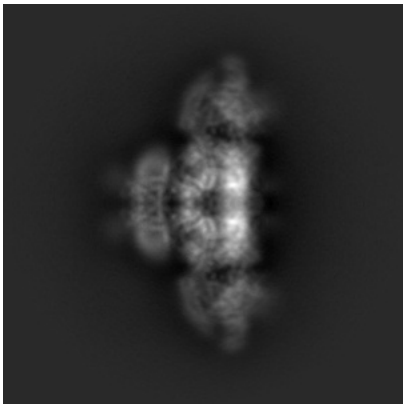


Z

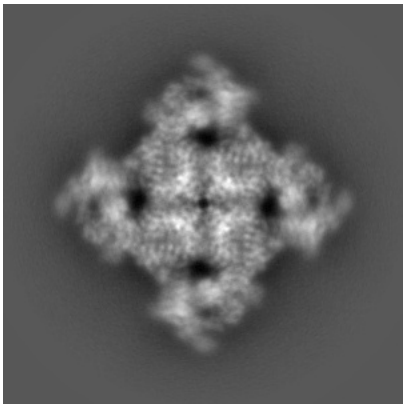
6.1.2 Raw map



X



Y

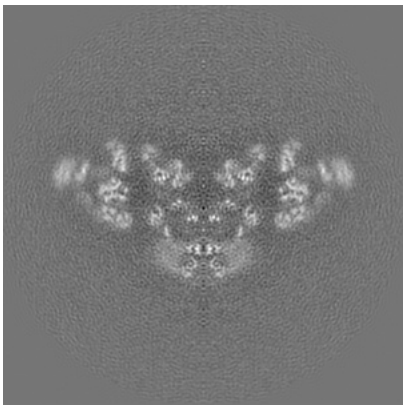


Z

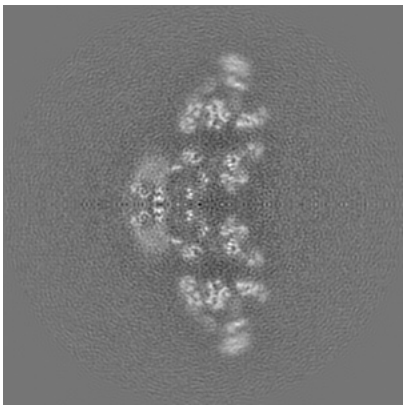
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

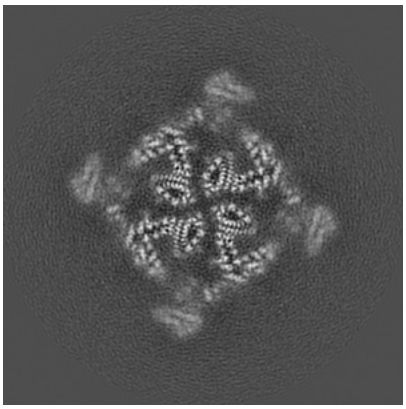
6.2.1 Primary map



X Index: 200

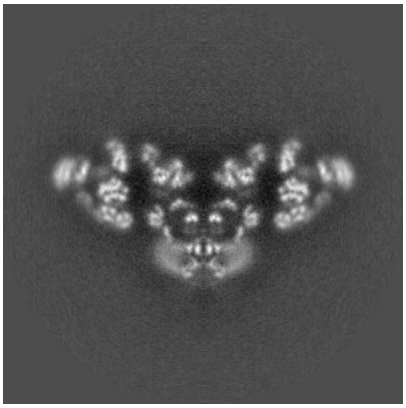


Y Index: 200

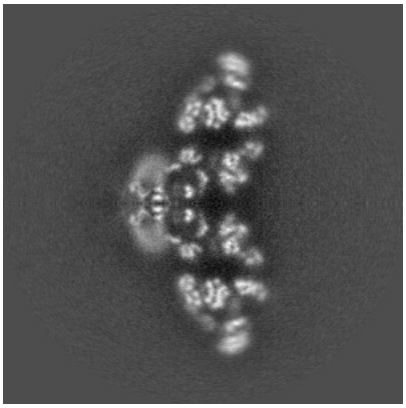


Z Index: 200

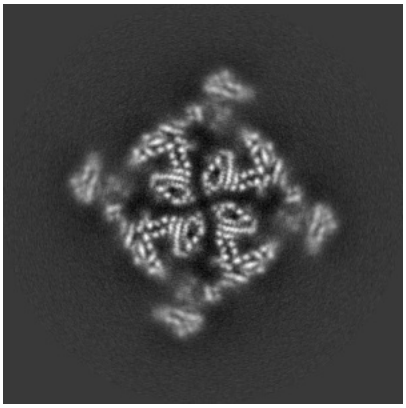
6.2.2 Raw map



X Index: 200



Y Index: 200

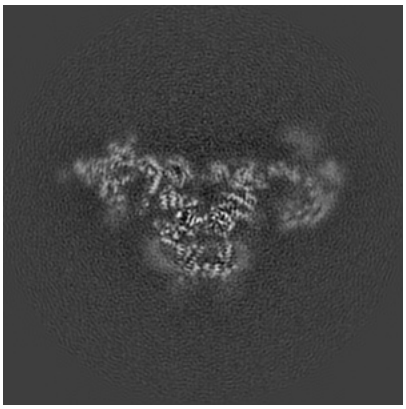


Z Index: 200

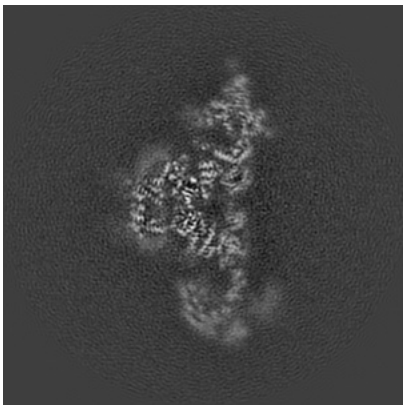
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

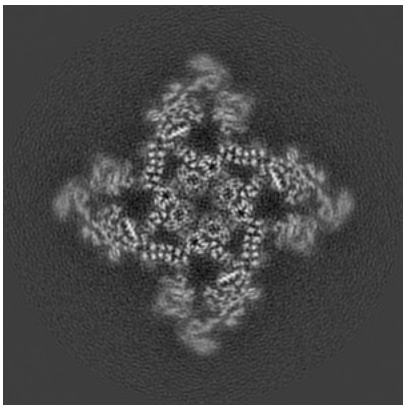
6.3.1 Primary map



X Index: 216

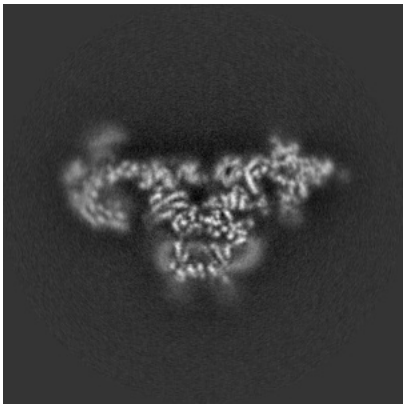


Y Index: 216

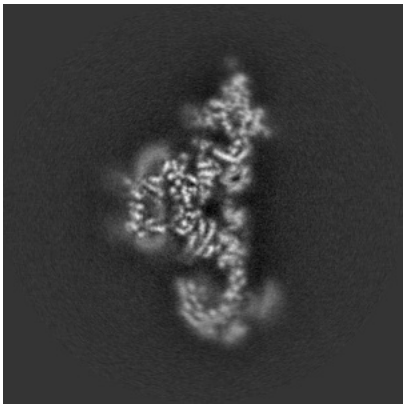


Z Index: 227

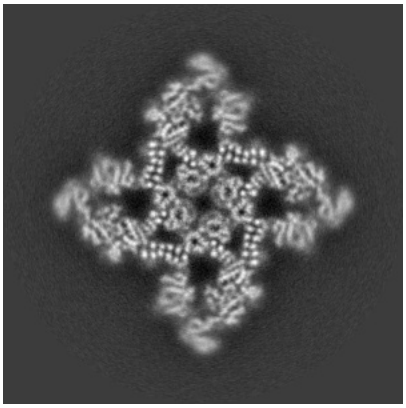
6.3.2 Raw map



X Index: 183



Y Index: 217

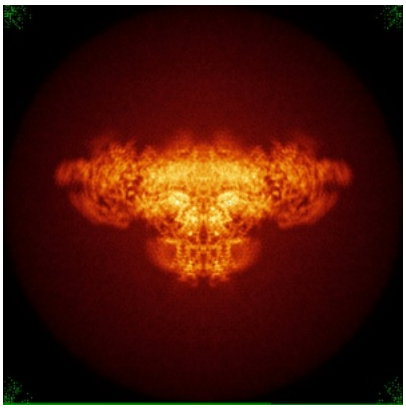


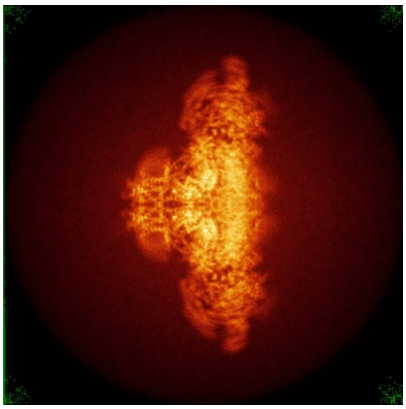
Z Index: 227

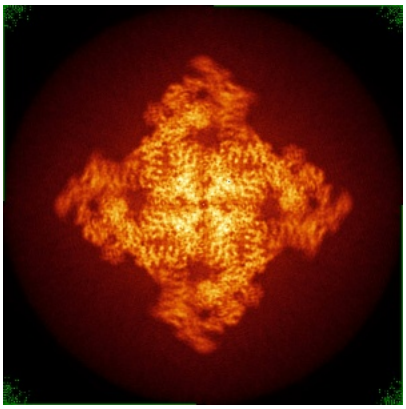
The images above show the largest variance slices of the map in three orthogonal directions.

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

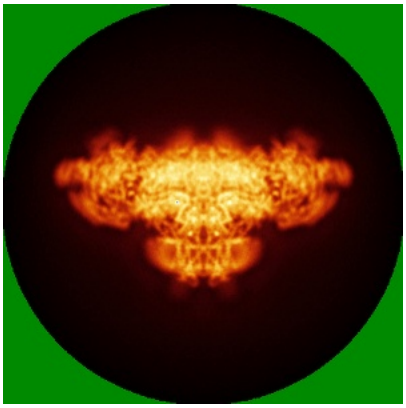
6.4.1 Primary map

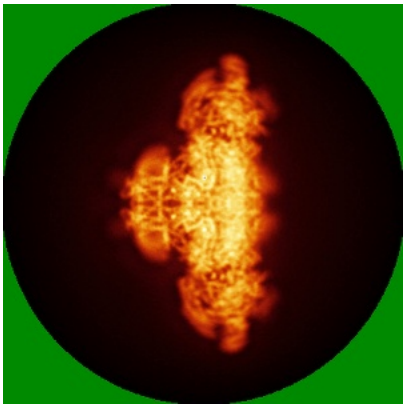

X

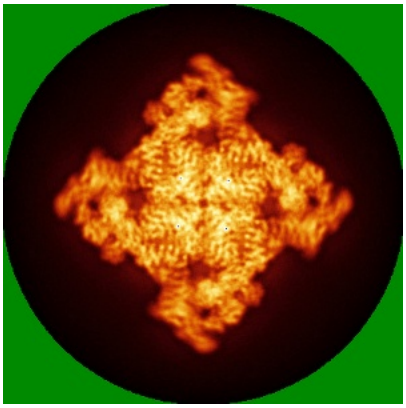

Y


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 0.035. 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.

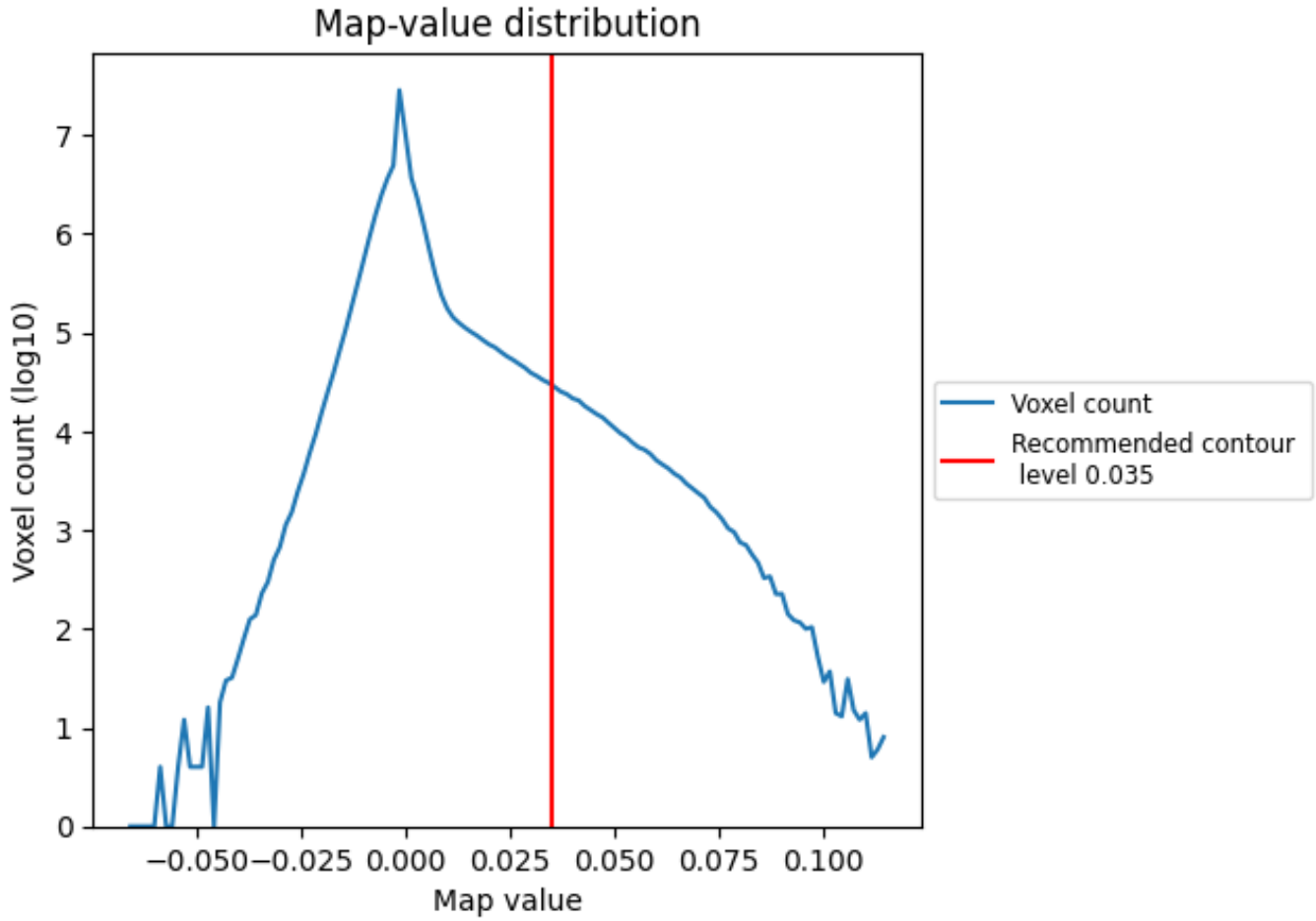
6.6 Mask visualisation (i)

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

7 Map analysis

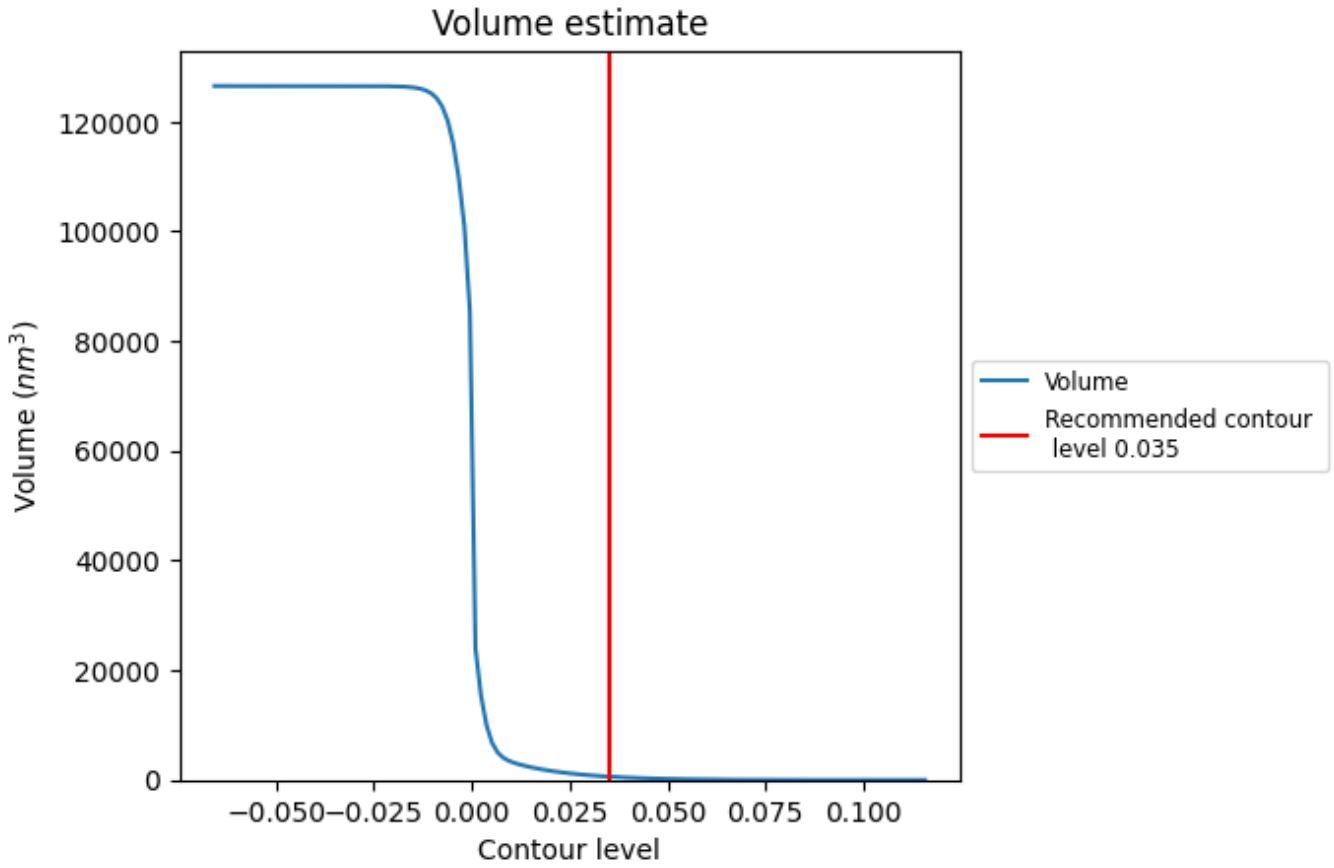
This section contains the results of statistical analysis of the map.

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.

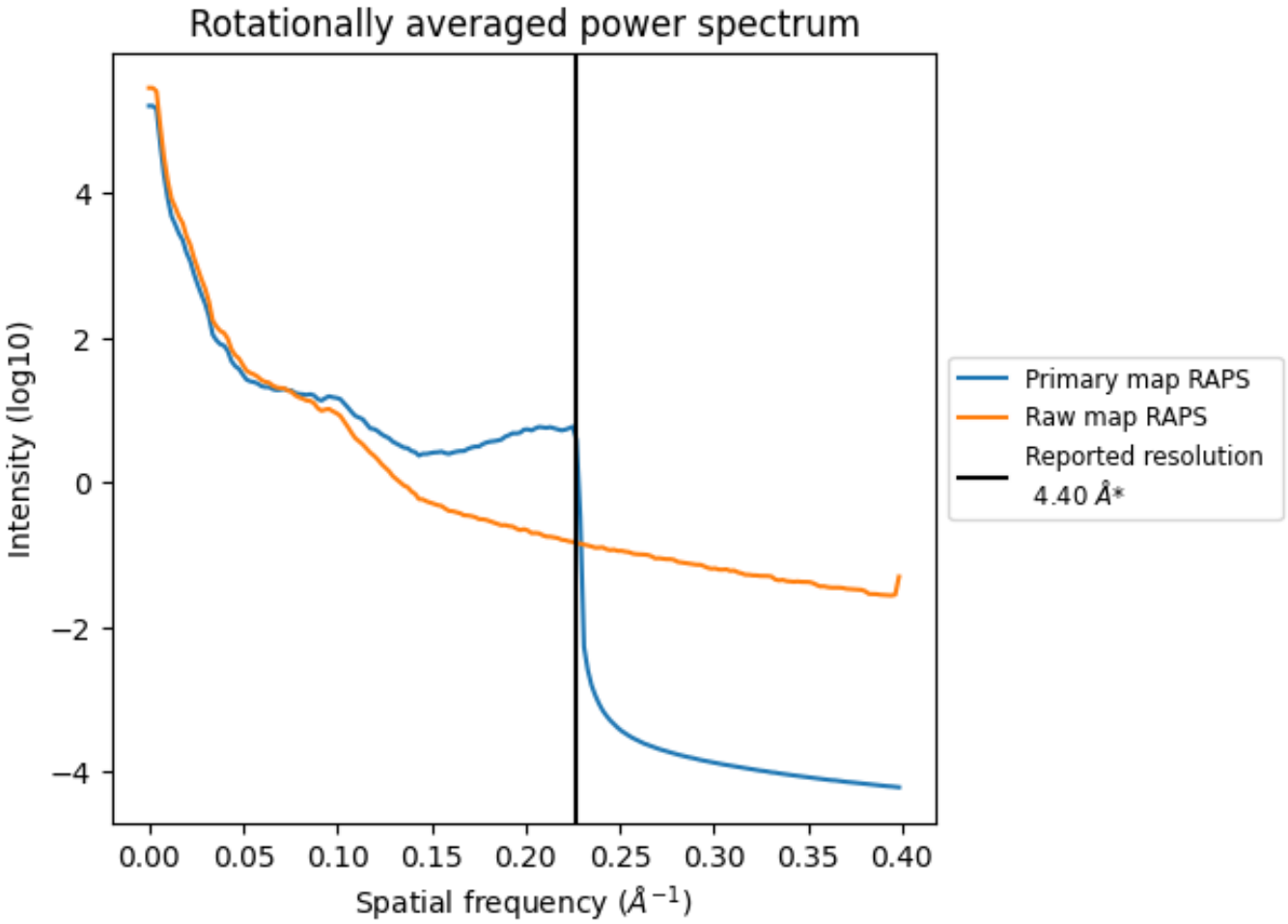
7.2 Volume estimate



The volume at the recommended contour level is 610 nm^3; this corresponds to an approximate mass of 551 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)

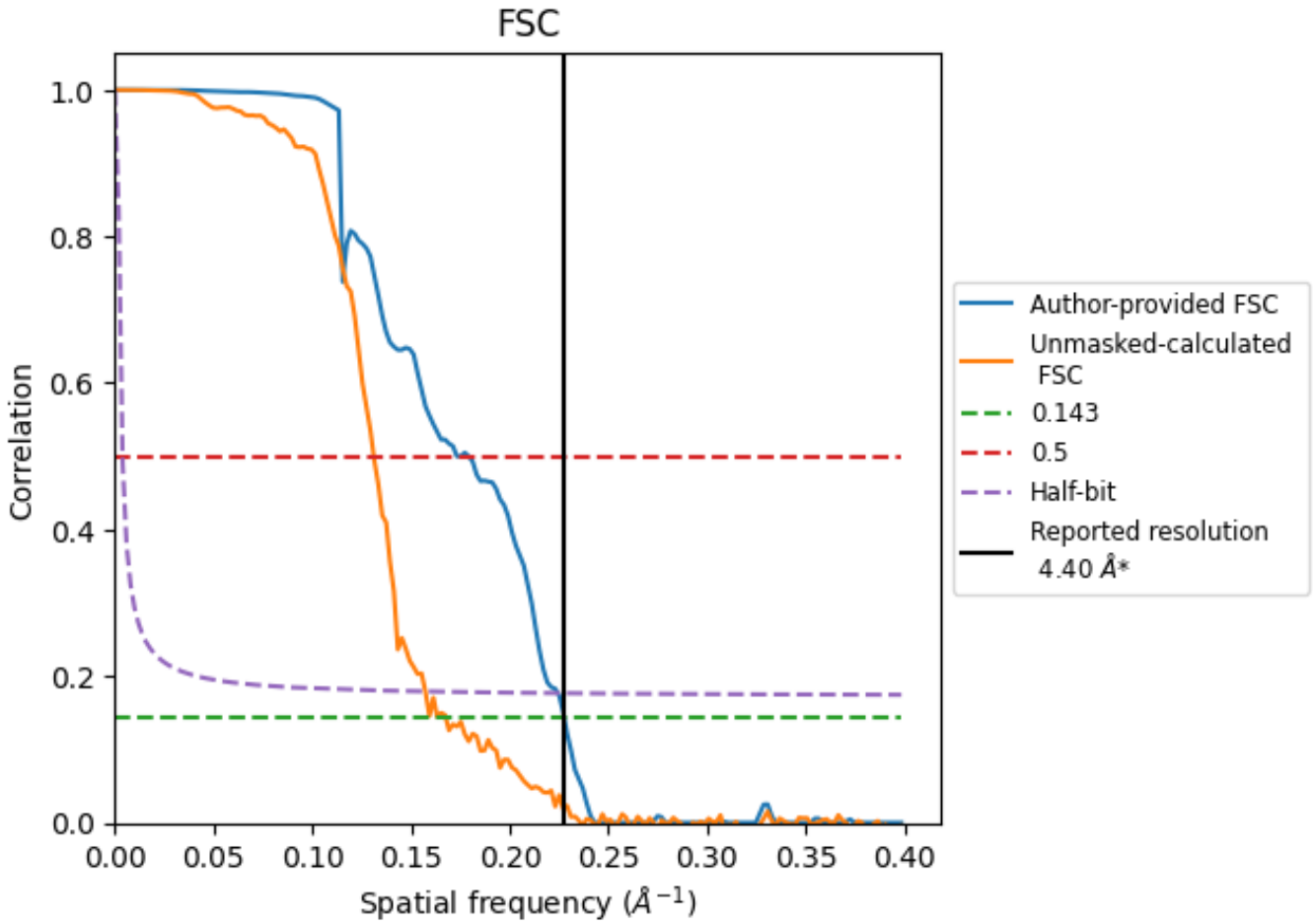


*Reported resolution corresponds to spatial frequency of 0.227 Å^{-1}

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 0.227 Å^{-1}

8.2 Resolution estimates (i)

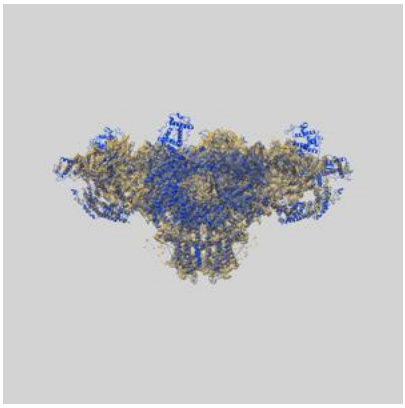
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.39	5.58	4.46
Unmasked-calculated*	5.96	7.62	6.36

*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 5.96 differs from the reported value 4.4 by more than 10 %

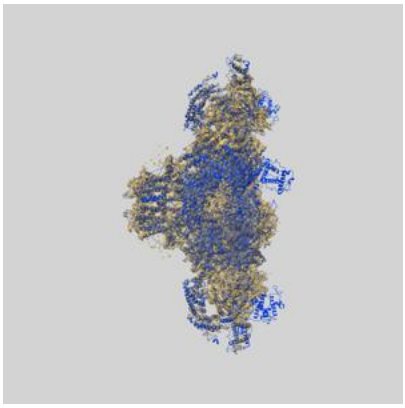
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8381 and PDB model 5TAP. Per-residue inclusion information can be found in section 3 on page 6.

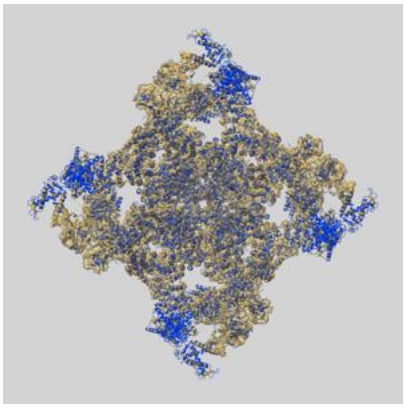
9.1 Map-model overlay



X



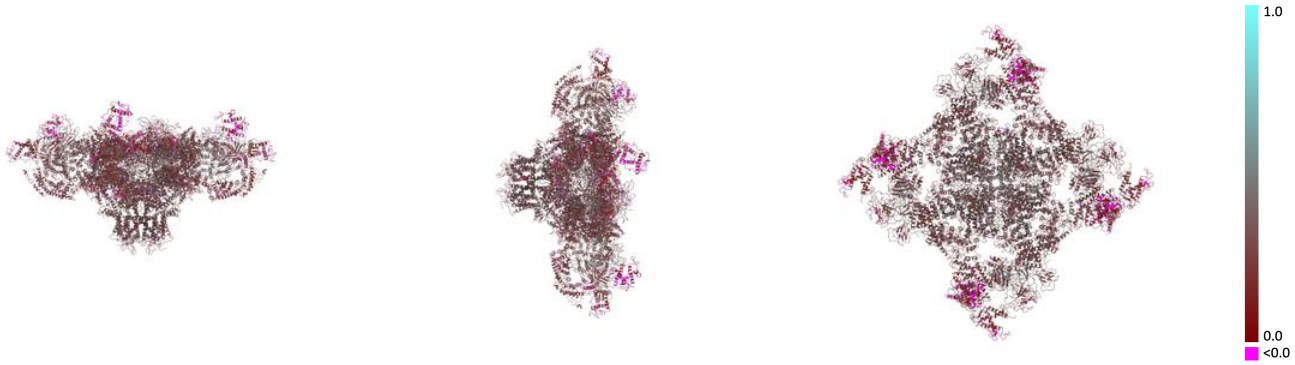
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.035 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.

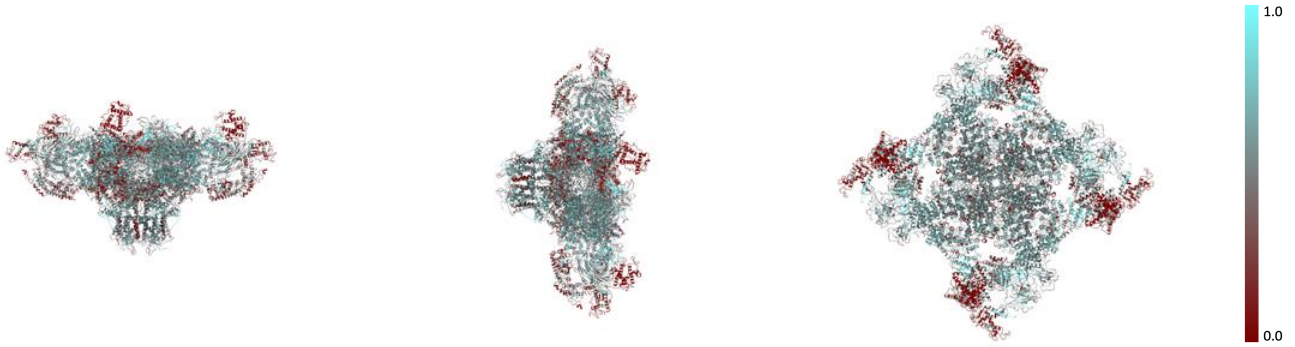
9.2 Q-score mapped to coordinate model (i)



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.

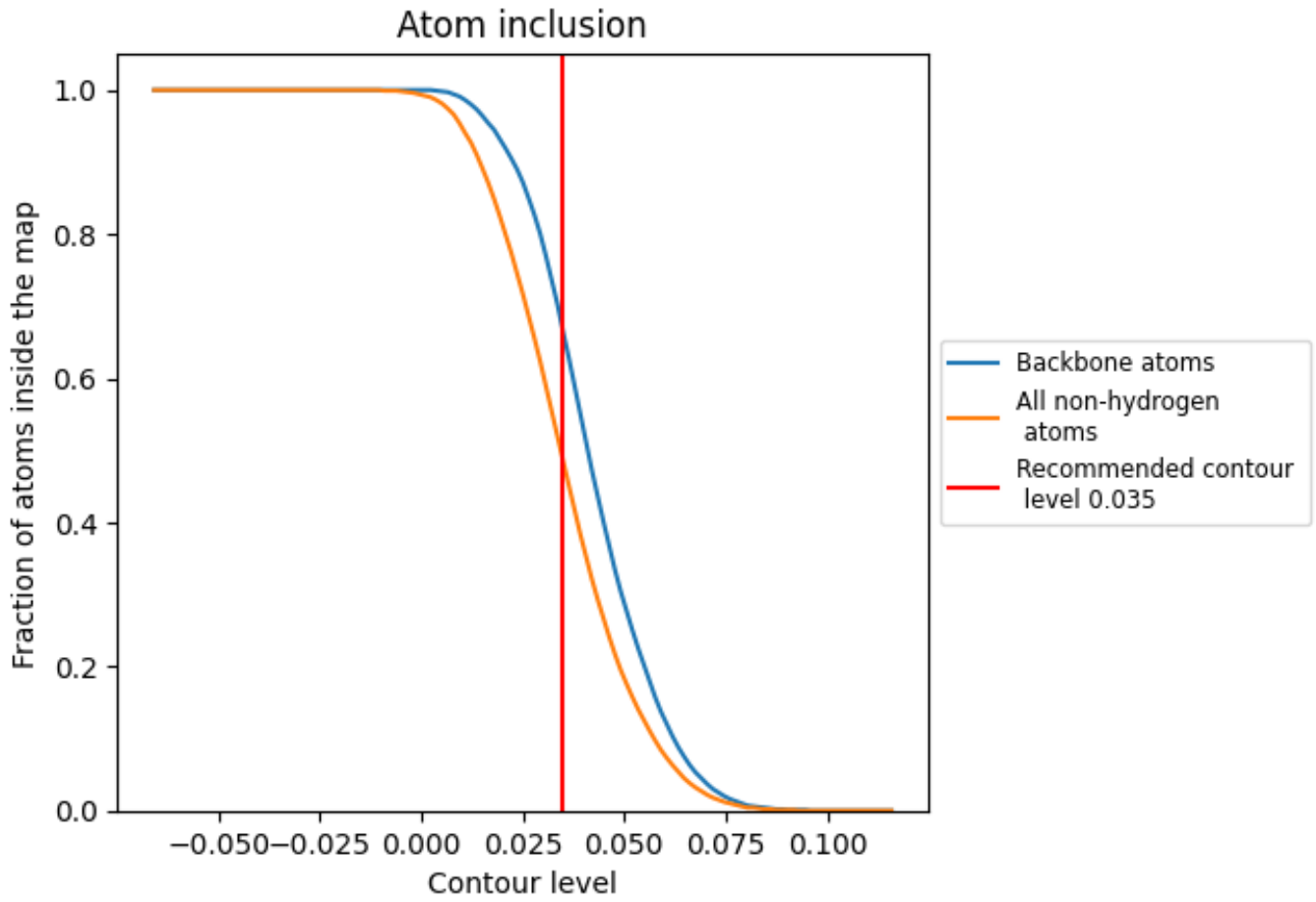
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.035).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 48% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4840	0.2940
A	0.4900	0.3030
B	0.4840	0.2940
E	0.4840	0.2930
F	0.4940	0.3070
G	0.4830	0.2930
H	0.4890	0.3040
I	0.4830	0.2930
J	0.4900	0.3020