Full wwPDB EM Validation Report ⓘ

Nov 2, 2022 – 05:59 AM EDT

PDB ID	:	5TAV
EMDB ID	:	EMD-8386
Title	:	Structure of rabbit RyR1 (Caffeine/ATP/EGTA dataset, class 4)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-10
Resolution	:	4.80 Å(reported)

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

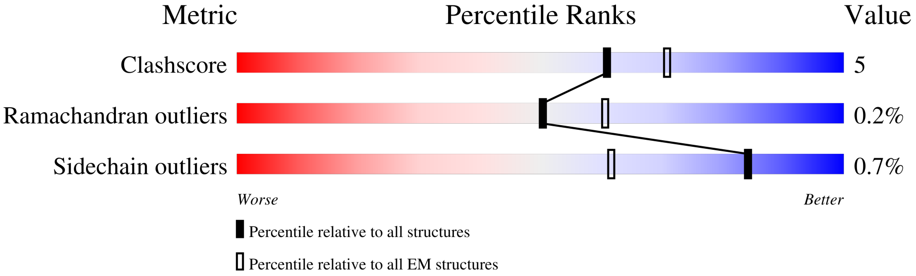
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

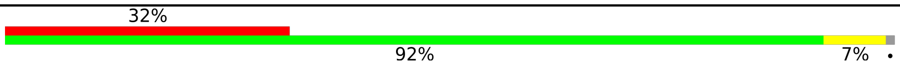
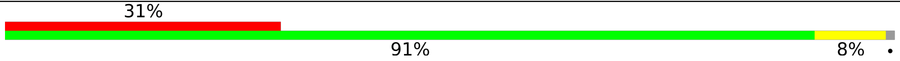
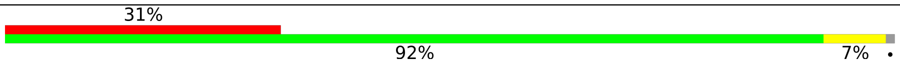
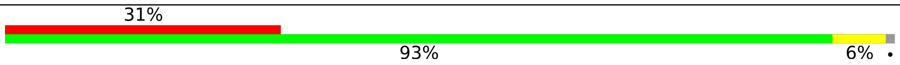
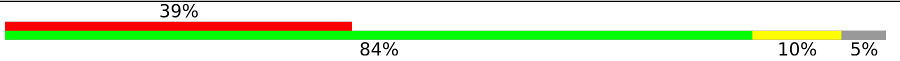
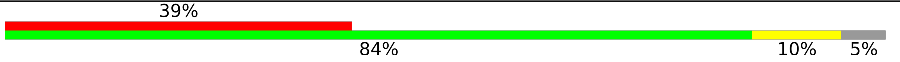
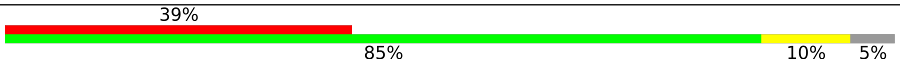
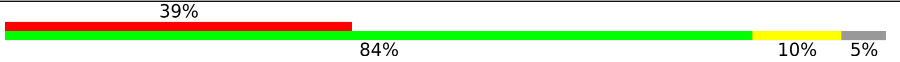
The reported resolution of this entry is 4.80 Å.

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	
1	F	108	
1	H	108	
1	J	108	
2	B	4416	
2	E	4416	
2	G	4416	
2	I	4416	

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.

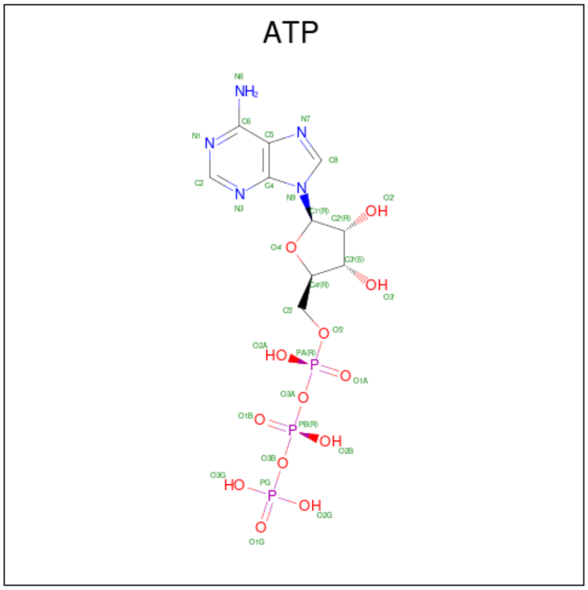
- Molecule 1 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 2 is a protein called Ryanodine receptor 1.

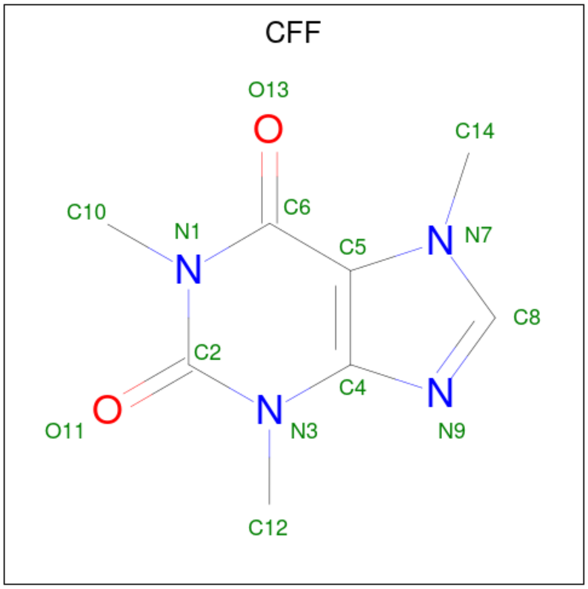
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total 29499	C 18686	N 5228	O 5428	S 157	0	0
2	E	4194	Total 29499	C 18686	N 5228	O 5428	S 157	0	0
2	I	4194	Total 29499	C 18686	N 5228	O 5428	S 157	0	0
2	G	4194	Total 29499	C 18686	N 5228	O 5428	S 157	0	0

- 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
			Total	C	N	O	P	
3	B	1	31	10	5	13	3	0
3	E	1	31	10	5	13	3	0
3	I	1	31	10	5	13	3	0
3	G	1	31	10	5	13	3	0

- 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 14 8 4 2	0
4	E	1	Total C N O 14 8 4 2	0
4	I	1	Total C N O 14 8 4 2	0
4	G	1	Total C N O 14 8 4 2	0

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

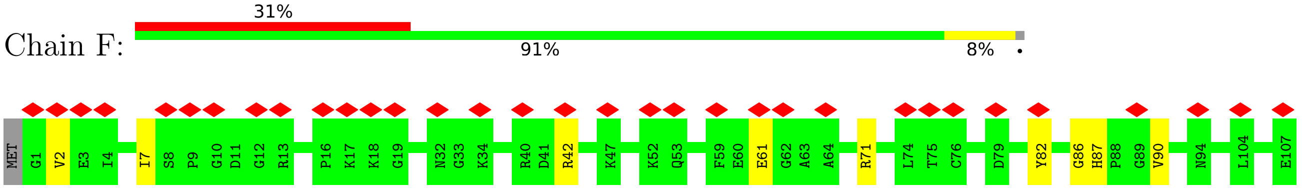
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Zn 1 1	0
5	E	1	Total Zn 1 1	0
5	I	1	Total Zn 1 1	0
5	G	1	Total Zn 1 1	0

3 Residue-property plots

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

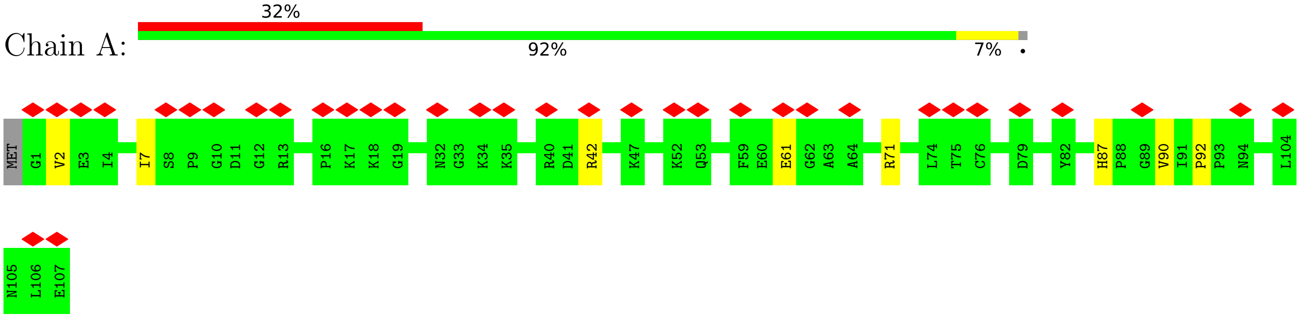
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



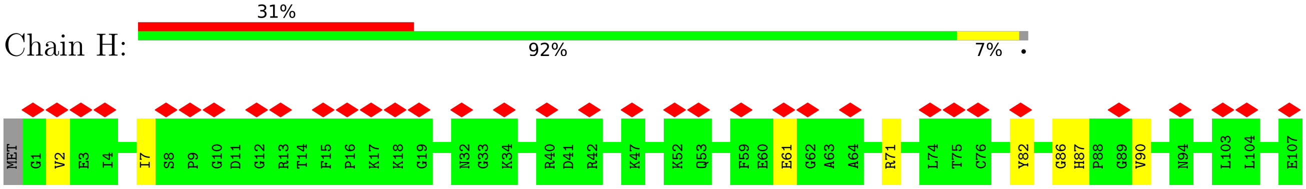
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



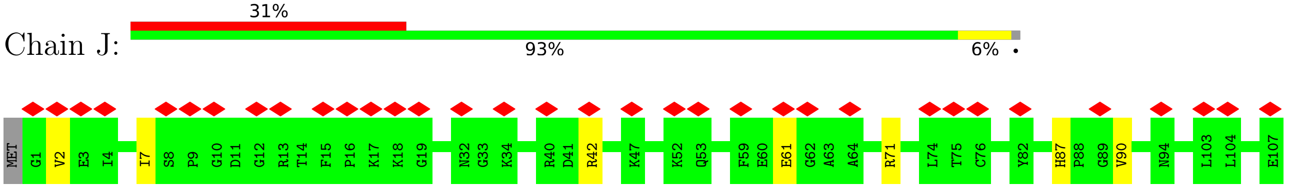
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



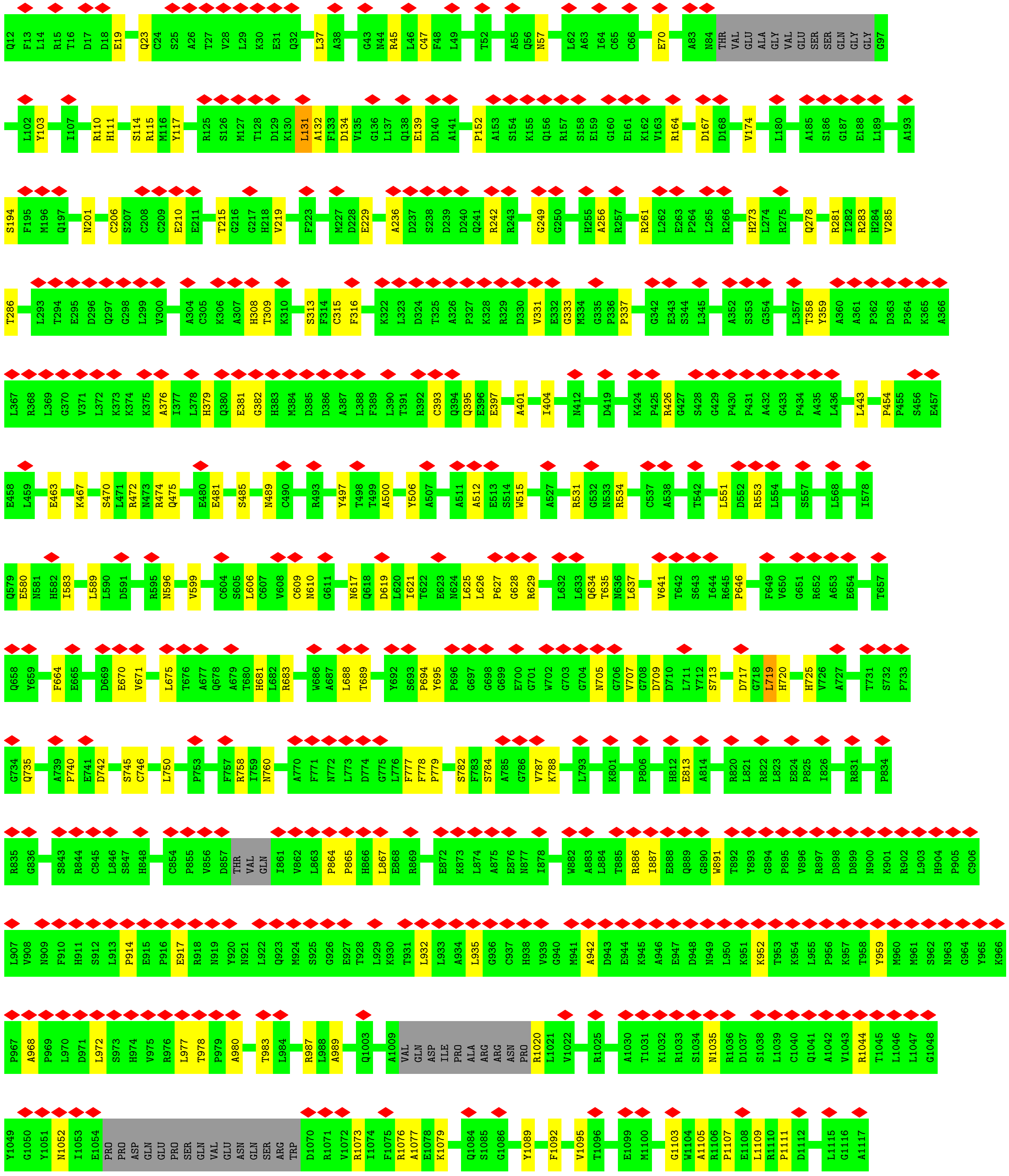
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J:



- Molecule 2: Ryanodine receptor 1

Chain B: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L102 Y103 I107 R110 H111 S114 R115 M116 Y117 R125 S126 M127 T128 D129 K130 L131 A132 F133 D134 V135 G136 L137 Q138 E139 D140 A141 P152 A153 S154 K155 Q156 R157 S158 E159 G160 E161 K162 V163 R164 D167 D168 V174 L180 A185 S186 G187 E188 L189 A193
S194 F195 M196 Q197 N201 C206 S207 C208 C209 E210 E211 T215 G216 G217 H218 V219 F223 M227 D228 E229 A236 D237 S238 D239 D240 Q241 R242 R243 G249 G250 H255 A256 R257 R261 L262 E263 P264 L265 R266 H273 L274 R275 Q278 R281 I282 R283 H284 V285
T286 L293 T294 E295 D296 Q297 G298 L299 V300 A304 C305 K306 A307 H308 T309 K310 S313 F314 C315 F316 K322 L323 D324 T325 A326 P327 K328 R329 D330 V331 E332 G333 M334 G335 P336 P337 G342 E343 S344 L345 A352 S353 G354 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366
L367 R368 L369 G370 V371 L372 K373 K374 K375 A376 I377 L378 H379 Q380 E381 G382 H383 M384 D385 D386 A387 L388 F389 L390 T391 R392 C393 Q394 Q395 E396 E397 A401 I404 N412 D419 K424 P425 R426 G427 S428 G429 P430 P431 A432 G433 P434 A435 L436 L443 P454 P455 S456 E457
E458 L459 E463 K467 S470 L471 R472 N473 R474 Q475 F480 E481 S485 N489 C490 R493 Y497 T498 T499 A500 Y506 A507 A511 A512 E513 S514 W515 A527 R531 G532 N533 R534 C537 A538 T542 L551 D552 R553 L554 S557 L568 I578
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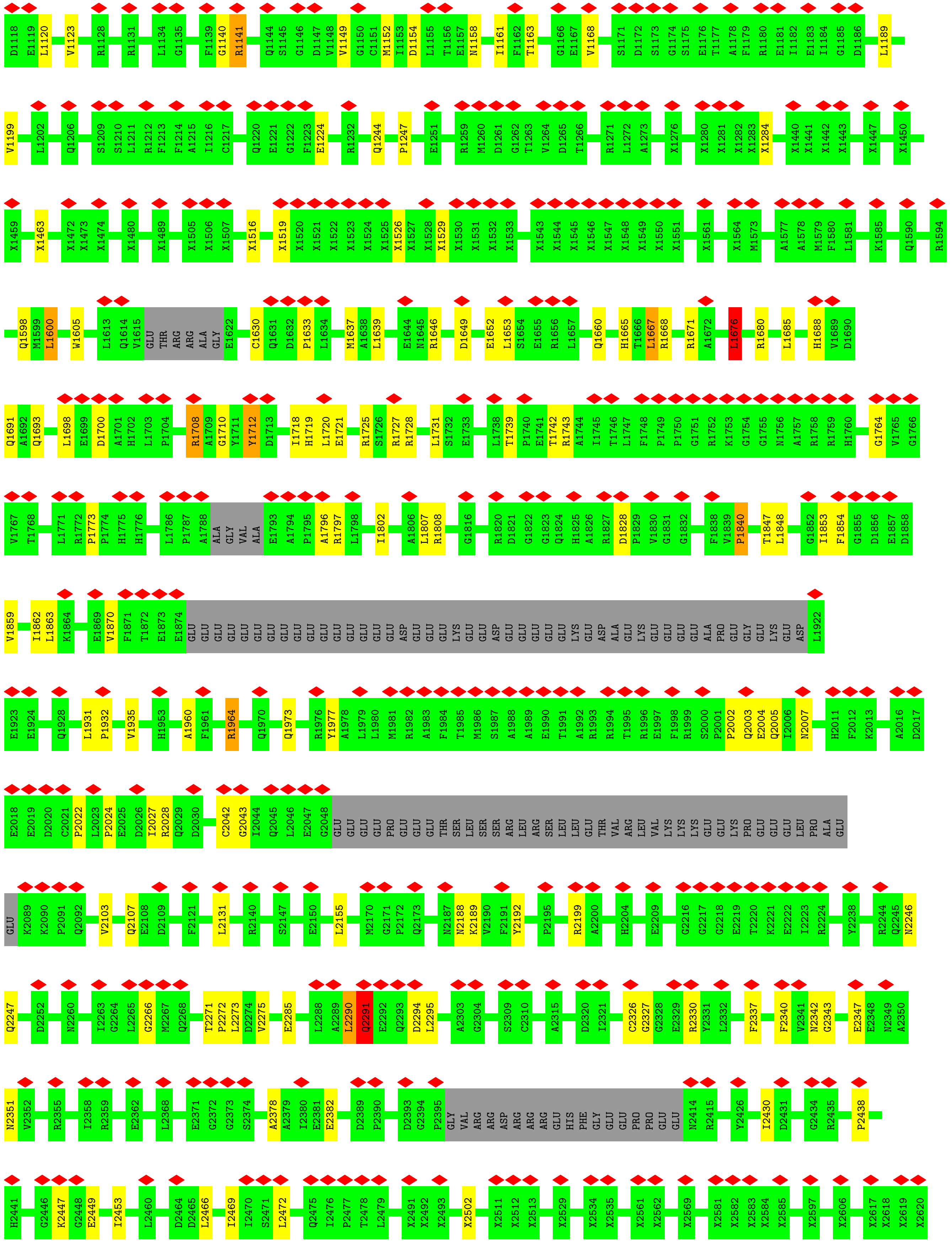
R835 G836 S843 R844 C845 L846 S847 H848 C854 P855 V856 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 E872 K873 L874 A875 E876 N877 I878 W882 A883 L884 T885 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906
L907 V908 N909 F910 H911 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 K957 T958 Y959 M960 M961 S962 N963 G964 Y965 K966
P967 A968 P969 L970 D971 L972 S973 H974 V975 R976 L977 T978 P979 A980 T983 L984 R987 L988 A989 Q1003 A1009 VAL GLN ASP ILE PRO ALA ARG ARG ASN PRO R1020 L1021 V1022 R1025 A1030 T1031 K1032 R1033 S1034 N1035 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 I1074 F1075 R1076 A1077 E1078 K1079 Q1084 S1085 G1086 Y1089 F1092 V1095 T1096 E1099 M1100 G1103 W1104 A1105 R1106 P1107 E1108 L1109 R1110 P1111 D1112 L1115 G1116 A1117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V1859 I1862 L1863 K1864 E1869 V1870 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922
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E2018 E2019 D2020 C2021 P2022 L2023 P2024 E2025 D2026 I2027 R2028 Q2029 D2030 C2042 G2043 I2044 Q2045 L2046 E2047 G2048 GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU
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N2351 V2352 R2355 I2358 R2359 E2362 L2368 E2371 G2372 G2373 S2374 A2378 A2379 I2380 E2381 E2382 D2389 P2390 D2393 G2394 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 R2415 Y2426 I2430 D2431 G2434 R2435 P2438
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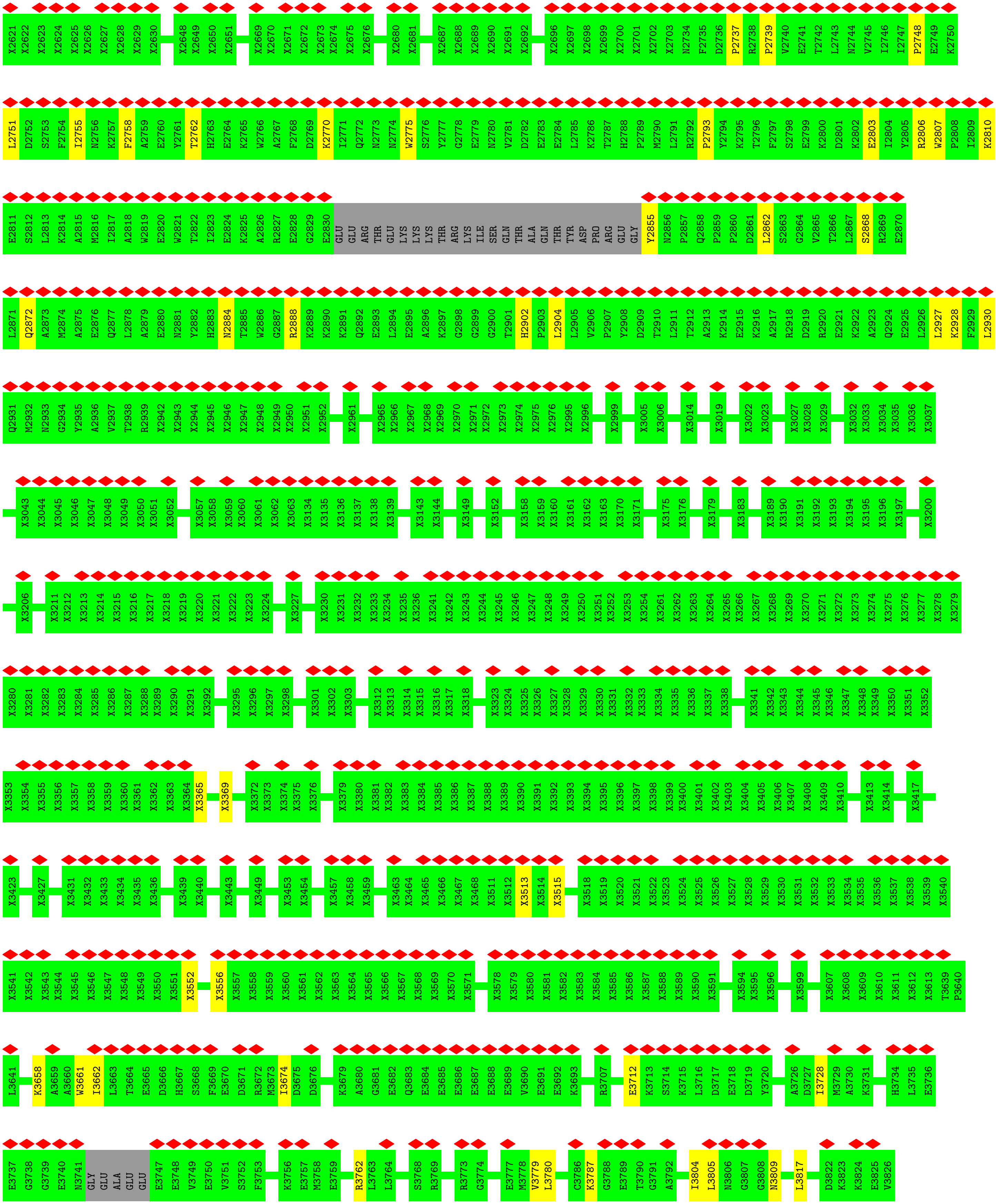
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E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870
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- Molecule 2: Ryanodine receptor 1

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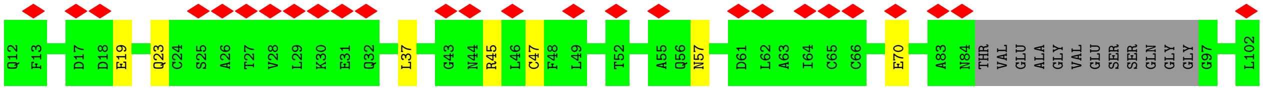

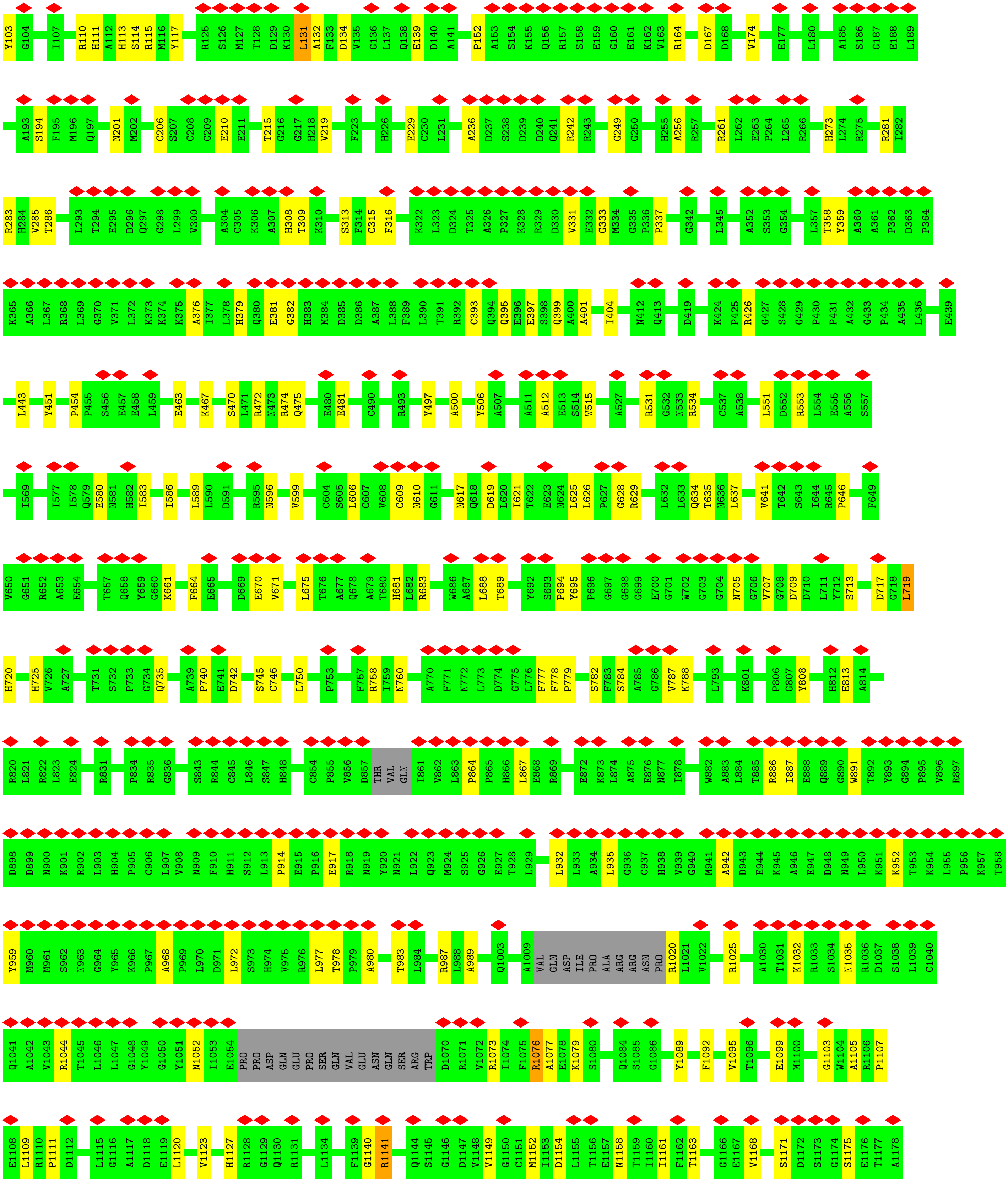
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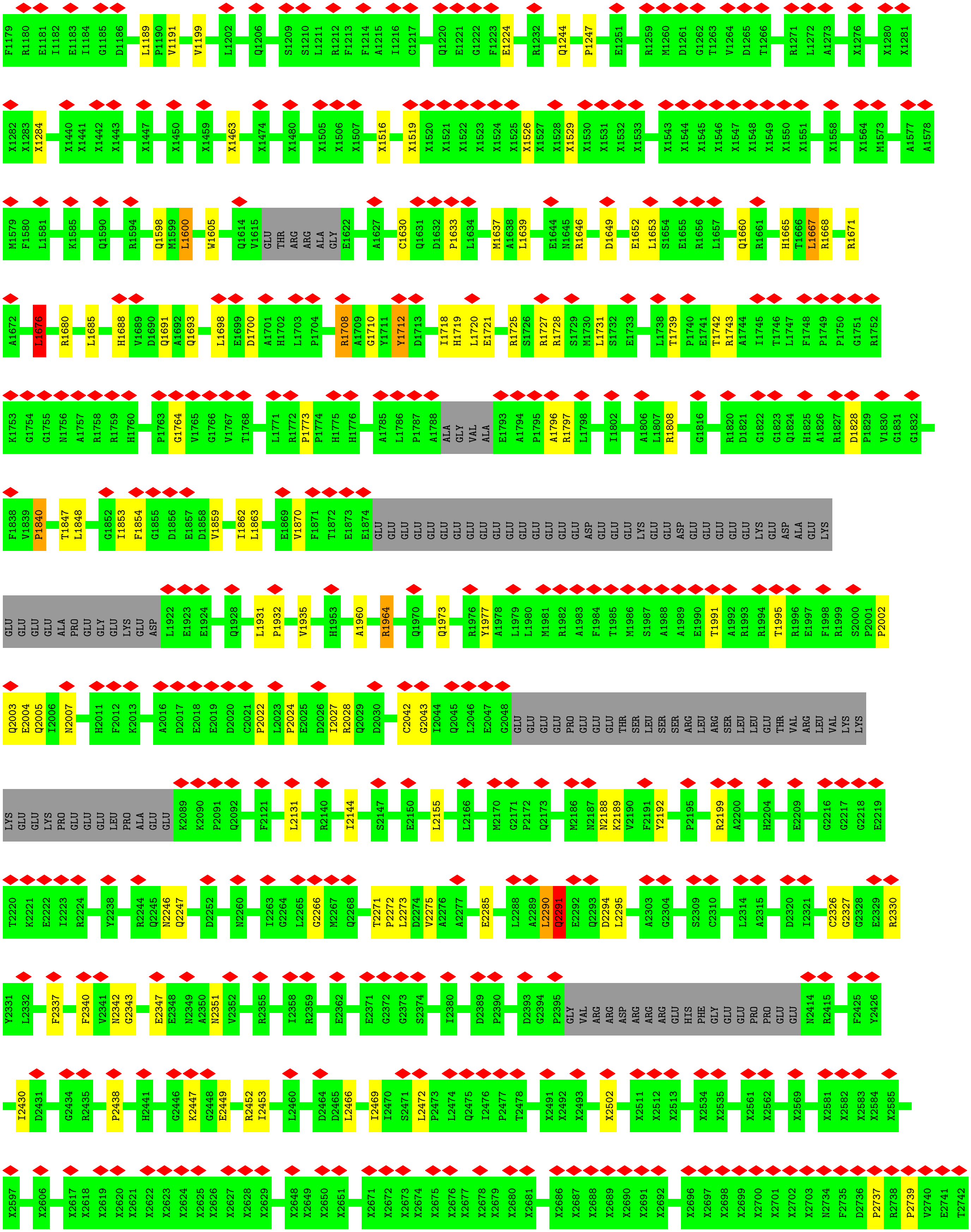
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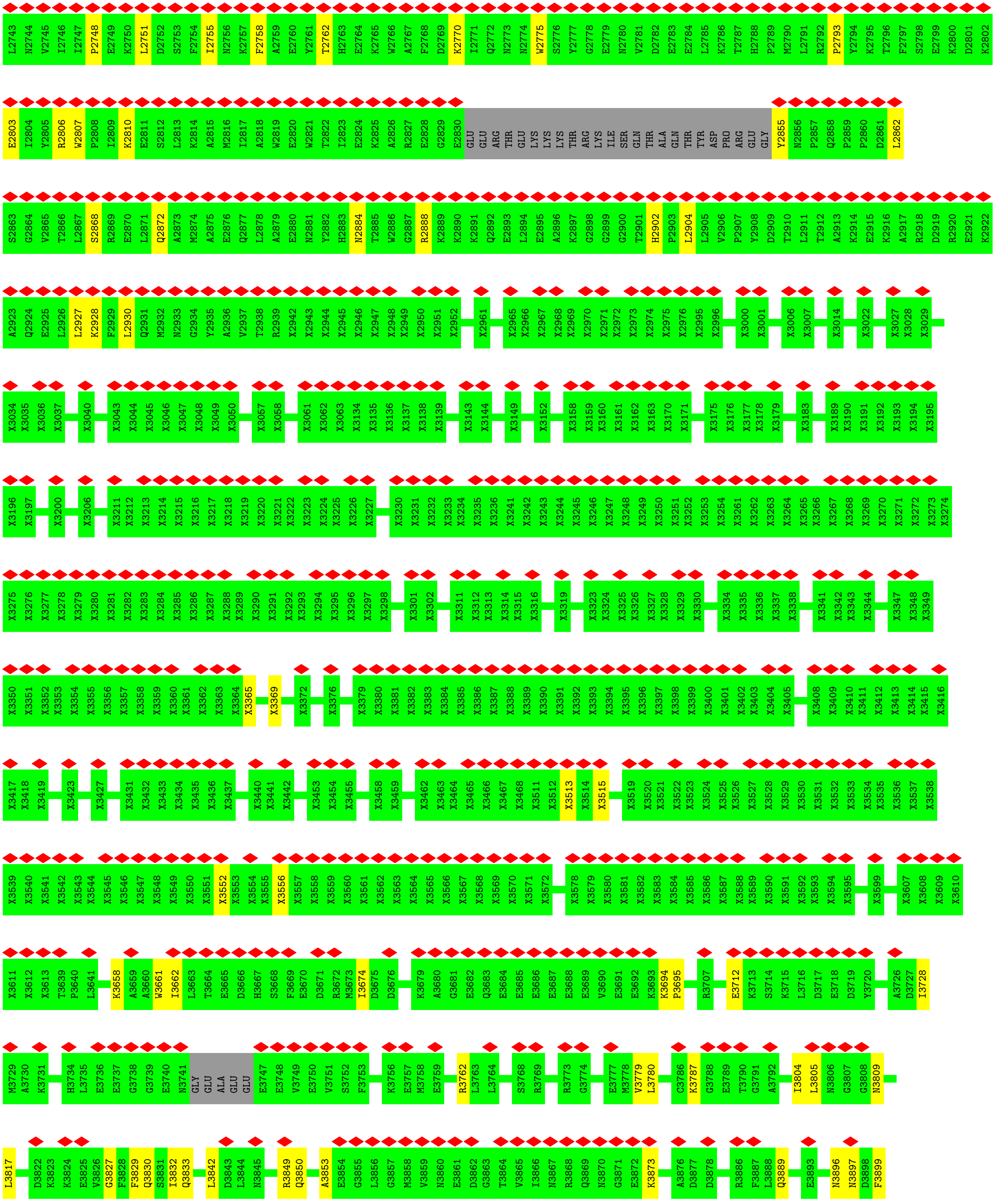
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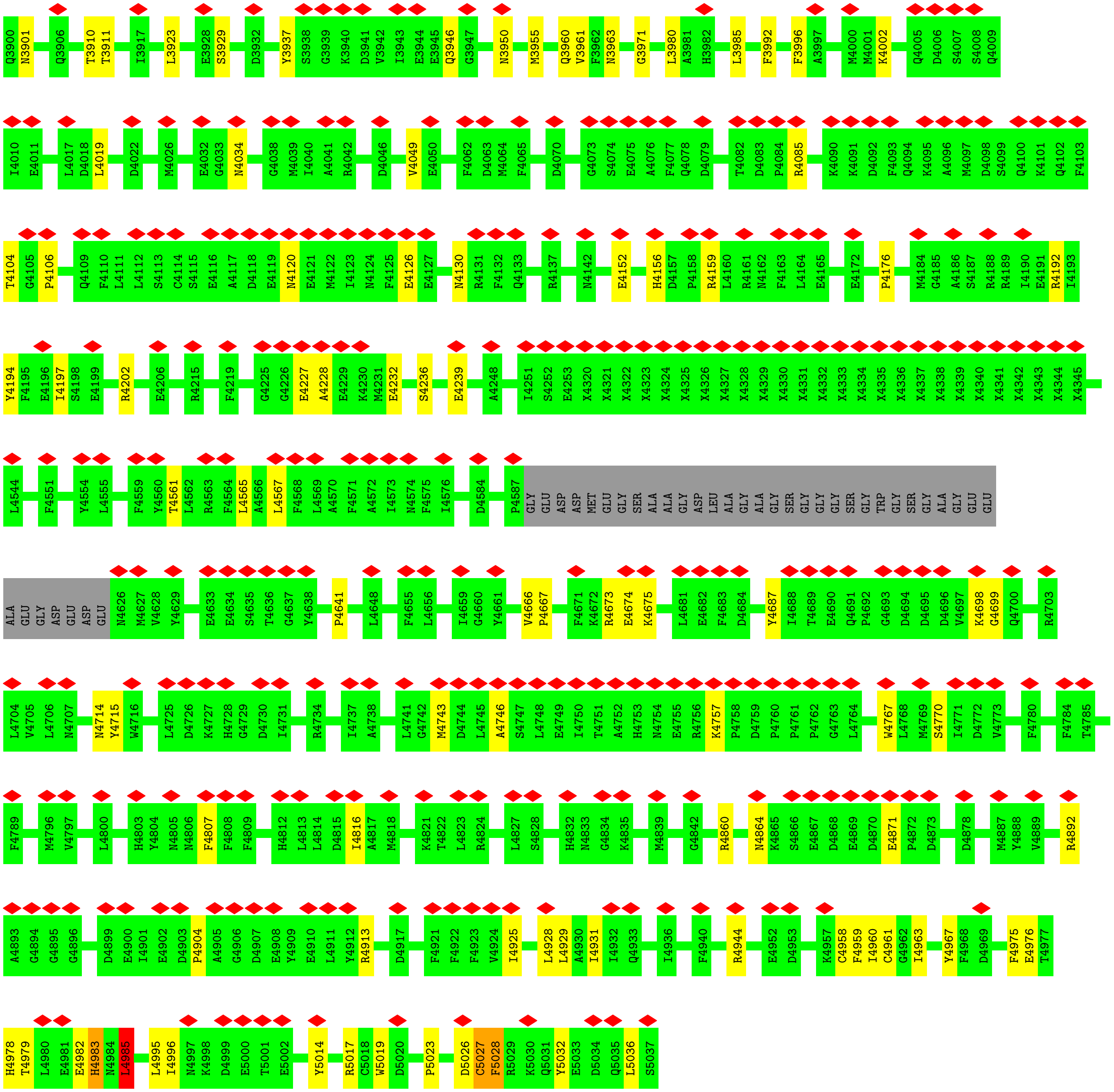

- Molecule 2: Ryanodine receptor 1

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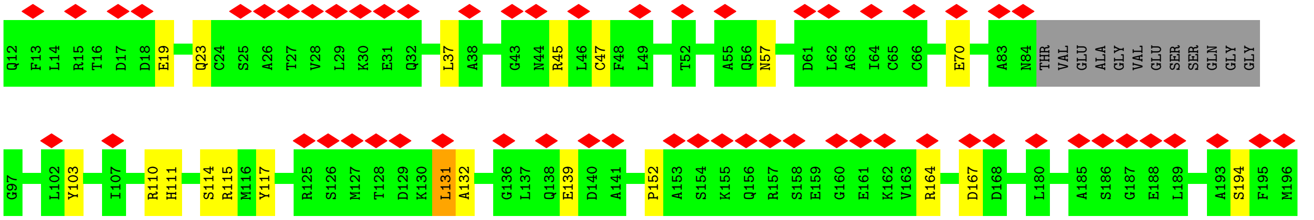

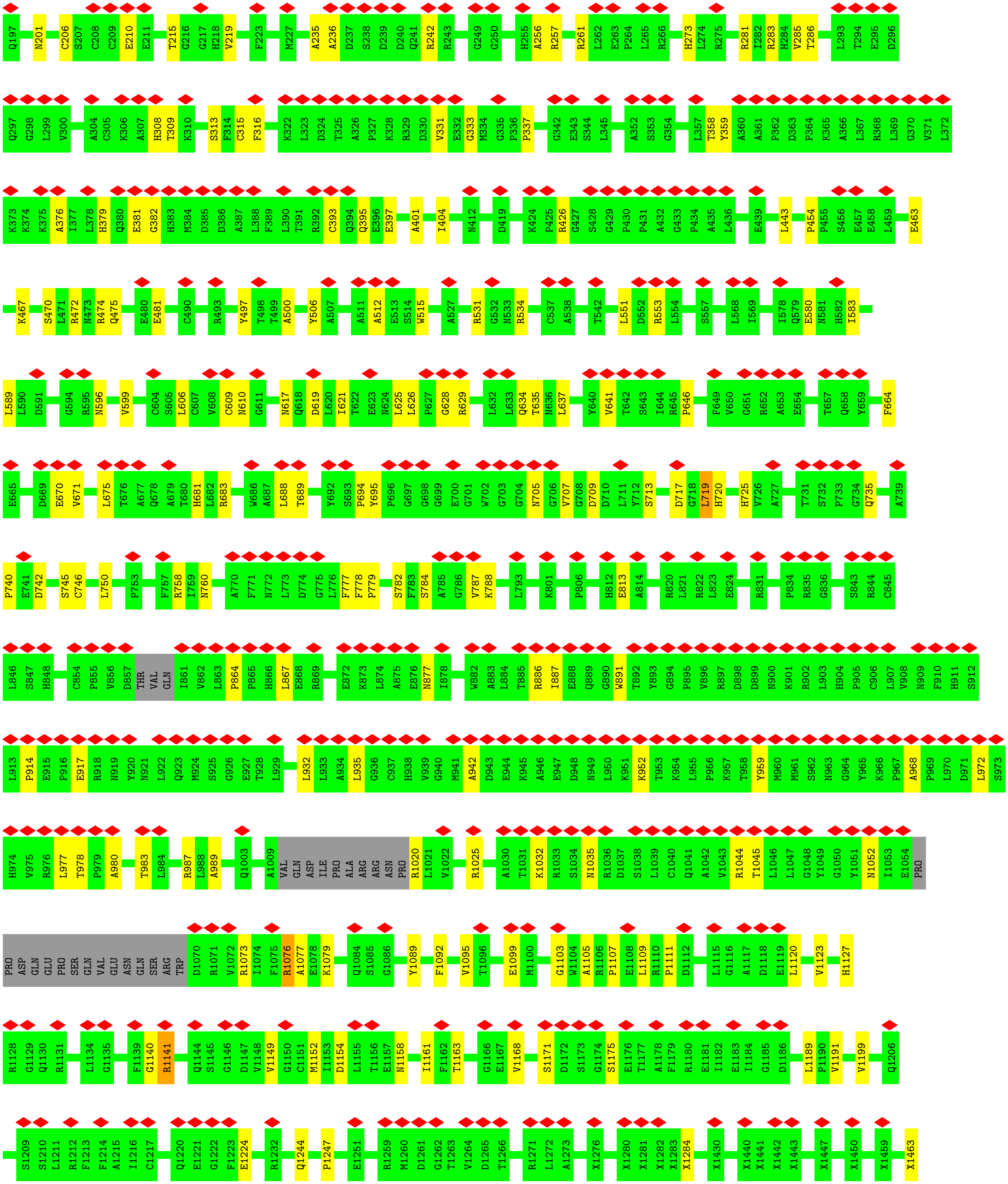
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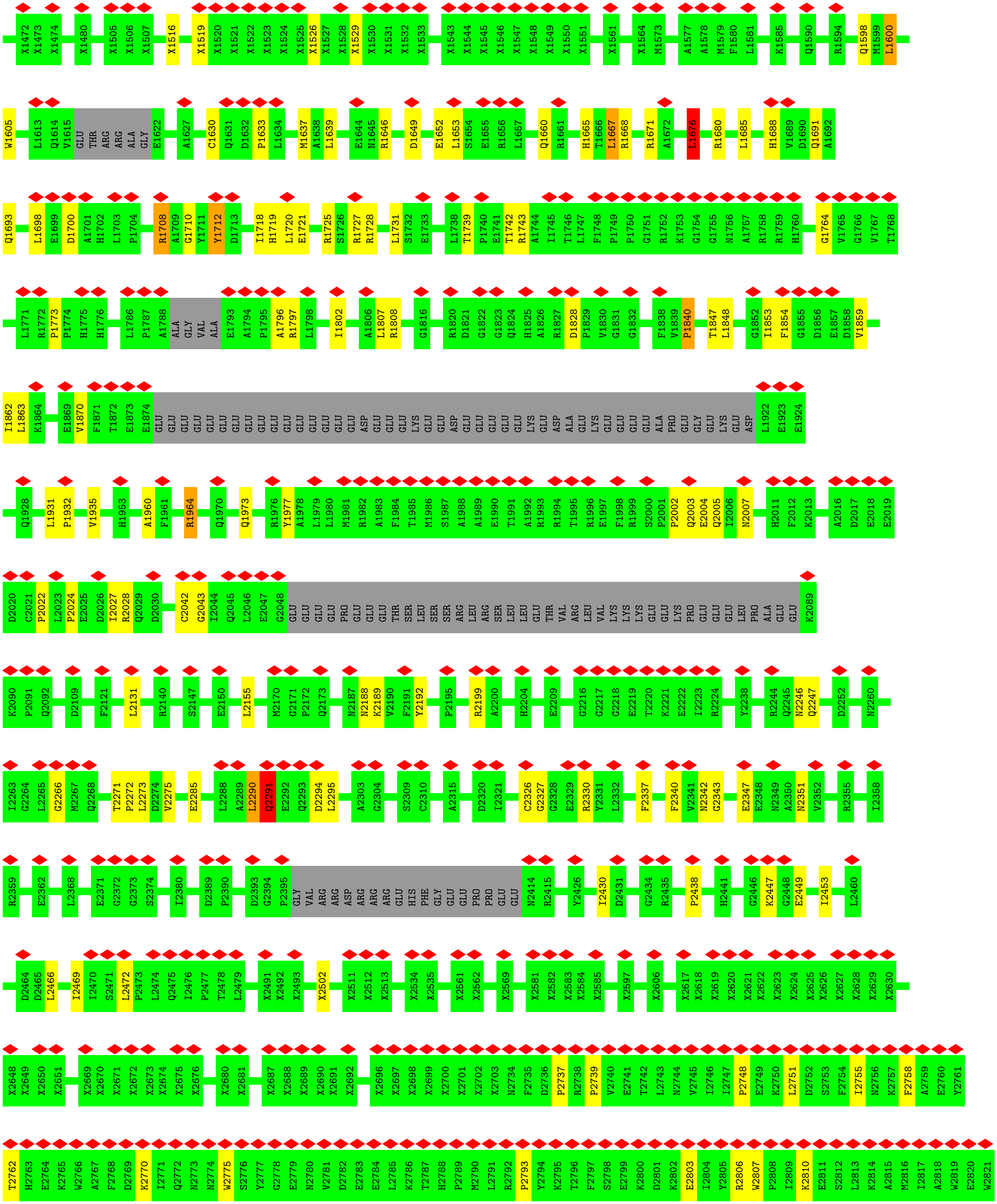
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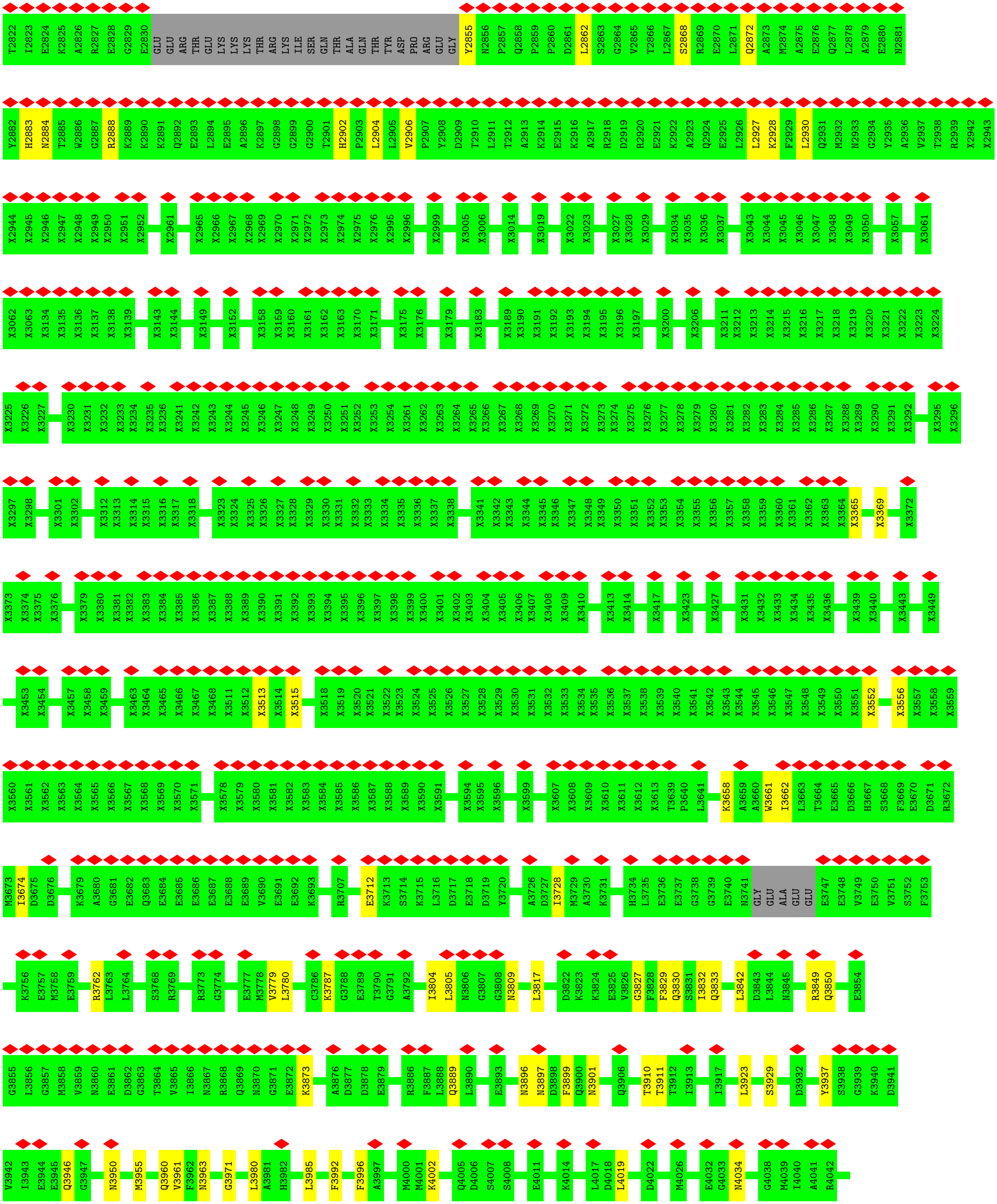
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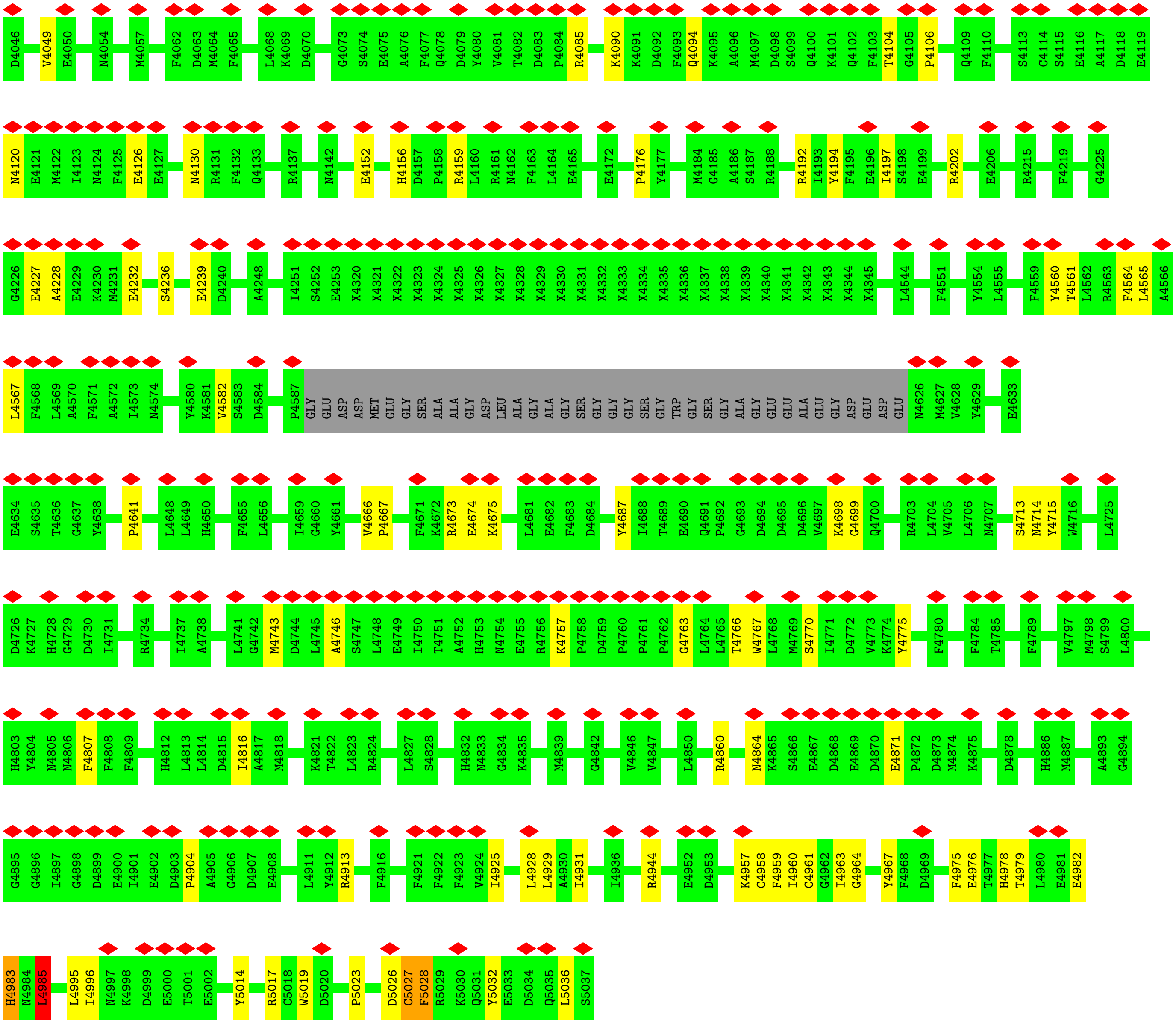

- Molecule 2: Ryanodine receptor 1

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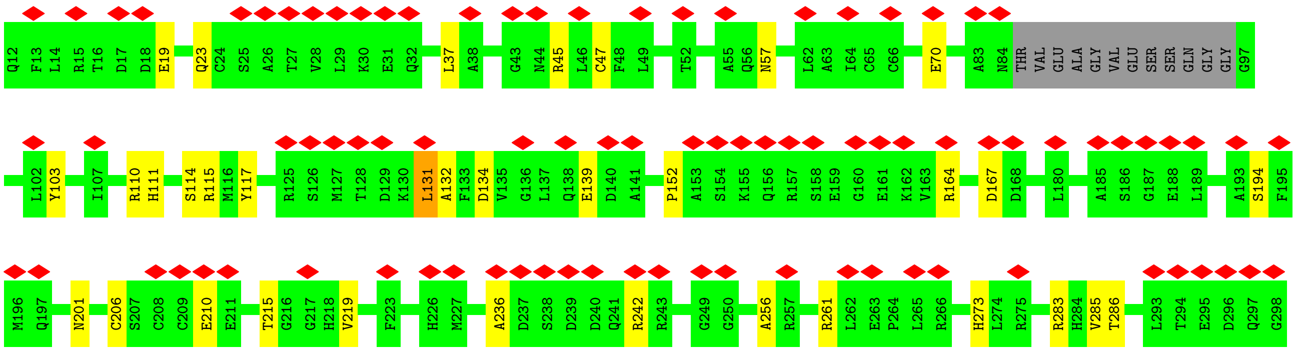

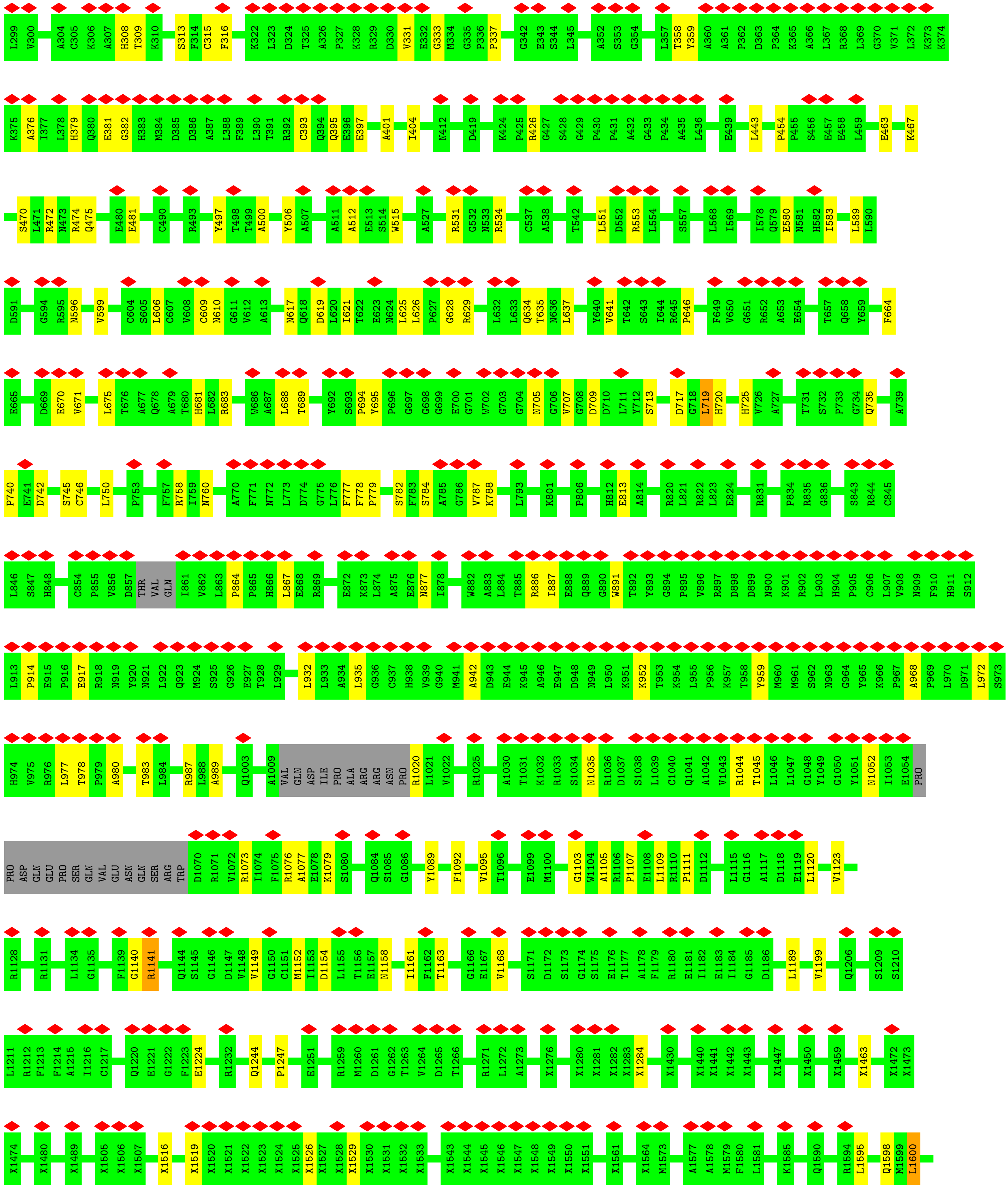
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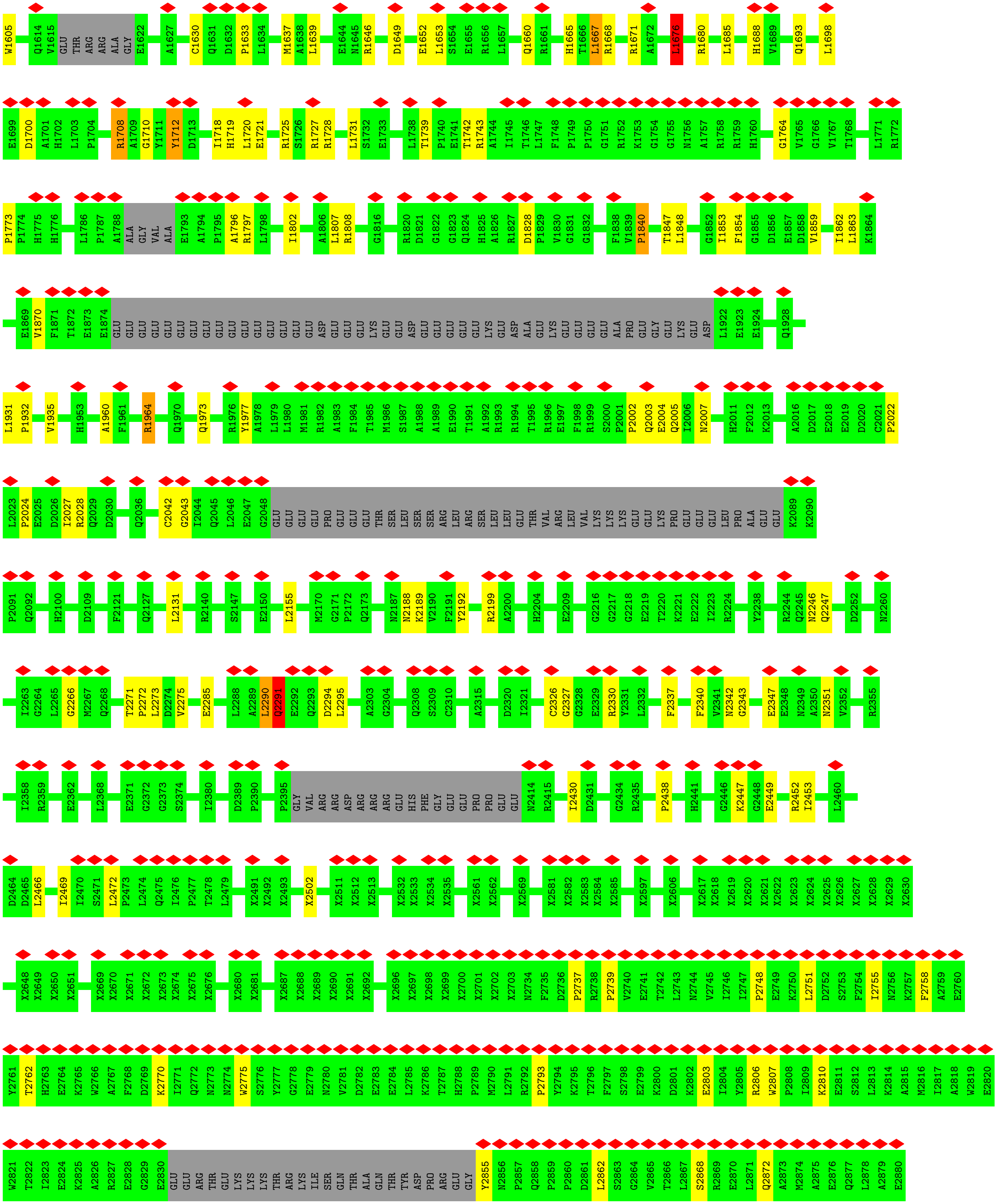
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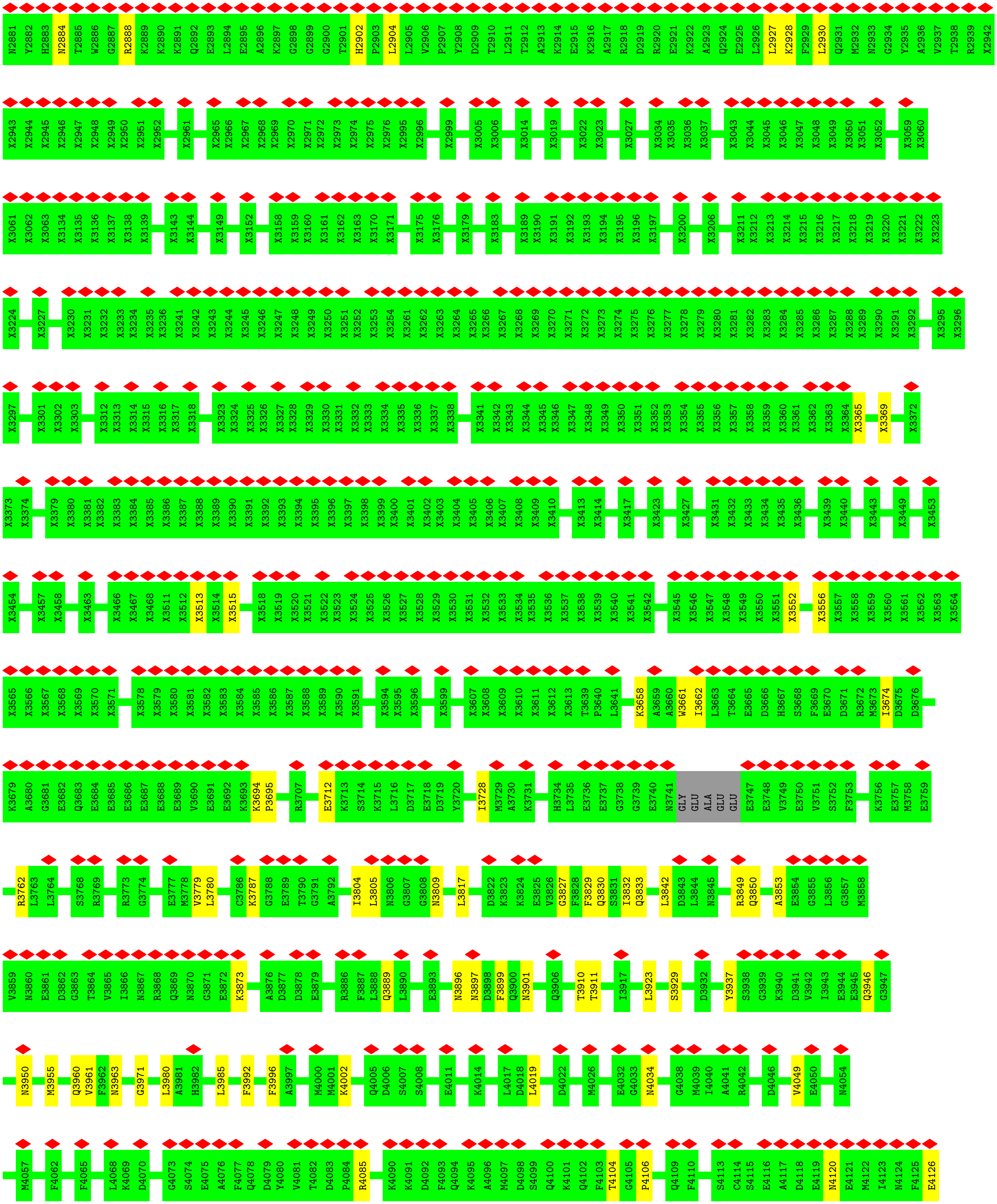
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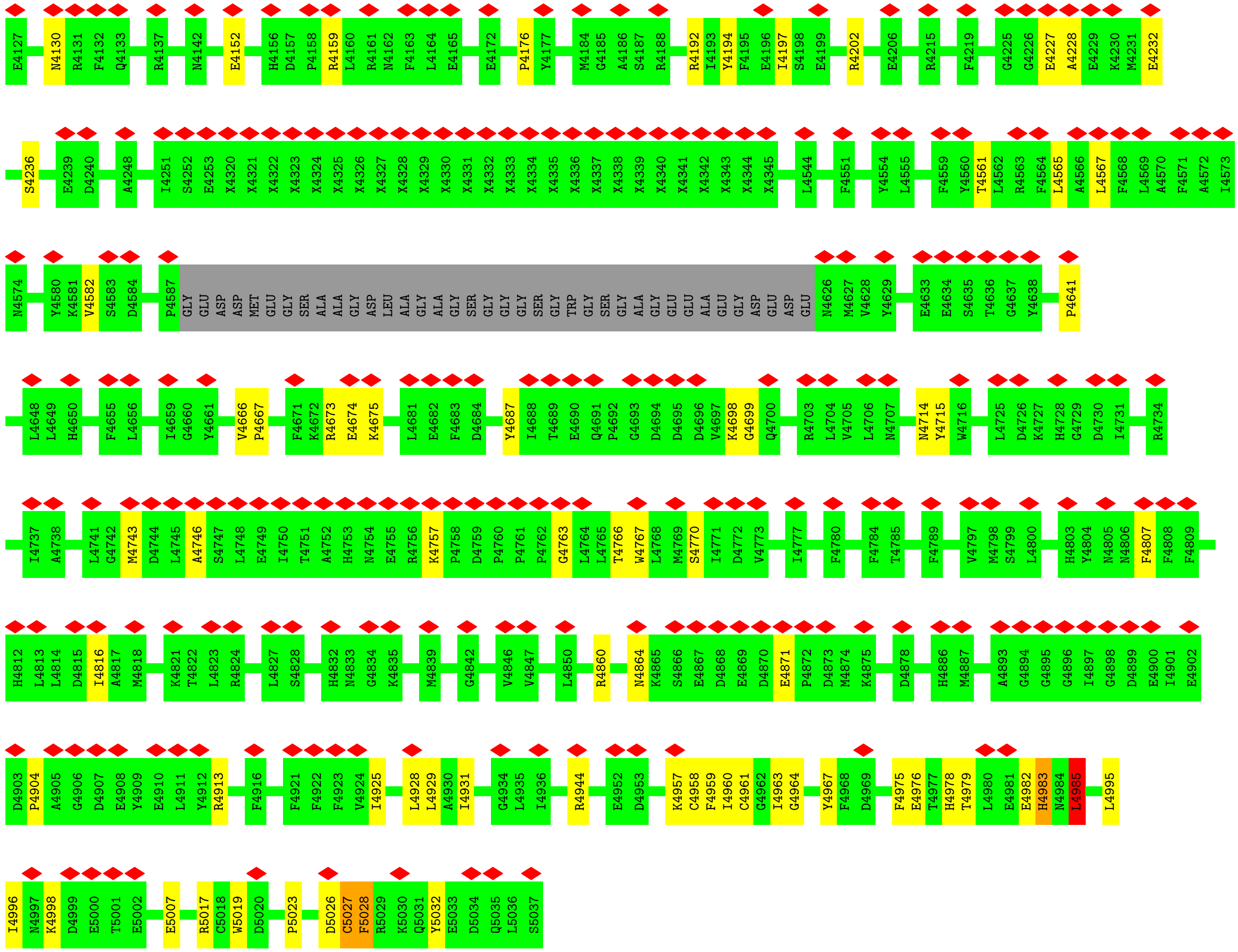
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4 Experimental information ⓘ

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 $(e^-/\text{Å}^2)$	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	0.105	Depositor
Minimum map value	-0.051	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	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: ZN, ATP, CFF

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	0.29	0/834	0.52	0/1123
1	F	0.29	0/834	0.52	0/1123
1	H	0.29	0/834	0.52	0/1123
1	J	0.29	0/834	0.52	0/1123
2	B	0.29	0/25428	0.54	10/34534 (0.0%)
2	E	0.29	0/25428	0.54	10/34534 (0.0%)
2	G	0.29	0/25428	0.54	10/34534 (0.0%)
2	I	0.29	0/25428	0.54	10/34534 (0.0%)
All	All	0.29	0/105048	0.54	40/142628 (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
2	B	0	13
2	E	0	13
2	G	0	13
2	I	0	13
All	All	0	52

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	131	LEU	CA-CB-CG	8.42	134.66	115.30
2	B	131	LEU	CA-CB-CG	8.41	134.65	115.30
2	E	131	LEU	CA-CB-CG	8.41	134.63	115.30
2	I	131	LEU	CA-CB-CG	8.39	134.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1600	LEU	CA-CB-CG	6.97	131.33	115.30
2	G	1600	LEU	CA-CB-CG	6.96	131.31	115.30
2	E	1600	LEU	CA-CB-CG	6.96	131.31	115.30
2	I	1600	LEU	CA-CB-CG	6.96	131.30	115.30
2	E	4985	LEU	CA-CB-CG	6.75	130.83	115.30
2	B	4985	LEU	CA-CB-CG	6.74	130.79	115.30
2	I	4985	LEU	CA-CB-CG	6.73	130.79	115.30
2	G	4985	LEU	CA-CB-CG	6.73	130.78	115.30
2	G	1676	LEU	CA-CB-CG	6.73	130.77	115.30
2	E	1676	LEU	CA-CB-CG	6.72	130.76	115.30
2	I	1676	LEU	CA-CB-CG	6.71	130.75	115.30
2	B	1676	LEU	CA-CB-CG	6.71	130.74	115.30
2	E	1140	GLY	C-N-CA	5.96	136.60	121.70
2	I	1140	GLY	C-N-CA	5.96	136.59	121.70
2	B	1140	GLY	C-N-CA	5.95	136.57	121.70
2	G	1140	GLY	C-N-CA	5.94	136.55	121.70
2	G	2290	LEU	CA-CB-CG	5.83	128.70	115.30
2	B	2290	LEU	CA-CB-CG	5.82	128.69	115.30
2	I	2290	LEU	CA-CB-CG	5.81	128.67	115.30
2	E	2290	LEU	CA-CB-CG	5.80	128.65	115.30
2	E	688	LEU	CA-CB-CG	5.55	128.07	115.30
2	B	688	LEU	CA-CB-CG	5.53	128.03	115.30
2	G	688	LEU	CA-CB-CG	5.53	128.02	115.30
2	I	688	LEU	CA-CB-CG	5.52	127.99	115.30
2	G	719	LEU	CA-CB-CG	5.35	127.60	115.30
2	B	719	LEU	CA-CB-CG	5.34	127.58	115.30
2	I	719	LEU	CA-CB-CG	5.34	127.57	115.30
2	E	719	LEU	CA-CB-CG	5.33	127.56	115.30
2	G	977	LEU	CA-CB-CG	5.08	126.98	115.30
2	B	977	LEU	CA-CB-CG	5.08	126.97	115.30
2	G	1667	LEU	CA-CB-CG	5.06	126.94	115.30
2	E	977	LEU	CA-CB-CG	5.06	126.94	115.30
2	I	977	LEU	CA-CB-CG	5.06	126.94	115.30
2	E	1667	LEU	CA-CB-CG	5.05	126.92	115.30
2	B	1667	LEU	CA-CB-CG	5.05	126.91	115.30
2	I	1667	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1712	TYR	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	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1712	TYR	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	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide

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Mol	Chain	Res	Type	Group
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	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	5	0
1	F	818	0	824	5	0
1	H	818	0	824	4	0
1	J	818	0	824	4	0
2	B	29499	0	24746	252	0
2	E	29499	0	24746	258	0
2	G	29499	0	24746	248	0
2	I	29499	0	24746	255	0
3	B	31	0	12	0	0
3	E	31	0	12	0	0
3	G	31	0	12	0	0
3	I	31	0	12	0	0
4	B	14	0	10	1	0
4	E	14	0	10	1	0
4	G	14	0	10	1	0
4	I	14	0	10	1	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	102368	1020	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1020) 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:G:5028:PHE:HE1	2:G:5032:TYR:CD2	1.87	0.93
2:I:5028:PHE:HE1	2:I:5032:TYR:CD2	1.87	0.93
2:B:5028:PHE:HE1	2:B:5032:TYR:CD2	1.87	0.92
2:E:5028:PHE:HE1	2:E:5032:TYR:CD2	1.87	0.92
2:I:5028:PHE:CE1	2:I:5032:TYR:CD2	2.58	0.92
2:G:5028:PHE:CE1	2:G:5032:TYR:CD2	2.58	0.92
2:B:5028:PHE:CE1	2:B:5032:TYR:CD2	2.58	0.92
2:E:5028:PHE:CE1	2:E:5032:TYR:CD2	2.58	0.91
2:G:5028:PHE:HE1	2:G:5032:TYR:CE2	1.99	0.81
2:E:5028:PHE:HE1	2:E:5032:TYR:CE2	1.99	0.80
2:G:5028:PHE:CE1	2:G:5032:TYR:HD2	1.99	0.79
2:I:5028:PHE:HE1	2:I:5032:TYR:CE2	1.99	0.79
2:B:5028:PHE:HE1	2:B:5032:TYR:CE2	1.99	0.79
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.63	0.79
2:I:5028:PHE:CE1	2:I:5032:TYR:HD2	1.99	0.79
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.63	0.79
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.63	0.78
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.64	0.78
2:E:5028:PHE:CE1	2:E:5032:TYR:HD2	2.00	0.77
2:B:5028:PHE:CE1	2:B:5032:TYR:HD2	2.00	0.76
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.74	0.70
2:E:379:HIS:HD2	2:E:382:GLY:H	1.41	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.74	0.69
2:I:4904:PRO:HB3	2:I:4913:ARG:HD3	1.75	0.69
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.74	0.69
2:I:379:HIS:HD2	2:I:382:GLY:H	1.41	0.69
2:G:4904:PRO:HB3	2:G:4913:ARG:HD3	1.75	0.69
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.74	0.68
2:E:4904:PRO:HB3	2:E:4913:ARG:HD3	1.75	0.68
2:B:4904:PRO:HB3	2:B:4913:ARG:HD3	1.75	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.41	0.68
2:B:379:HIS:HD2	2:B:382:GLY:H	1.41	0.68
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.59	0.68
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.59	0.68
2:I:4975:PHE:O	2:I:4979:THR:HG23	1.95	0.67
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.78	0.66
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.59	0.66
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.77	0.66
2:B:4975:PHE:O	2:B:4979:THR:HG23	1.95	0.66
2:G:4975:PHE:O	2:G:4979:THR:HG23	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.78	0.66
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.78	0.66
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.78	0.66
2:E:4975:PHE:O	2:E:4979:THR:HG23	1.95	0.65
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.78	0.65
2:E:4983:HIS:CD2	2:E:4983:HIS:H	2.13	0.65
2:I:4983:HIS:H	2:I:4983:HIS:CD2	2.13	0.65
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.59	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:B:4983:HIS:CD2	2:B:4983:HIS:H	2.13	0.64
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.64
2:G:4983:HIS:CD2	2:G:4983:HIS:H	2.13	0.64
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.62	0.64
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.31	0.64
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.62	0.64
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.63	0.63
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.31	0.63
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.31	0.63
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.31	0.63
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.63	0.62
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.62
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.62
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.82	0.62
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.82	0.61
2:B:2266:GLY:O	2:B:2330:ARG:NH2	2.33	0.61
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.61
2:I:683:ARG:HB2	2:I:782:SER:HB3	1.82	0.61
2:I:4192:ARG:HD2	2:I:5028:PHE:CD2	2.35	0.61
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.82	0.61
2:G:2266:GLY:O	2:G:2330:ARG:NH2	2.33	0.61
2:B:4192:ARG:HD2	2:B:5028:PHE:CD2	2.35	0.61
2:E:4192:ARG:HD2	2:E:5028:PHE:CD2	2.35	0.61
2:I:2266:GLY:O	2:I:2330:ARG:NH2	2.33	0.61
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.60
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.60
2:B:683:ARG:HB2	2:B:782:SER:HB3	1.82	0.60
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.60
2:G:4192:ARG:HD2	2:G:5028:PHE:CD2	2.35	0.60
2:E:2266:GLY:O	2:E:2330:ARG:NH2	2.33	0.60
2:G:683:ARG:NH1	2:G:707:VAL:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.67	0.60
2:E:683:ARG:HB2	2:E:782:SER:HB3	1.82	0.60
2:G:683:ARG:HB2	2:G:782:SER:HB3	1.82	0.59
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.82	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:B:683:ARG:NH1	2:B:707:VAL:O	2.35	0.59
2:G:609:CYS:SG	2:G:610:ASN:N	2.76	0.59
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.84	0.59
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.85	0.59
2:B:5028:PHE:CE1	2:B:5032:TYR:CE2	2.88	0.59
2:E:609:CYS:SG	2:E:610:ASN:N	2.76	0.59
2:E:683:ARG:NH1	2:E:707:VAL:O	2.35	0.59
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.67	0.59
2:B:609:CYS:SG	2:B:610:ASN:N	2.76	0.59
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.59
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.85	0.59
2:I:609:CYS:SG	2:I:610:ASN:N	2.76	0.59
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.85	0.58
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.84	0.58
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.58
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.85	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.58
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.85	0.58
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.67	0.58
2:G:331:VAL:HG12	2:G:333:GLY:H	1.68	0.58
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.85	0.58
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.85	0.58
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.58
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.84	0.58
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.86	0.58
2:I:331:VAL:HG12	2:I:333:GLY:H	1.68	0.58
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.85	0.58
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.58
2:B:4674:GLU:HB3	2:B:4715:TYR:HB2	1.86	0.58
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.85	0.58
2:B:331:VAL:HG12	2:B:333:GLY:H	1.68	0.58
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.37	0.58
2:I:683:ARG:NH1	2:I:707:VAL:O	2.35	0.57
2:I:315:CYS:SG	2:I:316:PHE:N	2.77	0.57
2:B:4104:THR:HG22	2:B:4106:PRO:HD2	1.86	0.57
2:E:315:CYS:SG	2:E:316:PHE:N	2.77	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57
2:I:4104:THR:HG22	2:I:4106:PRO:HD2	1.86	0.57
2:I:4674:GLU:HG3	2:I:4714:ASN:HB3	1.87	0.57
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.37	0.57
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.37	0.57
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.86	0.57
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.38	0.57
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.37	0.57
2:E:331:VAL:HG12	2:E:333:GLY:H	1.68	0.57
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.37	0.57
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.86	0.57
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.38	0.57
2:G:315:CYS:SG	2:G:316:PHE:N	2.77	0.57
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.38	0.57
2:G:4104:THR:HG22	2:G:4106:PRO:HD2	1.86	0.57
2:B:315:CYS:SG	2:B:316:PHE:N	2.77	0.57
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.38	0.57
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.85	0.57
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.85	0.57
2:E:4104:THR:HG22	2:E:4106:PRO:HD2	1.86	0.57
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.37	0.57
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.38	0.57
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.67	0.57
2:I:4674:GLU:HB3	2:I:4715:TYR:HB2	1.86	0.57
2:B:132:ALA:HA	2:B:194:SER:HB2	1.86	0.57
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.37	0.57
2:I:359:TYR:HA	2:I:376:ALA:HA	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.38	0.57
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.38	0.57
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.39	0.56
2:B:4674:GLU:HG3	2:B:4714:ASN:HB3	1.87	0.56
2:E:4983:HIS:CD2	2:E:4983:HIS:N	2.73	0.56
2:G:4983:HIS:CD2	2:G:4983:HIS:N	2.73	0.56
2:B:4983:HIS:CD2	2:B:4983:HIS:N	2.73	0.56
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:132:ALA:HA	2:G:194:SER:HB2	1.86	0.56
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.39	0.56
2:G:4674:GLU:HG3	2:G:4714:ASN:HB3	1.87	0.56
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.87	0.56
2:G:4674:GLU:HB3	2:G:4715:TYR:HB2	1.86	0.56
2:B:359:TYR:HA	2:B:376:ALA:HA	1.87	0.56
2:E:132:ALA:HA	2:E:194:SER:HB2	1.86	0.56
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.38	0.56
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.37	0.56
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.39	0.56
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.71	0.56
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.88	0.56
2:E:4674:GLU:HB3	2:E:4715:TYR:HB2	1.86	0.56
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.39	0.56
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.87	0.56
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.71	0.56
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.38	0.56
2:E:4674:GLU:HG3	2:E:4714:ASN:HB3	1.86	0.56
2:G:359:TYR:HA	2:G:376:ALA:HA	1.86	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.54	0.56
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.87	0.56
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.88	0.56
2:I:132:ALA:HA	2:I:194:SER:HB2	1.86	0.56
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.37	0.56
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.38	0.56
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.39	0.56
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.39	0.56
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.37	0.55
2:B:111:HIS:HD2	2:B:114:SER:H	1.54	0.55
2:E:359:TYR:HA	2:E:376:ALA:HA	1.86	0.55
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.88	0.55
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.89	0.55
2:E:23:GLN:HB3	2:E:201:ASN:HB2	1.89	0.55
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.89	0.55
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.40	0.55
2:E:4232:GLU:OE2	2:E:5017:ARG:NH1	2.39	0.55
2:G:111:HIS:HD2	2:G:114:SER:H	1.54	0.55
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.89	0.55
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.40	0.55
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.87	0.55
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.39	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.79	0.55
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.89	0.55
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.79	0.55
2:B:23:GLN:HB3	2:B:201:ASN:HB2	1.89	0.54
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.79	0.54
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.90	0.54
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.71	0.54
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.88	0.54
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.90	0.54
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.89	0.54
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.90	0.54
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.37	0.54
2:I:2868:SER:O	2:I:2872:GLN:N	2.38	0.54
2:I:4232:GLU:OE2	2:I:5017:ARG:NH1	2.39	0.54
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.71	0.54
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.88	0.54
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.89	0.54
2:G:4232:GLU:OE2	2:G:5017:ARG:NH1	2.39	0.54
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.40	0.54
2:I:23:GLN:HB3	2:I:201:ASN:HB2	1.89	0.54
2:I:111:HIS:HD2	2:I:114:SER:H	1.54	0.54
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.89	0.54
2:G:23:GLN:HB3	2:G:201:ASN:HB2	1.89	0.54
2:E:470:SER:O	2:E:474:ARG:NE	2.39	0.54
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.90	0.54
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.89	0.54
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.89	0.54
1:J:7:ILE:HB	1:J:71:ARG:HB3	1.90	0.54
2:B:4232:GLU:OE2	2:B:5017:ARG:NH1	2.39	0.54
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.89	0.54
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.90	0.54
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.41	0.54
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.90	0.54
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.90	0.54
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.41	0.54
2:E:5028:PHE:CE1	2:E:5032:TYR:CE2	2.88	0.54
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.90	0.54
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.89	0.54
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.89	0.53
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.90	0.53
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.53
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.53
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.40	0.53
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.73	0.53
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.42	0.53
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.73	0.53
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.42	0.53
1:F:7:ILE:HB	1:F:71:ARG:HB3	1.90	0.53
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.42	0.53
1:A:7:ILE:HB	1:A:71:ARG:HB3	1.90	0.53
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.90	0.53
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.39	0.53
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.42	0.53
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.41	0.53
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.42	0.53
2:I:3897:ASN:O	2:I:3901:ASN:ND2	2.42	0.53
2:I:4983:HIS:CD2	2:I:4983:HIS:N	2.73	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.38	0.53
2:G:470:SER:O	2:G:474:ARG:NE	2.39	0.53
2:E:3897:ASN:O	2:E:3901:ASN:ND2	2.42	0.53
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.90	0.53
2:G:4687:TYR:OH	2:G:4699:GLY:O	2.27	0.52
2:E:4687:TYR:OH	2:E:4699:GLY:O	2.27	0.52
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.73	0.52
2:B:3897:ASN:O	2:B:3901:ASN:ND2	2.42	0.52
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.41	0.52
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.90	0.52
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.38	0.52
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.91	0.52
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.52
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.52
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.52
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.90	0.52
2:B:1727:ARG:NH2	2:B:1773:PRO:O	2.40	0.52
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.73	0.52
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.42	0.52
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.91	0.52
2:I:5028:PHE:CE1	2:I:5032:TYR:CE2	2.88	0.52
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.91	0.52
2:G:3842:LEU:O	2:G:3929:SER:OG	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3897:ASN:O	2:G:3901:ASN:ND2	2.42	0.52
1:H:7:ILE:HB	1:H:71:ARG:HB3	1.90	0.52
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.42	0.52
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.92	0.52
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.90	0.52
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.92	0.52
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.92	0.52
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.91	0.52
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.92	0.52
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.52
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.91	0.52
2:B:3842:LEU:O	2:B:3929:SER:OG	2.26	0.51
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.91	0.51
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.51
2:G:1516:UNK:N	2:G:1529:UNK:O	2.43	0.51
2:G:5028:PHE:CE1	2:G:5032:TYR:CE2	2.88	0.51
2:B:1516:UNK:N	2:B:1529:UNK:O	2.43	0.51
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.91	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.43	0.51
2:E:3842:LEU:O	2:E:3929:SER:OG	2.27	0.51
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.92	0.51
2:B:470:SER:O	2:B:474:ARG:NE	2.39	0.51
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.90	0.51
2:E:2868:SER:O	2:E:2872:GLN:N	2.38	0.51
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.44	0.51
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.92	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.92	0.51
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.91	0.51
2:I:4236:SER:OG	2:I:4675:LYS:NZ	2.41	0.51
2:I:4687:TYR:OH	2:I:4699:GLY:O	2.27	0.51
2:B:978:THR:HB	2:B:980:ALA:H	1.75	0.51
2:I:3842:LEU:O	2:I:3929:SER:OG	2.27	0.51
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.44	0.51
2:B:4687:TYR:OH	2:B:4699:GLY:O	2.27	0.51
2:E:813:GLU:OE2	2:E:1020:ARG:N	2.44	0.51
2:E:1727:ARG:NH2	2:E:1773:PRO:O	2.40	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.43	0.51
2:I:1727:ARG:NH2	2:I:1773:PRO:O	2.40	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.92	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:4958:CYS:SG	2:I:4961:CYS:N	2.84	0.51
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.44	0.51
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.76	0.51
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.76	0.51
2:B:670:GLU:HG3	2:B:787:VAL:HG13	1.93	0.51
2:B:4958:CYS:SG	2:B:4961:CYS:N	2.84	0.51
2:I:626:LEU:HG	2:I:628:GLY:H	1.76	0.51
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.44	0.51
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.51
2:E:978:THR:HB	2:E:980:ALA:H	1.75	0.51
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.93	0.51
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.93	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.93	0.50
2:I:813:GLU:OE2	2:I:1020:ARG:N	2.44	0.50
2:G:813:GLU:OE2	2:G:1020:ARG:N	2.44	0.50
2:B:813:GLU:OE2	2:B:1020:ARG:N	2.44	0.50
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.44	0.50
2:E:4236:SER:OG	2:E:4675:LYS:NZ	2.41	0.50
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.91	0.50
2:G:626:LEU:HG	2:G:628:GLY:H	1.76	0.50
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.76	0.50
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.76	0.50
2:E:45:ARG:HG2	2:E:443:LEU:HD21	1.93	0.50
2:E:395:GLN:HG3	2:E:397:GLU:H	1.77	0.50
2:E:670:GLU:HG3	2:E:787:VAL:HG13	1.93	0.50
2:E:3804:ILE:O	2:E:3809:ASN:ND2	2.45	0.50
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.50
2:I:3992:PHE:O	2:I:3996:PHE:N	2.40	0.50
2:E:626:LEU:HG	2:E:628:GLY:H	1.76	0.50
2:I:629:ARG:HD3	2:I:634:GLN:HG2	1.94	0.50
2:I:978:THR:HB	2:I:980:ALA:H	1.75	0.50
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.93	0.50
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.77	0.50
2:B:629:ARG:HD3	2:B:634:GLN:HG2	1.94	0.50
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.93	0.50
2:B:3804:ILE:O	2:B:3809:ASN:ND2	2.45	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:E:4176:PRO:O	2:E:4202:ARG:NH2	2.45	0.50
2:G:670:GLU:HG3	2:G:787:VAL:HG13	1.93	0.50
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4236:SER:OG	2:B:4675:LYS:NZ	2.41	0.50
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.44	0.50
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.50
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.45	0.50
2:B:626:LEU:HG	2:B:628:GLY:H	1.76	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.93	0.49
2:E:621:ILE:O	2:E:625:LEU:N	2.45	0.49
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.45	0.49
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.77	0.49
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.94	0.49
2:I:395:GLN:HG3	2:I:397:GLU:H	1.77	0.49
2:G:395:GLN:HG3	2:G:397:GLU:H	1.77	0.49
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.49
2:I:3804:ILE:O	2:I:3809:ASN:ND2	2.45	0.49
2:G:621:ILE:O	2:G:625:LEU:N	2.45	0.49
2:B:395:GLN:HG3	2:B:397:GLU:H	1.77	0.49
2:I:470:SER:O	2:I:474:ARG:NE	2.39	0.49
2:I:3827:GLY:HA2	2:I:3830:GLN:HE21	1.78	0.49
2:G:3804:ILE:O	2:G:3809:ASN:ND2	2.45	0.49
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.79	0.49
2:E:2342:ASN:N	2:E:2342:ASN:OD1	2.44	0.49
2:I:670:GLU:HG3	2:I:787:VAL:HG13	1.93	0.49
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.45	0.49
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.49
2:G:4958:CYS:SG	2:G:4961:CYS:N	2.84	0.49
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.95	0.49
2:E:1796:ALA:HB1	2:E:1797:ARG:HH21	1.78	0.49
2:G:629:ARG:HD3	2:G:634:GLN:HG2	1.94	0.49
2:E:629:ARG:HD3	2:E:634:GLN:HG2	1.94	0.49
2:I:1796:ALA:HB1	2:I:1797:ARG:HH21	1.78	0.49
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.45	0.49
2:B:4228:ALA:O	2:B:4232:GLU:N	2.46	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.95	0.49
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	1.95	0.49
2:I:621:ILE:O	2:I:625:LEU:N	2.45	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.46	0.49
2:B:404:ILE:HG21	2:B:481:GLU:HG3	1.95	0.49
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.45	0.49
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3827:GLY:HA2	2:G:3830:GLN:HE21	1.78	0.49
2:I:1863:LEU:HB3	2:I:1870:VAL:HG21	1.95	0.49
2:I:2347:GLU:O	2:I:2351:ASN:N	2.39	0.49
2:I:4228:ALA:O	2:I:4232:GLU:N	2.46	0.49
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.77	0.48
2:I:4976:GLU:HA	2:I:4979:THR:HG23	1.95	0.48
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.95	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.95	0.48
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.95	0.48
2:B:4176:PRO:O	2:B:4202:ARG:NH2	2.45	0.48
2:B:4976:GLU:HA	2:B:4979:THR:HG23	1.95	0.48
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.46	0.48
2:E:4958:CYS:SG	2:E:4961:CYS:N	2.84	0.48
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.46	0.48
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	1.95	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.95	0.48
2:I:404:ILE:HG21	2:I:481:GLU:HG3	1.95	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.95	0.48
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.46	0.48
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	1.95	0.48
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.95	0.48
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.46	0.48
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.95	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.93	0.48
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.78	0.48
2:G:1863:LEU:HB3	2:G:1870:VAL:HG21	1.95	0.48
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.78	0.48
2:B:4960:ILE:HD11	2:B:4985:LEU:HD23	1.96	0.48
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.48
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.95	0.48
2:E:3980:LEU:HD22	2:E:3985:LEU:HD22	1.96	0.48
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.95	0.48
2:G:37:LEU:HD11	2:G:47:CYS:HB3	1.96	0.48
2:G:404:ILE:HG21	2:G:481:GLU:HG3	1.95	0.48
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.46	0.48
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.77	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.46	0.48
2:E:4228:ALA:O	2:E:4232:GLU:N	2.46	0.48
2:I:4713:SER:HG	2:I:4775:TYR:HH	1.59	0.48
2:G:1105:ALA:HB1	2:G:1109:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2347:GLU:O	2:G:2351:ASN:N	2.39	0.48
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.45	0.48
2:B:3827:GLY:HA2	2:B:3830:GLN:HE21	1.78	0.48
2:B:3980:LEU:HD22	2:B:3985:LEU:HD22	1.96	0.48
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.49	0.48
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.47	0.48
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.96	0.48
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	1.95	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.38	0.48
2:G:4176:PRO:O	2:G:4202:ARG:NH2	2.45	0.48
2:G:4228:ALA:O	2:G:4232:GLU:N	2.46	0.48
2:B:1796:ALA:HB1	2:B:1797:ARG:HH21	1.78	0.48
2:I:37:LEU:HD11	2:I:47:CYS:HB3	1.96	0.48
2:I:4960:ILE:HD11	2:I:4985:LEU:HD23	1.96	0.48
2:I:4963:ILE:HG21	2:I:4967:TYR:HD2	1.79	0.48
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.48
2:B:1863:LEU:HB3	2:B:1870:VAL:HG21	1.95	0.48
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.95	0.48
2:I:4176:PRO:O	2:I:4202:ARG:NH2	2.45	0.48
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.45	0.48
2:G:3980:LEU:HD22	2:G:3985:LEU:HD22	1.96	0.48
2:E:4976:GLU:HA	2:E:4979:THR:HG23	1.95	0.48
2:I:3980:LEU:HD22	2:I:3985:LEU:HD22	1.96	0.48
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.95	0.47
2:E:4963:ILE:HG21	2:E:4967:TYR:HD2	1.79	0.47
2:G:1796:ALA:HB1	2:G:1797:ARG:HH21	1.78	0.47
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.47	0.47
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.79	0.47
2:E:404:ILE:HG21	2:E:481:GLU:HG3	1.95	0.47
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:E:3827:GLY:HA2	2:E:3830:GLN:HE21	1.78	0.47
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.95	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.95	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.47
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.79	0.47
2:I:1105:ALA:HB1	2:I:1109:LEU:HD21	1.96	0.47
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.47
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.79	0.47
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4976:GLU:HA	2:G:4979:THR:HG23	1.95	0.47
2:E:1863:LEU:HB3	2:E:1870:VAL:HG21	1.95	0.47
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.78	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.96	0.47
2:G:3889:GLN:HE22	2:G:3963:ASN:HB3	1.79	0.47
2:G:4192:ARG:HD2	2:G:5028:PHE:CE2	2.50	0.47
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.46	0.47
2:B:1105:ALA:HB1	2:B:1109:LEU:HD21	1.96	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.47	0.47
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.49	0.47
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	1.97	0.47
2:B:2868:SER:O	2:B:2872:GLN:N	2.38	0.47
2:B:3992:PHE:O	2:B:3996:PHE:N	2.40	0.47
2:B:4898:GLY:O	2:E:4892:ARG:NH2	2.47	0.47
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.79	0.47
2:E:5023:PRO:HB3	2:E:5026:ASP:O	2.14	0.47
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.47
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.47	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:G:5023:PRO:HB3	2:G:5026:ASP:O	2.15	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.47
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	1.97	0.47
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.47
2:B:4192:ARG:HD2	2:B:5028:PHE:CE2	2.50	0.47
2:B:4963:ILE:HG21	2:B:4967:TYR:HD2	1.79	0.47
2:E:750:LEU:HD21	2:E:777:PHE:HE2	1.80	0.47
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.47	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.97	0.47
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.78	0.47
2:G:4960:ILE:HD11	2:G:4985:LEU:HD23	1.96	0.47
2:G:4963:ILE:HG21	2:G:4967:TYR:HD2	1.79	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.96	0.47
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	1.97	0.47
2:B:750:LEU:HD21	2:B:777:PHE:HE2	1.80	0.47
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.96	0.47
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.47	0.47
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.79	0.47
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.97	0.47
2:B:5023:PRO:HB3	2:B:5026:ASP:O	2.15	0.47
2:E:1105:ALA:HB1	2:E:1109:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4192:ARG:HD2	2:E:5028:PHE:CE2	2.50	0.47
2:E:4960:ILE:HD11	2:E:4985:LEU:HD23	1.96	0.47
2:I:750:LEU:HD21	2:I:777:PHE:HE2	1.80	0.47
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.47
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.80	0.47
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.47	0.46
2:E:70:GLU:HG3	2:E:117:TYR:HE1	1.80	0.46
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	1.97	0.46
2:I:5023:PRO:HB3	2:I:5026:ASP:O	2.15	0.46
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.79	0.46
2:B:472:ARG:HA	2:B:475:GLN:HB2	1.98	0.46
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.46
2:E:37:LEU:HD11	2:E:47:CYS:HB3	1.96	0.46
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.97	0.46
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.96	0.46
2:E:3889:GLN:HE22	2:E:3963:ASN:HB3	1.79	0.46
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.47	0.46
2:G:70:GLU:HG3	2:G:117:TYR:HE1	1.80	0.46
2:E:4561:THR:O	2:E:4565:LEU:N	2.46	0.46
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.46
2:G:1727:ARG:NH2	2:G:1773:PRO:O	2.41	0.46
2:B:37:LEU:HD11	2:B:47:CYS:HB3	1.96	0.46
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.98	0.46
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.96	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.49	0.46
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.81	0.46
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.98	0.46
2:I:3889:GLN:HE22	2:I:3963:ASN:HB3	1.79	0.46
2:I:4192:ARG:HD2	2:I:5028:PHE:CE2	2.50	0.46
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.81	0.46
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.79	0.46
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.81	0.46
2:I:675:LEU:HD11	2:I:1633:PRO:HB3	1.97	0.46
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.81	0.46
2:B:621:ILE:O	2:B:625:LEU:N	2.45	0.46
2:I:512:ALA:HA	2:I:515:TRP:HB2	1.98	0.46
2:I:4561:THR:O	2:I:4565:LEU:N	2.46	0.46
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.46
2:E:472:ARG:HA	2:E:475:GLN:HB2	1.98	0.46
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.98	0.46
2:I:70:GLU:HG3	2:I:117:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.97	0.46
2:B:379:HIS:CD2	2:B:381:GLU:H	2.34	0.46
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.98	0.46
2:B:1973:GLN:O	2:B:1977:TYR:N	2.48	0.46
2:I:472:ARG:HA	2:I:475:GLN:HB2	1.98	0.46
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.98	0.46
2:G:750:LEU:HD21	2:G:777:PHE:HE2	1.80	0.46
2:G:1973:GLN:O	2:G:1977:TYR:N	2.48	0.46
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.81	0.46
2:E:675:LEU:HD11	2:E:1633:PRO:HB3	1.97	0.46
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.98	0.46
2:B:675:LEU:HD11	2:B:1633:PRO:HB3	1.97	0.46
2:B:3889:GLN:HE22	2:B:3963:ASN:HB3	1.79	0.46
2:E:236:ALA:HA	2:E:242:ARG:HD2	1.98	0.46
2:E:379:HIS:CD2	2:E:381:GLU:H	2.34	0.46
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.81	0.46
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.81	0.46
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.98	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.80	0.45
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.96	0.45
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.81	0.45
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.98	0.45
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.81	0.45
2:B:174:VAL:O	2:E:2452:ARG:NH1	2.49	0.45
2:B:2247:GLN:NE2	2:B:2285:GLU:OE2	2.49	0.45
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.97	0.45
2:G:512:ALA:HA	2:G:515:TRP:HB2	1.98	0.45
2:G:3365:UNK:O	2:G:3369:UNK:N	2.50	0.45
2:G:4236:SER:OG	2:G:4675:LYS:NZ	2.41	0.45
2:B:70:GLU:HG3	2:B:117:TYR:HE1	1.80	0.45
2:B:236:ALA:HA	2:B:242:ARG:HD2	1.99	0.45
2:E:3992:PHE:O	2:E:3996:PHE:N	2.40	0.45
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.98	0.45
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.98	0.45
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.99	0.45
2:E:1973:GLN:O	2:E:1977:TYR:N	2.48	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.98	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.97	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.34	0.45
2:G:675:LEU:HD11	2:G:1633:PRO:HB3	1.97	0.45
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:914:PRO:HD2	2:E:917:GLU:HB2	1.98	0.45
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.99	0.45
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.99	0.45
2:G:472:ARG:HA	2:G:475:GLN:HB2	1.98	0.45
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.98	0.45
2:B:19:GLU:HB2	2:B:206:CYS:HB3	1.99	0.45
2:B:4561:THR:O	2:B:4565:LEU:N	2.46	0.45
2:E:932:LEU:HA	2:E:935:LEU:HD12	1.98	0.45
2:I:2247:GLN:NE2	2:I:2285:GLU:OE2	2.49	0.45
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.99	0.45
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.98	0.45
2:B:2758:PHE:O	2:B:2762:THR:N	2.49	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.50	0.45
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.99	0.45
2:E:512:ALA:HA	2:E:515:TRP:HB2	1.98	0.45
2:I:236:ALA:HA	2:I:242:ARG:HD2	1.99	0.45
2:B:932:LEU:HA	2:B:935:LEU:HD12	1.98	0.45
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.98	0.45
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.98	0.45
2:E:4963:ILE:HD13	2:E:5027:CYS:SG	2.57	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.34	0.45
2:I:4232:GLU:OE1	2:I:5019:TRP:NE1	2.50	0.45
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.81	0.45
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.98	0.45
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.45
2:E:4959:PHE:O	2:E:4959:PHE:CG	2.70	0.45
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.99	0.45
2:I:5028:PHE:O	2:I:5028:PHE:CD1	2.70	0.45
2:G:215:THR:HG22	2:G:273:HIS:HA	1.99	0.45
2:G:4963:ILE:HD13	2:G:5027:CYS:SG	2.57	0.45
2:B:886:ARG:HB3	2:B:891:TRP:HB2	1.99	0.45
2:B:914:PRO:HD2	2:B:917:GLU:HB2	1.98	0.45
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.81	0.45
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.81	0.45
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.99	0.45
2:E:886:ARG:HB3	2:E:891:TRP:HB2	1.99	0.45
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.98	0.45
2:I:1171:SER:OG	2:I:1175:SER:N	2.45	0.45
2:I:4959:PHE:O	2:I:4959:PHE:CD1	2.70	0.45
2:G:2247:GLN:NE2	2:G:2285:GLU:OE2	2.49	0.45
2:G:4959:PHE:O	2:G:4959:PHE:CG	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:512:ALA:HA	2:B:515:TRP:HB2	1.98	0.44
2:B:4963:ILE:HD13	2:B:5027:CYS:SG	2.57	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CG	2.70	0.44
2:E:1099:GLU:OE2	2:E:1127:HIS:ND1	2.34	0.44
2:E:2247:GLN:NE2	2:E:2285:GLU:OE2	2.50	0.44
2:I:914:PRO:HD2	2:I:917:GLU:HB2	1.98	0.44
2:I:4963:ILE:HD13	2:I:5027:CYS:SG	2.57	0.44
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.99	0.44
2:G:914:PRO:HD2	2:G:917:GLU:HB2	1.98	0.44
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CD1	2.70	0.44
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.98	0.44
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.50	0.44
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.82	0.44
2:E:3365:UNK:O	2:E:3369:UNK:N	2.50	0.44
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.99	0.44
2:I:19:GLU:HB2	2:I:206:CYS:HB3	1.99	0.44
2:I:3365:UNK:O	2:I:3369:UNK:N	2.50	0.44
2:I:5028:PHE:O	2:I:5028:PHE:CG	2.70	0.44
2:G:236:ALA:HA	2:G:242:ARG:HD2	1.99	0.44
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.83	0.44
2:B:2347:GLU:O	2:B:2351:ASN:N	2.39	0.44
2:E:4959:PHE:O	2:E:4959:PHE:CD1	2.70	0.44
2:I:1973:GLN:O	2:I:1977:TYR:N	2.48	0.44
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.00	0.44
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.98	0.44
2:G:5028:PHE:O	2:G:5028:PHE:CG	2.70	0.44
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.99	0.44
2:B:4959:PHE:CG	2:B:4959:PHE:O	2.70	0.44
2:E:580:GLU:HG2	2:E:583:ILE:HD11	2.00	0.44
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.99	0.44
2:E:3762:ARG:NH2	2:E:4757:LYS:O	2.51	0.44
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.45	0.44
2:I:932:LEU:HA	2:I:935:LEU:HD12	1.98	0.44
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.50	0.44
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.91	0.44
2:G:3762:ARG:NH2	2:G:4757:LYS:O	2.51	0.44
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.00	0.44
2:B:983:THR:O	2:B:987:ARG:N	2.50	0.44
2:B:4232:GLU:OE1	2:B:5019:TRP:NE1	2.50	0.44
2:E:983:THR:O	2:E:987:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.00	0.44
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	2.00	0.44
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.99	0.44
2:G:4232:GLU:OE1	2:G:5019:TRP:NE1	2.50	0.44
2:B:164:ARG:N	2:B:167:ASP:OD2	2.51	0.44
2:B:485:SER:O	2:B:489:ASN:N	2.42	0.44
2:B:3762:ARG:NH2	2:B:4757:LYS:O	2.51	0.44
2:B:4959:PHE:O	2:B:4959:PHE:CD1	2.70	0.44
2:E:215:THR:HG22	2:E:273:HIS:HA	1.99	0.44
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.91	0.44
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	1.99	0.44
2:I:1739:THR:H	2:I:1742:THR:HB	1.83	0.44
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	1.99	0.44
2:B:2447:LYS:HG3	2:B:2449:GLU:H	1.83	0.44
2:B:4998:LYS:NZ	2:B:5007:GLU:OE1	2.46	0.44
2:B:5028:PHE:O	2:B:5028:PHE:CD1	2.70	0.44
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.50	0.44
2:E:5028:PHE:CG	2:E:5028:PHE:O	2.70	0.44
2:I:215:THR:HG22	2:I:273:HIS:HA	1.99	0.44
2:I:4959:PHE:O	2:I:4959:PHE:CG	2.70	0.44
2:G:932:LEU:HA	2:G:935:LEU:HD12	1.98	0.44
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.00	0.44
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	1.99	0.44
2:G:4959:PHE:O	2:G:4959:PHE:CD1	2.70	0.44
2:B:864:PRO:HD2	2:B:867:LEU:HD12	2.00	0.44
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.99	0.44
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.00	0.44
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.99	0.44
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.82	0.44
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.99	0.44
2:E:5028:PHE:O	2:E:5028:PHE:CD1	2.70	0.44
2:I:164:ARG:N	2:I:167:ASP:OD2	2.51	0.44
2:I:2447:LYS:HG3	2:I:2449:GLU:H	1.83	0.44
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.99	0.44
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.99	0.44
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.50	0.44
2:G:4561:THR:O	2:G:4565:LEU:N	2.46	0.44
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.91	0.43
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.99	0.43
2:E:1739:THR:H	2:E:1742:THR:HB	1.83	0.43
2:E:4232:GLU:OE1	2:E:5019:TRP:NE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.99	0.43
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	2.00	0.43
2:I:3762:ARG:NH2	2:I:4757:LYS:O	2.51	0.43
2:G:19:GLU:HB2	2:G:206:CYS:HB3	1.99	0.43
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	2.00	0.43
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.99	0.43
2:B:1154:ASP:O	2:B:1158:ASN:N	2.51	0.43
2:B:1739:THR:H	2:B:1742:THR:HB	1.83	0.43
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.99	0.43
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.99	0.43
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.99	0.43
2:B:2466:LEU:HD23	2:B:2469:ILE:HD12	2.00	0.43
2:E:19:GLU:HB2	2:E:206:CYS:HB3	1.99	0.43
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.00	0.43
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.99	0.43
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.52	0.43
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.99	0.43
2:I:1154:ASP:O	2:I:1158:ASN:N	2.51	0.43
2:G:164:ARG:N	2:G:167:ASP:OD2	2.51	0.43
2:G:864:PRO:HD2	2:G:867:LEU:HD12	2.00	0.43
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.83	0.43
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.91	0.43
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.84	0.43
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	2.00	0.43
2:I:2466:LEU:HD23	2:I:2469:ILE:HD12	2.00	0.43
2:G:2447:LYS:HG3	2:G:2449:GLU:H	1.83	0.43
2:E:2447:LYS:HG3	2:E:2449:GLU:H	1.83	0.43
2:I:1284:UNK:HA	2:I:1463:UNK:HA	2.00	0.43
2:G:3992:PHE:O	2:G:3996:PHE:N	2.40	0.43
2:B:215:THR:HG22	2:B:273:HIS:HA	1.99	0.43
2:B:4899:ASP:OD1	2:E:4892:ARG:NH2	2.50	0.43
2:E:864:PRO:HD2	2:E:867:LEU:HD12	2.00	0.43
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	2.00	0.43
2:E:2347:GLU:O	2:E:2351:ASN:N	2.39	0.43
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.83	0.43
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.99	0.43
2:B:1284:UNK:HA	2:B:1463:UNK:HA	2.00	0.43
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	2.00	0.43
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.84	0.43
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	2.00	0.43
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:164:ARG:N	2:E:167:ASP:OD2	2.51	0.43
2:E:2290:LEU:HB3	2:E:3849:ARG:HH12	1.84	0.43
2:G:1154:ASP:O	2:G:1158:ASN:N	2.51	0.43
2:G:1739:THR:H	2:G:1742:THR:HB	1.83	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	1.99	0.43
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	2.00	0.43
2:B:1728:ARG:HA	2:B:1731:LEU:HB2	2.01	0.43
2:E:1284:UNK:HA	2:E:1463:UNK:HA	2.00	0.43
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	2.00	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	1.99	0.43
2:I:1728:ARG:HA	2:I:1731:LEU:HB2	2.01	0.43
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.84	0.43
2:G:983:THR:O	2:G:987:ARG:N	2.49	0.43
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.84	0.43
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.99	0.43
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	2.01	0.43
2:I:401:ALA:HA	2:I:404:ILE:HD12	2.01	0.43
2:I:983:THR:O	2:I:987:ARG:N	2.50	0.43
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.84	0.43
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	2.00	0.43
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.84	0.43
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	2.01	0.43
2:E:1154:ASP:O	2:E:1158:ASN:N	2.51	0.43
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	2.01	0.43
2:E:1859:VAL:HA	2:E:1862:ILE:HG12	2.01	0.43
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.83	0.43
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	2.01	0.43
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.00	0.43
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	2.01	0.43
2:G:886:ARG:HB3	2:G:891:TRP:HB2	1.99	0.43
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	2.01	0.43
2:G:2466:LEU:HD23	2:G:2469:ILE:HD12	2.00	0.43
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.00	0.42
2:E:2466:LEU:HD23	2:E:2469:ILE:HD12	2.00	0.42
2:I:1859:VAL:HA	2:I:1862:ILE:HG12	2.01	0.42
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.42
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	2.01	0.42
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	2.00	0.42
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.83	0.42
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	2.01	0.42
2:E:401:ALA:HA	2:E:404:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	2.01	0.42
2:I:864:PRO:HD2	2:I:867:LEU:HD12	2.00	0.42
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.53	0.42
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	2.00	0.42
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.83	0.42
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.53	0.42
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	2.01	0.42
1:H:82:TYR:O	1:H:86:GLY:N	2.52	0.42
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.52	0.42
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.53	0.42
2:G:2290:LEU:HB3	2:G:3849:ARG:HH12	1.84	0.42
2:B:2290:LEU:HB3	2:B:3849:ARG:HH12	1.84	0.42
2:B:2793:PRO:HG3	2:B:2855:TYR:CZ	2.55	0.42
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.42
2:I:2758:PHE:O	2:I:2762:THR:N	2.49	0.42
2:I:3513:UNK:O	2:I:3515:UNK:N	2.53	0.42
2:I:4560:TYR:O	2:I:4564:PHE:N	2.49	0.42
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	2.01	0.42
2:G:695:TYR:OH	2:G:1073:ARG:NH1	2.51	0.42
2:B:278:GLN:N	2:B:315:CYS:SG	2.92	0.42
2:B:401:ALA:HA	2:B:404:ILE:HD12	2.00	0.42
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	2.02	0.42
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	2.01	0.42
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.52	0.42
2:E:1105:ALA:N	2:E:1189:LEU:O	2.53	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:G:1105:ALA:N	2:G:1189:LEU:O	2.53	0.42
1:F:82:TYR:O	1:F:86:GLY:N	2.53	0.42
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.84	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	2.02	0.42
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.93	0.42
2:I:1025:ARG:O	2:I:1032:LYS:NZ	2.44	0.42
2:I:1099:GLU:OE2	2:I:1127:HIS:ND1	2.34	0.42
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	2.01	0.42
2:I:2290:LEU:HB3	2:I:3849:ARG:HH12	1.84	0.42
2:I:2793:PRO:HG3	2:I:2855:TYR:CZ	2.55	0.42
2:I:2902:HIS:CE1	2:I:2904:LEU:HB2	2.55	0.42
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	2.00	0.42
2:B:695:TYR:OH	2:B:1073:ARG:NH1	2.51	0.42
2:B:1105:ALA:N	2:B:1189:LEU:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	2.00	0.42
2:I:695:TYR:OH	2:I:1073:ARG:NH1	2.51	0.42
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.93	0.42
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	2.02	0.42
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	2.02	0.42
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.93	0.42
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	2.02	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.55	0.42
2:I:4239:GLU:OE2	2:I:5014:TYR:OH	2.32	0.42
2:G:1595:LEU:HD23	2:G:1595:LEU:HA	1.95	0.42
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	2.01	0.42
2:E:3513:UNK:O	2:E:3515:UNK:N	2.53	0.42
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.85	0.42
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.55	0.42
2:B:1141:ARG:H	2:B:1141:ARG:HD2	1.85	0.42
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	2.02	0.42
2:E:2902:HIS:CE1	2:E:2904:LEU:HB2	2.55	0.42
2:G:1728:ARG:HA	2:G:1731:LEU:HB2	2.01	0.42
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	2.01	0.41
2:B:2902:HIS:CE1	2:B:2904:LEU:HB2	2.55	0.41
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	2.01	0.41
2:E:635:THR:HG23	2:E:1693:GLN:HE22	1.85	0.41
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	2.01	0.41
2:E:2793:PRO:HG3	2:E:2855:TYR:CZ	2.55	0.41
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	2.02	0.41
2:I:1089:TYR:N	2:I:1224:GLU:O	2.53	0.41
2:I:1247:PRO:HA	2:I:1598:GLN:HA	2.02	0.41
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	2.02	0.41
2:G:2793:PRO:HG3	2:G:2855:TYR:CZ	2.55	0.41
2:G:3513:UNK:O	2:G:3515:UNK:N	2.53	0.41
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.02	0.41
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.02	0.41
2:B:1859:VAL:HA	2:B:1862:ILE:HG12	2.01	0.41
2:E:451:TYR:O	2:E:474:ARG:NH1	2.48	0.41
2:E:1089:TYR:N	2:E:1224:GLU:O	2.53	0.41
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.53	0.41
2:E:3694:LYS:HA	2:E:3695:PRO:HD3	1.93	0.41
2:E:4197:ILE:HG21	2:E:4202:ARG:HH21	1.85	0.41
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.84	0.41
2:E:4928:LEU:HD13	2:E:4931:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	2.01	0.41
2:I:2883:HIS:NE2	2:I:2906:VAL:O	2.50	0.41
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.85	0.41
2:G:1802:ILE:HG21	2:G:1807:LEU:HD22	2.02	0.41
2:G:1859:VAL:HA	2:G:1862:ILE:HG12	2.01	0.41
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.41
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.02	0.41
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.85	0.41
2:E:1247:PRO:HA	2:E:1598:GLN:HA	2.02	0.41
2:E:1728:ARG:HA	2:E:1731:LEU:HB2	2.01	0.41
2:I:1077:ALA:HB3	2:I:1189:LEU:HD11	2.03	0.41
2:I:4197:ILE:HG21	2:I:4202:ARG:HH21	1.85	0.41
2:G:1284:UNK:HA	2:G:1463:UNK:HA	2.00	0.41
2:G:2902:HIS:CE1	2:G:2904:LEU:HB2	2.55	0.41
2:B:261:ARG:HB3	2:B:283:ARG:HB3	2.02	0.41
2:B:1247:PRO:HA	2:B:1598:GLN:HA	2.02	0.41
2:B:4957:LYS:HG2	2:B:4964:GLY:HA2	2.03	0.41
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.93	0.41
2:G:401:ALA:HA	2:G:404:ILE:HD12	2.01	0.41
2:E:4239:GLU:OE2	2:E:5014:TYR:OH	2.32	0.41
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	2.01	0.41
2:E:4978:HIS:CA	2:E:4982:GLU:HB2	2.43	0.41
2:I:261:ARG:HB3	2:I:283:ARG:HB3	2.02	0.41
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.02	0.41
2:I:2272:PRO:HA	2:I:2275:VAL:HG12	2.03	0.41
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.29	0.41
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.54	0.41
2:G:1077:ALA:HB3	2:G:1189:LEU:HD11	2.03	0.41
2:G:1089:TYR:N	2:G:1224:GLU:O	2.54	0.41
2:G:4197:ILE:HG21	2:G:4202:ARG:HH21	1.85	0.41
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	2.03	0.41
2:B:3513:UNK:O	2:B:3515:UNK:N	2.53	0.41
2:B:3552:UNK:O	2:B:3556:UNK:N	2.54	0.41
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.56	0.41
2:E:1077:ALA:HB3	2:E:1189:LEU:HD11	2.03	0.41
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.56	0.41
2:I:4996:ILE:HD12	4:I:5102:CFF:H123	2.03	0.41
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.55	0.41
2:G:2758:PHE:O	2:G:2762:THR:N	2.49	0.41
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.02	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1077:ALA:HB3	2:B:1189:LEU:HD11	2.03	0.41
2:E:1025:ARG:O	2:E:1032:LYS:NZ	2.44	0.41
2:E:1141:ARG:H	2:E:1141:ARG:HD2	1.85	0.41
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.02	0.41
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.55	0.41
2:I:3552:UNK:O	2:I:3556:UNK:N	2.54	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.56	0.41
2:G:4996:ILE:HD12	4:G:5102:CFF:H123	2.03	0.41
2:G:4998:LYS:NZ	2:G:5007:GLU:OE1	2.46	0.41
1:A:92:PRO:HD3	2:B:627:PRO:HB2	2.02	0.41
2:B:4197:ILE:HG21	2:B:4202:ARG:HH21	1.85	0.41
2:E:1171:SER:OG	2:E:1175:SER:N	2.45	0.41
2:E:3552:UNK:O	2:E:3556:UNK:N	2.54	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.84	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.85	0.41
2:I:4928:LEU:HD13	2:I:4931:ILE:HD12	2.03	0.41
2:G:134:ASP:OD1	2:G:134:ASP:N	2.53	0.41
2:G:635:THR:HG23	2:G:1693:GLN:HE22	1.85	0.41
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	2.03	0.41
2:G:3552:UNK:O	2:G:3556:UNK:N	2.54	0.41
2:B:134:ASP:OD1	2:B:134:ASP:N	2.53	0.41
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.54	0.41
2:B:2378:ALA:O	2:B:2382:GLU:N	2.54	0.41
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	2.03	0.41
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.02	0.41
2:E:2272:PRO:HA	2:E:2275:VAL:HG12	2.03	0.41
2:I:1802:ILE:HG21	2:I:1807:LEU:HD22	2.02	0.41
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	2.03	0.41
2:G:1247:PRO:HA	2:G:1598:GLN:HA	2.02	0.41
2:G:2272:PRO:HA	2:G:2275:VAL:HG12	2.03	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.29	0.41
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.02	0.41
2:B:635:THR:HG23	2:B:1693:GLN:HE22	1.85	0.41
2:B:1089:TYR:N	2:B:1224:GLU:O	2.54	0.41
2:B:2103:VAL:O	2:B:2107:GLN:N	2.46	0.41
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	2.03	0.41
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.56	0.41
2:I:1105:ALA:N	2:I:1189:LEU:O	2.53	0.41
2:G:3658:LYS:HA	2:G:3661:TRP:CE2	2.56	0.41
2:G:4928:LEU:HD13	2:G:4931:ILE:HD12	2.03	0.41
2:B:1802:ILE:HG21	2:B:1807:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:583:ILE:HA	2:E:586:ILE:HD12	2.03	0.40
2:E:4156:HIS:CE1	2:E:5036:LEU:HD11	2.56	0.40
2:I:235:ALA:HA	2:I:257:ARG:HD3	2.03	0.40
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.54	0.40
2:I:683:ARG:HG2	2:I:717:ASP:HB3	2.04	0.40
2:I:1076:ARG:HB3	2:I:1191:VAL:HG23	2.03	0.40
2:I:4957:LYS:HG2	2:I:4964:GLY:HA2	2.03	0.40
2:G:3694:LYS:HA	2:G:3695:PRO:HD3	1.93	0.40
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.02	0.40
2:E:134:ASP:OD1	2:E:134:ASP:N	2.53	0.40
2:E:695:TYR:OH	2:E:1073:ARG:NH1	2.51	0.40
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	2.02	0.40
2:I:635:THR:HG23	2:I:1693:GLN:HE22	1.85	0.40
2:I:4090:LYS:O	2:I:4094:GLN:N	2.53	0.40
2:I:4156:HIS:CE1	2:I:5036:LEU:HD11	2.56	0.40
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.02	0.40
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.86	0.40
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	2.02	0.40
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.84	0.40
2:B:229:GLU:HA	2:B:249:GLY:HA2	2.03	0.40
2:B:2272:PRO:HA	2:B:2275:VAL:HG12	2.03	0.40
2:E:229:GLU:HA	2:E:249:GLY:HA2	2.03	0.40
2:E:261:ARG:HB3	2:E:283:ARG:HB3	2.02	0.40
2:E:1076:ARG:HB3	2:E:1191:VAL:HG23	2.03	0.40
2:E:4996:ILE:HD12	4:E:5102:CFF:H123	2.03	0.40
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.86	0.40
2:I:3658:LYS:HA	2:I:3661:TRP:CE2	2.56	0.40
2:G:683:ARG:HG2	2:G:717:ASP:HB3	2.04	0.40
2:B:4996:ILE:HD12	4:B:5102:CFF:H123	2.03	0.40
2:E:113:HIS:O	2:E:399:GLN:NE2	2.55	0.40
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.54	0.40
2:G:261:ARG:HB3	2:G:283:ARG:HB3	2.02	0.40
2:B:4156:HIS:CE1	2:B:5036:LEU:HD11	2.56	0.40
2:E:661:LYS:HB3	2:E:808:TYR:CD1	2.57	0.40
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.80	0.40
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.03	0.40
2:G:4957:LYS:HG2	2:G:4964:GLY:HA2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	F	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	H	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3235/4416 (73%)	2916 (90%)	311 (10%)	8 (0%)	47	81
2	E	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
2	G	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
2	I	3235/4416 (73%)	2915 (90%)	312 (10%)	8 (0%)	47	81
All	All	13360/18096 (74%)	12037 (90%)	1291 (10%)	32 (0%)	50	81

All (32) 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	B	2291	GLN
2	E	1840	PRO
2	E	2291	GLN
2	I	1840	PRO

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Mol	Chain	Res	Type
2	I	2291	GLN
2	G	1840	PRO
2	G	2291	GLN
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
2	B	4667	PRO
2	E	4667	PRO
2	I	4667	PRO
2	G	4667	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	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%)	2476 (99%)	17 (1%)	84	90
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	84	90
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	84	90

All (68) 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	3787	LYS
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4944	ARG
2	B	4983	HIS
2	B	4995	LEU
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	3787	LYS
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4944	ARG
2	E	4983	HIS
2	E	4995	LEU
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	3787	LYS

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Mol	Chain	Res	Type
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4944	ARG
2	I	4983	HIS
2	I	4995	LEU
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	3787	LYS
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4944	ARG
2	G	4983	HIS
2	G	4995	LEU
2	G	5027	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	113	HIS
2	B	224	HIS
2	B	379	HIS
2	B	395	GLN
2	B	413	GLN
2	B	479	GLN
2	B	582	HIS
2	B	1206	GLN

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Mol	Chain	Res	Type
2	B	1598	GLN
2	B	1688	HIS
2	B	1693	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	2858	GLN
2	B	3809	ASN
2	B	3830	GLN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4983	HIS
2	E	57	ASN
2	E	113	HIS
2	E	224	HIS
2	E	379	HIS
2	E	395	GLN
2	E	413	GLN
2	E	479	GLN
2	E	582	HIS
2	E	765	GLN
2	E	1206	GLN
2	E	1598	GLN
2	E	1688	HIS
2	E	1693	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	2858	GLN
2	E	3809	ASN
2	E	3830	GLN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN

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Mol	Chain	Res	Type
2	E	3960	GLN
2	E	3976	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4806	ASN
2	E	4983	HIS
2	I	57	ASN
2	I	113	HIS
2	I	224	HIS
2	I	379	HIS
2	I	395	GLN
2	I	413	GLN
2	I	479	GLN
2	I	582	HIS
2	I	765	GLN
2	I	1206	GLN
2	I	1598	GLN
2	I	1688	HIS
2	I	1693	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	2858	GLN
2	I	3809	ASN
2	I	3830	GLN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3976	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4983	HIS
2	G	57	ASN
2	G	113	HIS
2	G	224	HIS
2	G	379	HIS
2	G	395	GLN
2	G	413	GLN

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Mol	Chain	Res	Type
2	G	479	GLN
2	G	582	HIS
2	G	1206	GLN
2	G	1598	GLN
2	G	1688	HIS
2	G	1693	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	2858	GLN
2	G	3809	ASN
2	G	3830	GLN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3976	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4130	ASN
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	$\#\|Z\| > 2$
3	ATP	B	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.57	5 (16%)
3	ATP	G	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	E	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.26	1 (12%)
3	ATP	E	5101	-	26,33,33	0.88	1 (3%)	31,52,52	1.58	5 (16%)
4	CFF	G	5102	-	8,15,15	2.45	3 (37%)	8,23,23	1.27	1 (12%)
3	ATP	I	5101	-	26,33,33	0.87	1 (3%)	31,52,52	1.57	5 (16%)
4	CFF	I	5102	-	8,15,15	2.46	3 (37%)	8,23,23	1.26	1 (12%)
4	CFF	B	5102	-	8,15,15	2.45	3 (37%)	8,23,23	1.26	1 (12%)

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5102	CFF	C5-C4	-4.52	1.33	1.39
4	B	5102	CFF	C5-C4	-4.48	1.33	1.39
4	G	5102	CFF	C5-C4	-4.48	1.33	1.39
4	I	5102	CFF	C5-C4	-4.48	1.33	1.39
4	I	5102	CFF	C6-N1	-4.11	1.32	1.38
4	E	5102	CFF	C6-N1	-4.09	1.32	1.38
4	B	5102	CFF	C6-N1	-4.08	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5102	CFF	C6-N1	-4.08	1.32	1.38
3	B	5101	ATP	C5-C4	2.36	1.47	1.40
3	I	5101	ATP	C5-C4	2.36	1.47	1.40
3	G	5101	ATP	C5-C4	2.36	1.47	1.40
3	E	5101	ATP	C5-C4	2.35	1.47	1.40
4	B	5102	CFF	O13-C6	-2.32	1.18	1.24
4	I	5102	CFF	O13-C6	-2.32	1.18	1.24
4	G	5102	CFF	O13-C6	-2.32	1.18	1.24
4	E	5102	CFF	O13-C6	-2.30	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	5101	ATP	PB-O3B-PG	-3.89	119.47	132.83
3	I	5101	ATP	PB-O3B-PG	-3.89	119.49	132.83
3	B	5101	ATP	PB-O3B-PG	-3.88	119.51	132.83
3	G	5101	ATP	PB-O3B-PG	-3.88	119.51	132.83
3	E	5101	ATP	N3-C2-N1	-3.53	123.17	128.68
3	I	5101	ATP	N3-C2-N1	-3.49	123.22	128.68
3	B	5101	ATP	N3-C2-N1	-3.49	123.22	128.68
3	G	5101	ATP	N3-C2-N1	-3.49	123.22	128.68
3	E	5101	ATP	C3'-C2'-C1'	3.44	106.15	100.98
3	B	5101	ATP	C3'-C2'-C1'	3.42	106.12	100.98
3	G	5101	ATP	C3'-C2'-C1'	3.41	106.11	100.98
3	I	5101	ATP	C3'-C2'-C1'	3.39	106.08	100.98
3	G	5101	ATP	PA-O3A-PB	-2.80	123.23	132.83
3	I	5101	ATP	PA-O3A-PB	-2.80	123.23	132.83
3	B	5101	ATP	PA-O3A-PB	-2.79	123.25	132.83
3	E	5101	ATP	PA-O3A-PB	-2.79	123.25	132.83
4	G	5102	CFF	C14-N7-C8	-2.79	112.02	125.43
4	E	5102	CFF	C14-N7-C8	-2.78	112.03	125.43
4	B	5102	CFF	C14-N7-C8	-2.78	112.05	125.43
4	I	5102	CFF	C14-N7-C8	-2.77	112.08	125.43
3	B	5101	ATP	C4-C5-N7	-2.43	106.87	109.40
3	I	5101	ATP	C4-C5-N7	-2.43	106.87	109.40
3	G	5101	ATP	C4-C5-N7	-2.43	106.87	109.40
3	E	5101	ATP	C4-C5-N7	-2.40	106.90	109.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	5101	ATP	PB-O3A-PA-O5’
3	B	5101	ATP	C5’-O5’-PA-O3A
3	E	5101	ATP	PB-O3A-PA-O5’
3	E	5101	ATP	C5’-O5’-PA-O2A
3	E	5101	ATP	C5’-O5’-PA-O3A
3	I	5101	ATP	PB-O3A-PA-O5’
3	I	5101	ATP	C5’-O5’-PA-O3A
3	G	5101	ATP	PB-O3A-PA-O5’
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	C5’-O5’-PA-O1A
3	I	5101	ATP	C5’-O5’-PA-O1A
3	G	5101	ATP	C5’-O5’-PA-O1A
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

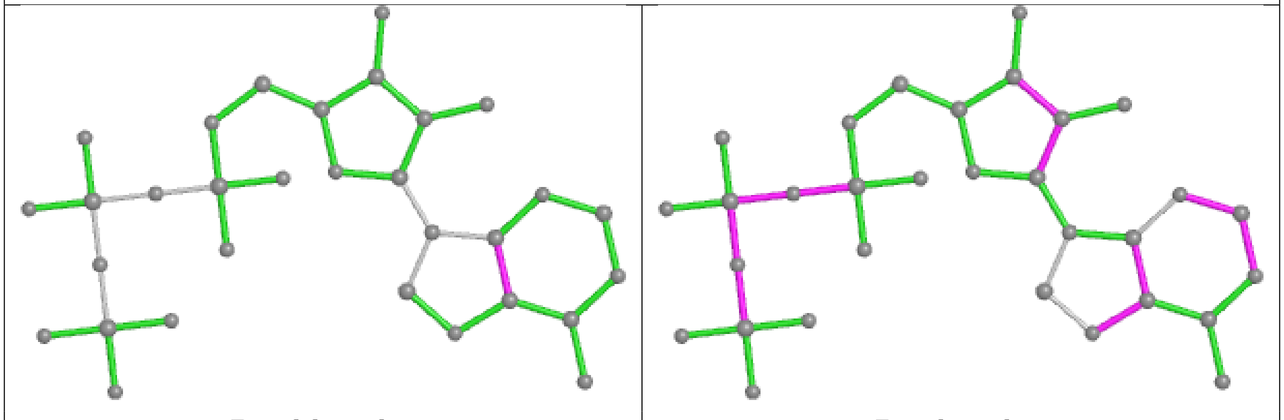
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5102	CFF	1	0
4	G	5102	CFF	1	0
4	I	5102	CFF	1	0
4	B	5102	CFF	1	0

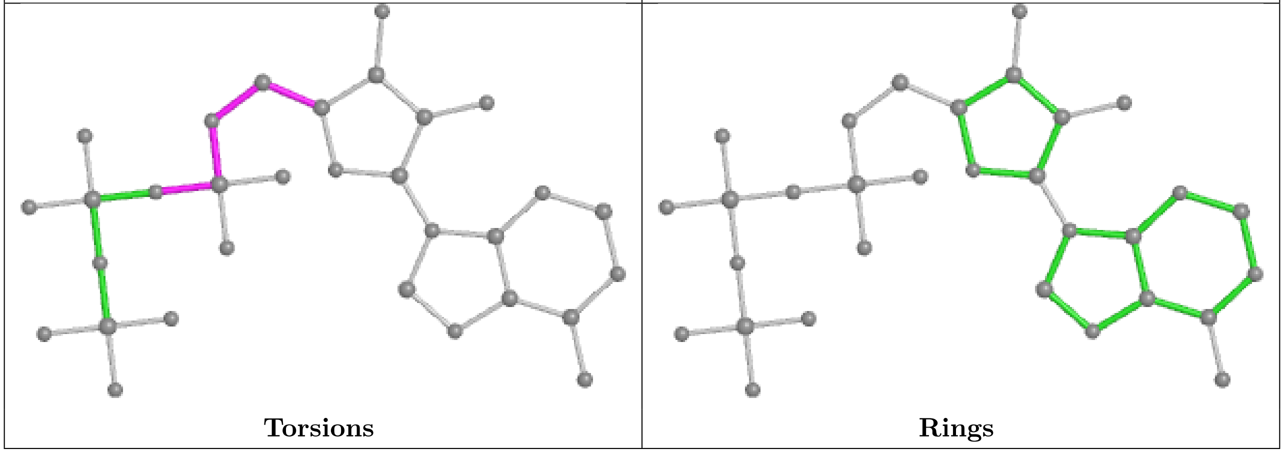
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ATP B 5101



Bond lengths

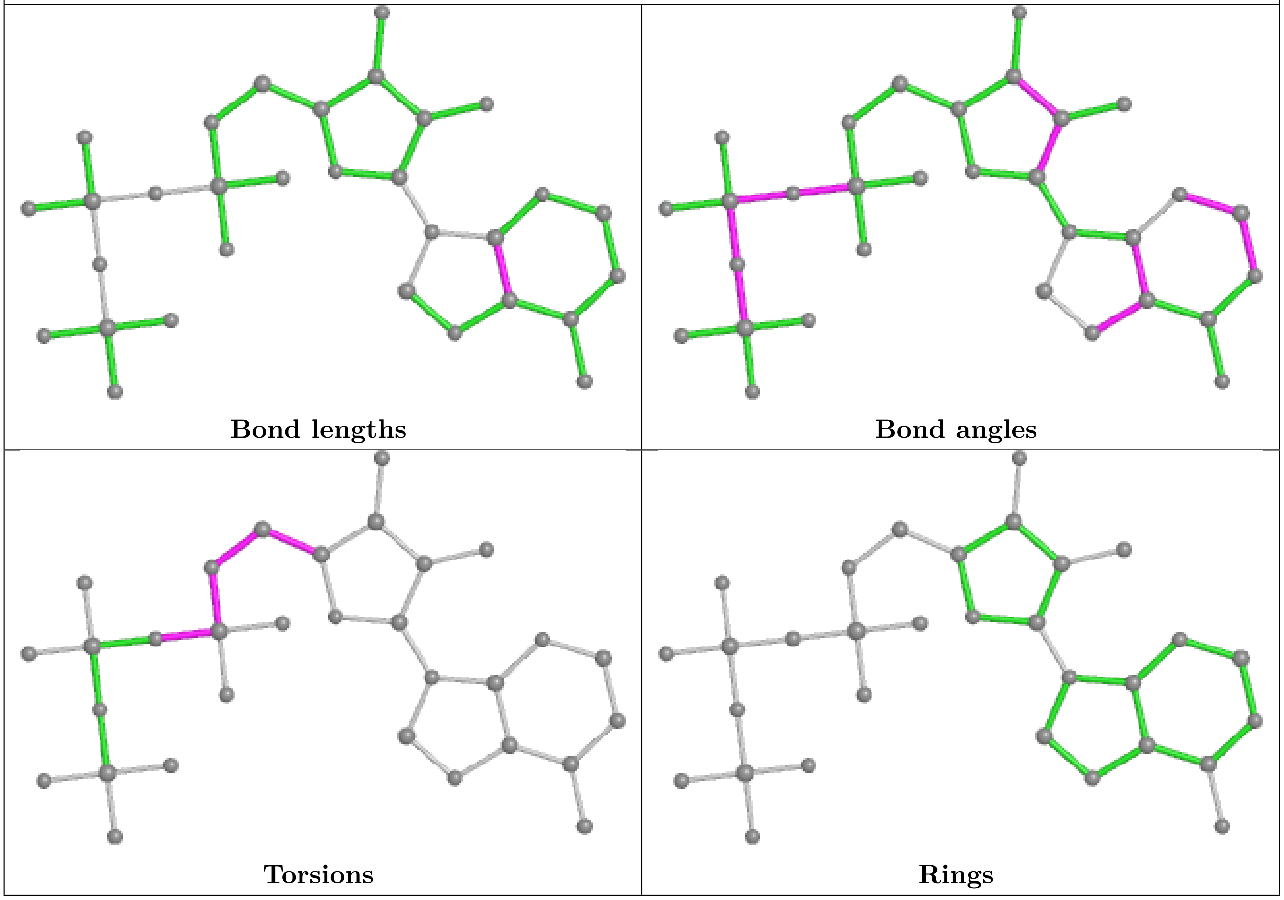
Bond angles



Torsions

Rings

Ligand ATP G 5101



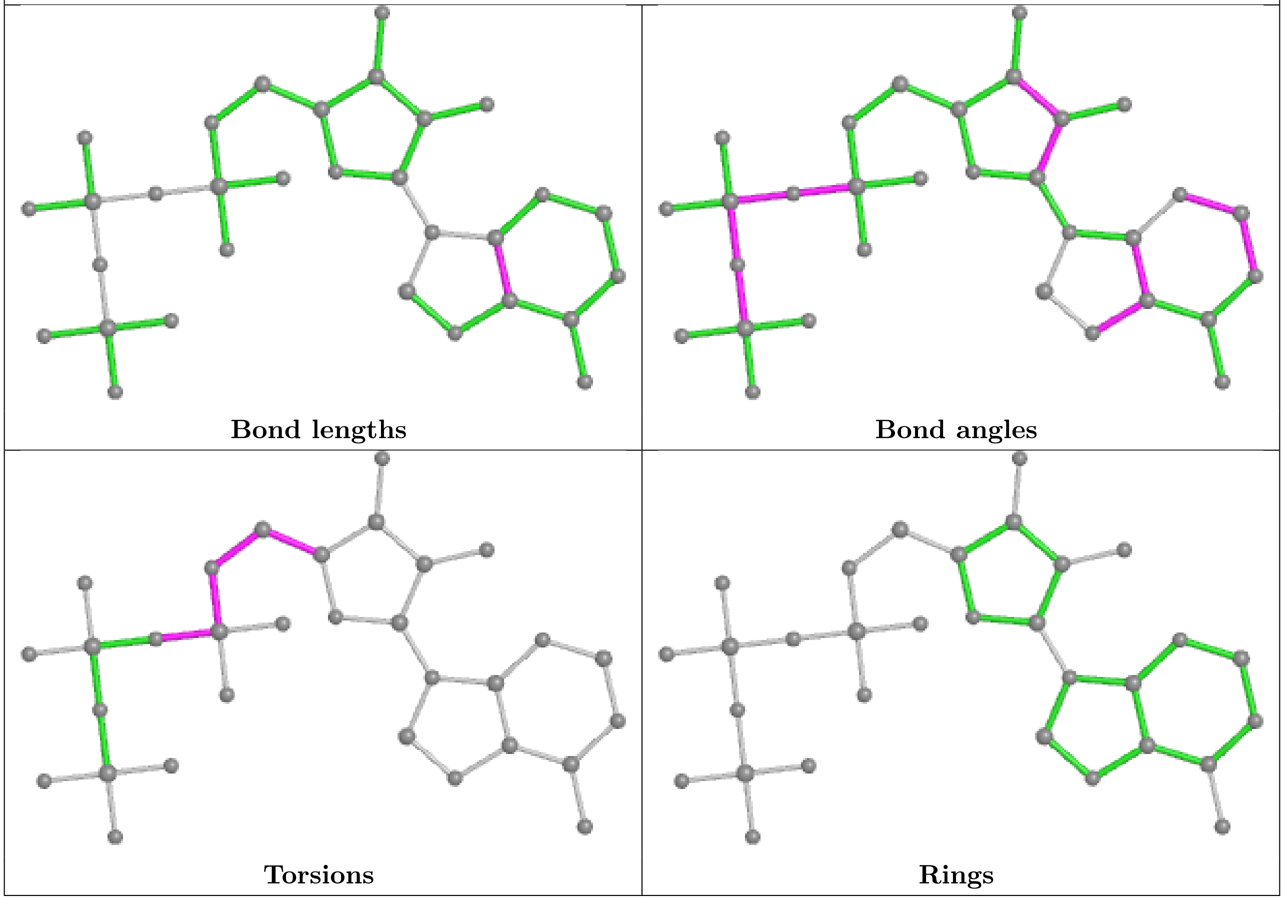
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP E 5101



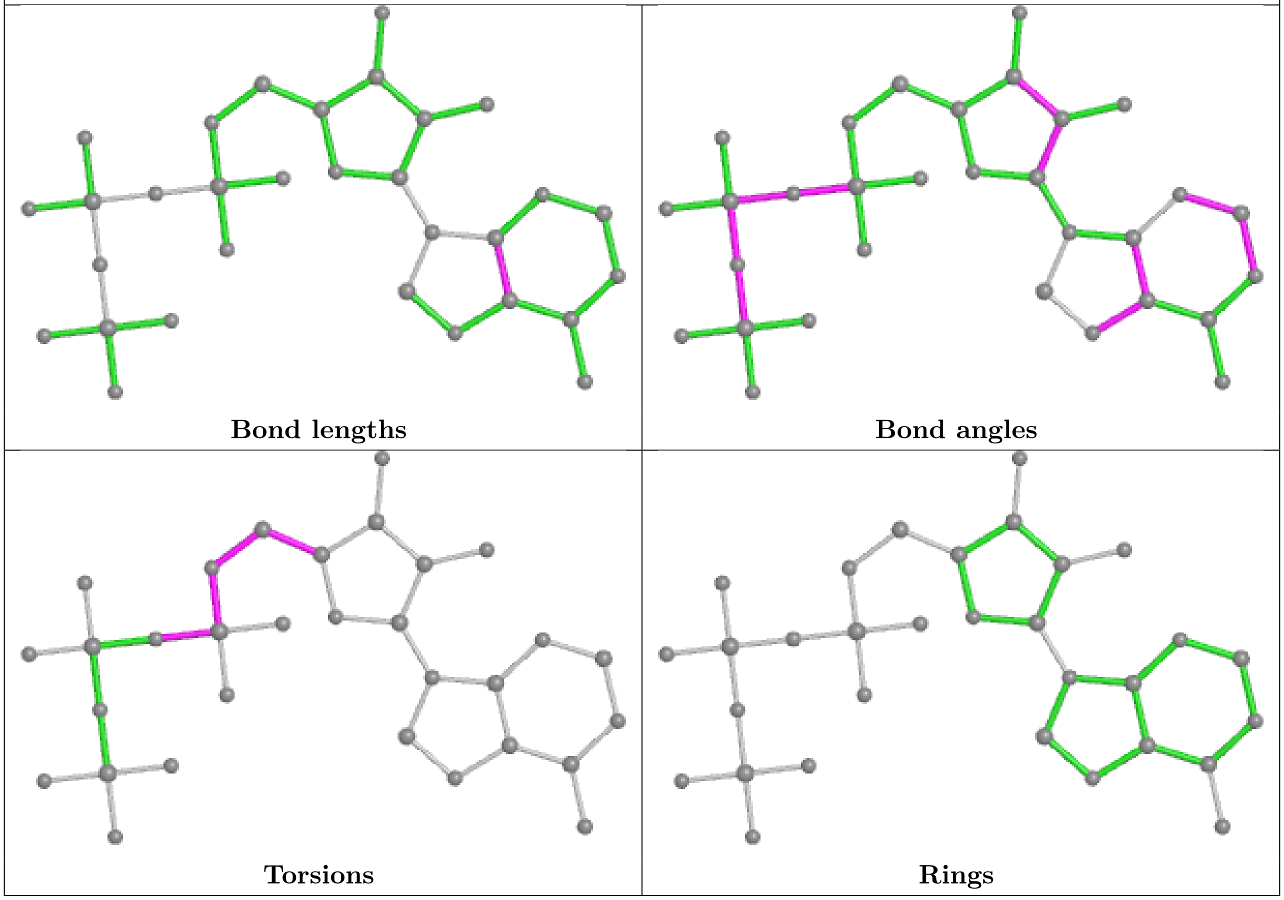
Bond lengths

Bond angles

Torsions

Rings

Ligand ATP I 5101



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	72.89
1	E	4345:UNK	C	4540:PHE	N	72.89

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	4345:UNK	C	4540:PHE	N	72.89
1	G	4345:UNK	C	4540:PHE	N	72.89
1	B	3613:UNK	C	3639:THR	N	44.63
1	E	3613:UNK	C	3639:THR	N	44.63
1	I	3613:UNK	C	3639:THR	N	44.63
1	G	3613:UNK	C	3639:THR	N	44.63
1	B	4253:GLU	C	4320:UNK	N	25.42
1	E	4253:GLU	C	4320:UNK	N	25.42
1	I	4253:GLU	C	4320:UNK	N	25.42
1	G	4253:GLU	C	4320:UNK	N	25.42
1	B	3163:UNK	C	3170:UNK	N	15.89
1	E	3163:UNK	C	3170:UNK	N	15.89
1	I	3163:UNK	C	3170:UNK	N	15.89
1	G	3163:UNK	C	3170:UNK	N	15.89
1	B	3063:UNK	C	3134:UNK	N	15.28
1	E	3063:UNK	C	3134:UNK	N	15.28
1	I	3063:UNK	C	3134:UNK	N	15.28
1	G	3063:UNK	C	3134:UNK	N	15.28
1	B	3468:UNK	C	3511:UNK	N	14.58
1	E	3468:UNK	C	3511:UNK	N	14.58
1	I	3468:UNK	C	3511:UNK	N	14.58
1	G	3468:UNK	C	3511:UNK	N	14.58
1	I	2703:UNK	C	2734:ASN	N	13.79
1	B	2703:UNK	C	2734:ASN	N	13.78
1	E	2703:UNK	C	2734:ASN	N	13.78
1	G	2703:UNK	C	2734:ASN	N	13.78
1	B	3236:UNK	C	3241:UNK	N	13.29
1	E	3236:UNK	C	3241:UNK	N	13.29
1	I	3236:UNK	C	3241:UNK	N	13.29
1	G	3236:UNK	C	3241:UNK	N	13.29
1	B	2976:UNK	C	2995:UNK	N	12.55
1	E	2976:UNK	C	2995:UNK	N	12.55
1	I	2976:UNK	C	2995:UNK	N	12.55
1	G	2976:UNK	C	2995:UNK	N	12.55
1	B	1564:UNK	C	1573:MET	N	12.52
1	E	1564:UNK	C	1573:MET	N	12.52
1	I	1564:UNK	C	1573:MET	N	12.52
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	3254:UNK	C	3261:UNK	N	8.35
1	E	3254:UNK	C	3261:UNK	N	8.35
1	I	3254:UNK	C	3261:UNK	N	8.35
1	G	3254:UNK	C	3261:UNK	N	8.35

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1297:UNK	C	1430:UNK	N	6.00
1	E	1297:UNK	C	1430:UNK	N	6.00
1	I	1297:UNK	C	1430:UNK	N	6.00
1	G	1297:UNK	C	1430:UNK	N	6.00
1	B	2939:ARG	C	2942:UNK	N	3.26
1	E	2939:ARG	C	2942:UNK	N	3.26
1	I	2939:ARG	C	2942:UNK	N	3.26
1	G	2939:ARG	C	2942:UNK	N	3.26
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

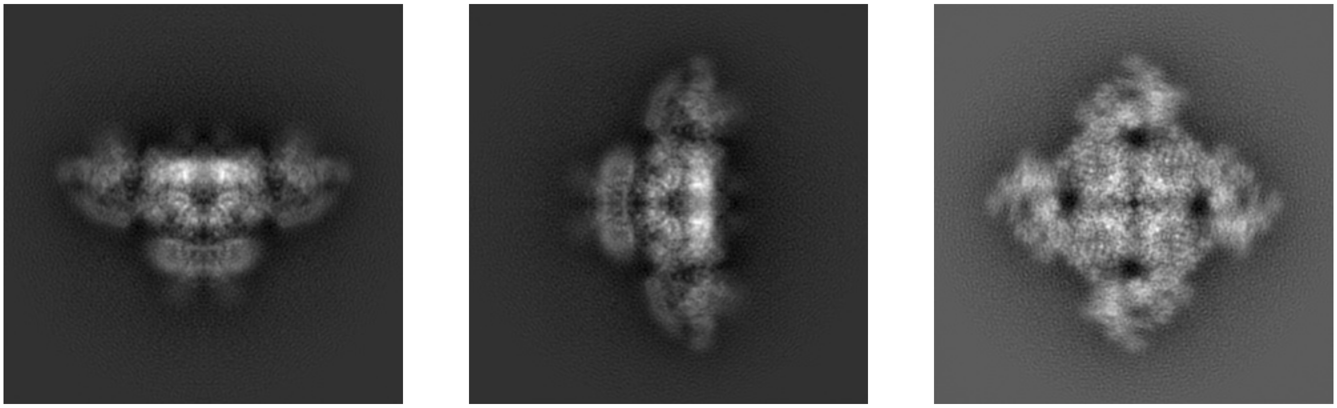
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-8386. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

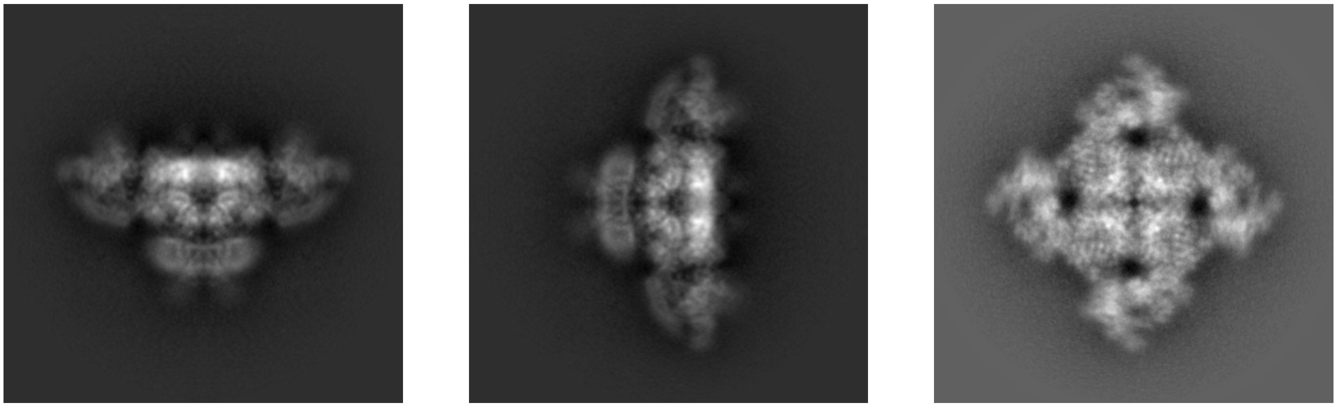
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

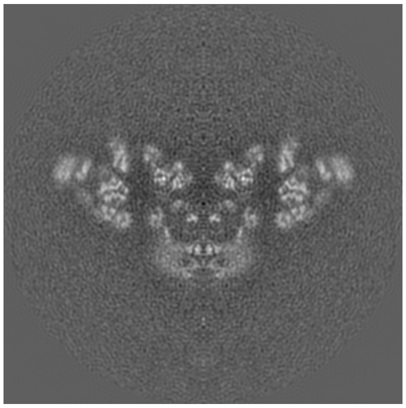


X Y Z

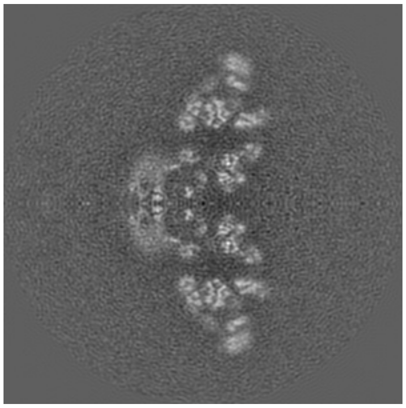
The images above show the map projected in three orthogonal directions.

6.2 Central slices

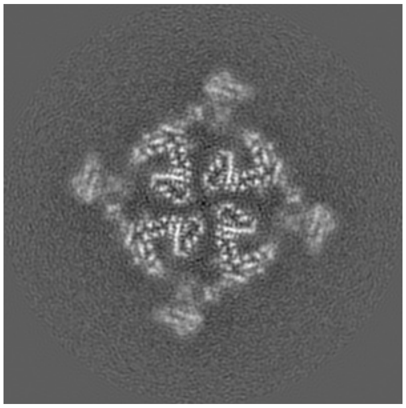
6.2.1 Primary map



X Index: 200

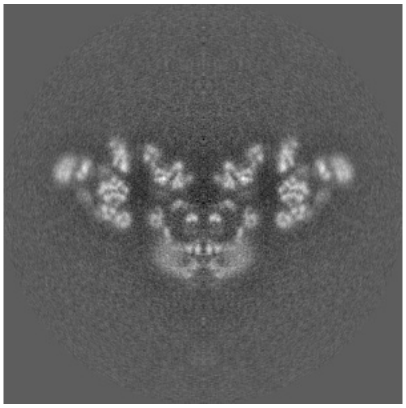


Y Index: 200

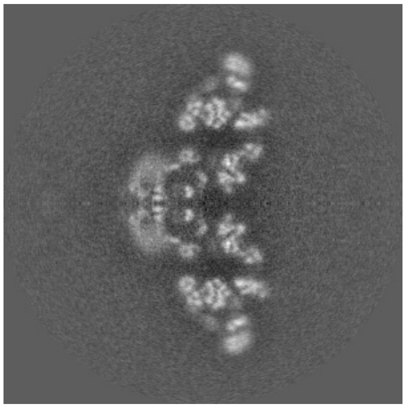


Z Index: 200

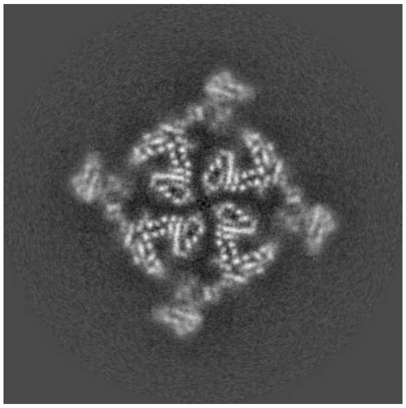
6.2.2 Raw map



X Index: 200



Y Index: 200

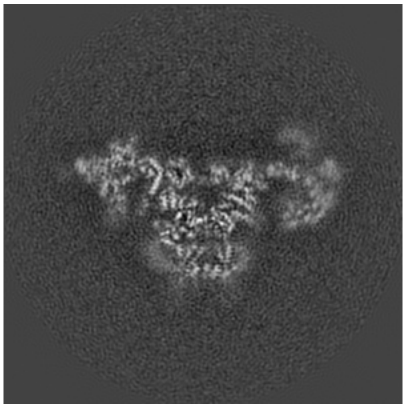


Z Index: 200

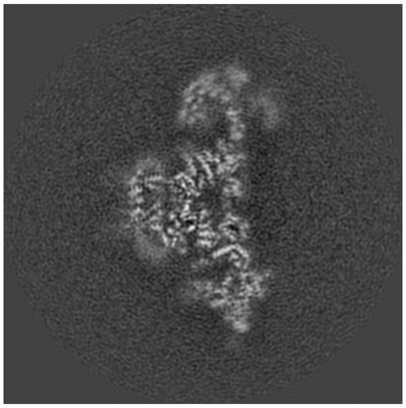
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

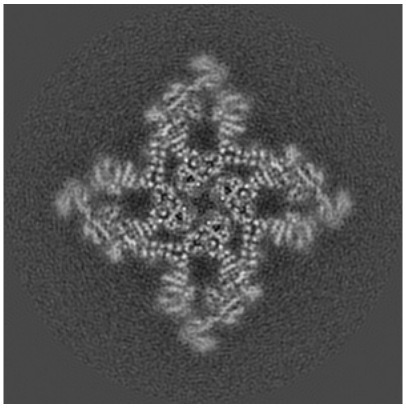
6.3.1 Primary map



X Index: 216

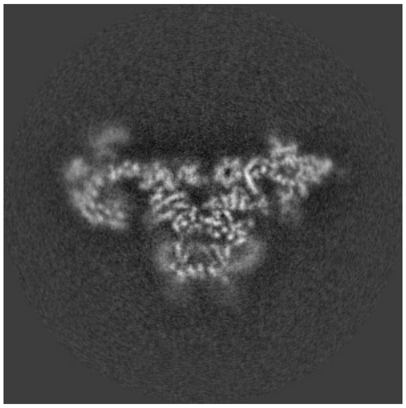


Y Index: 184

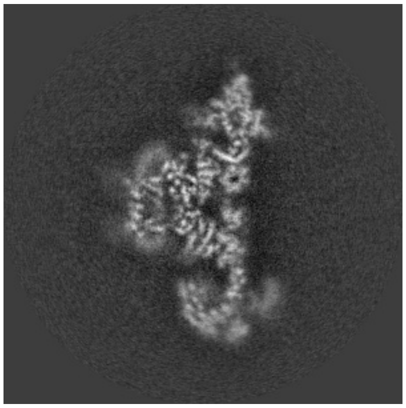


Z Index: 228

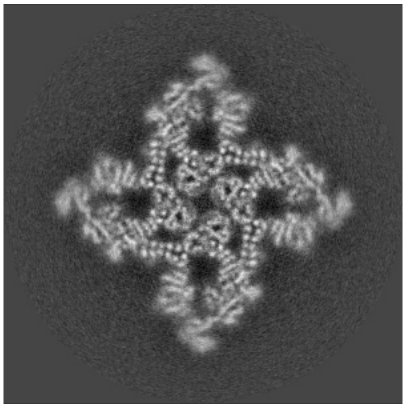
6.3.2 Raw map



X Index: 183



Y Index: 217



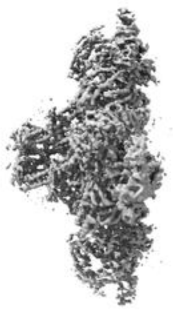
Z Index: 228

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

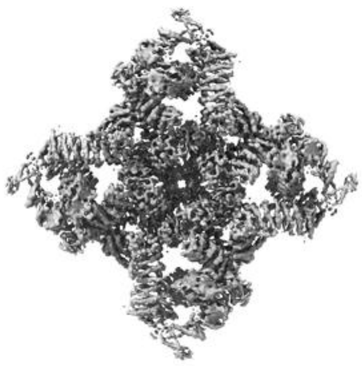
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y

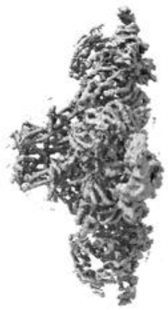


Z

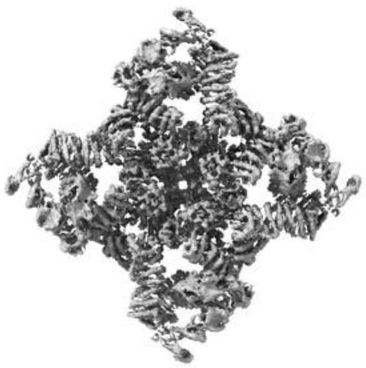
The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

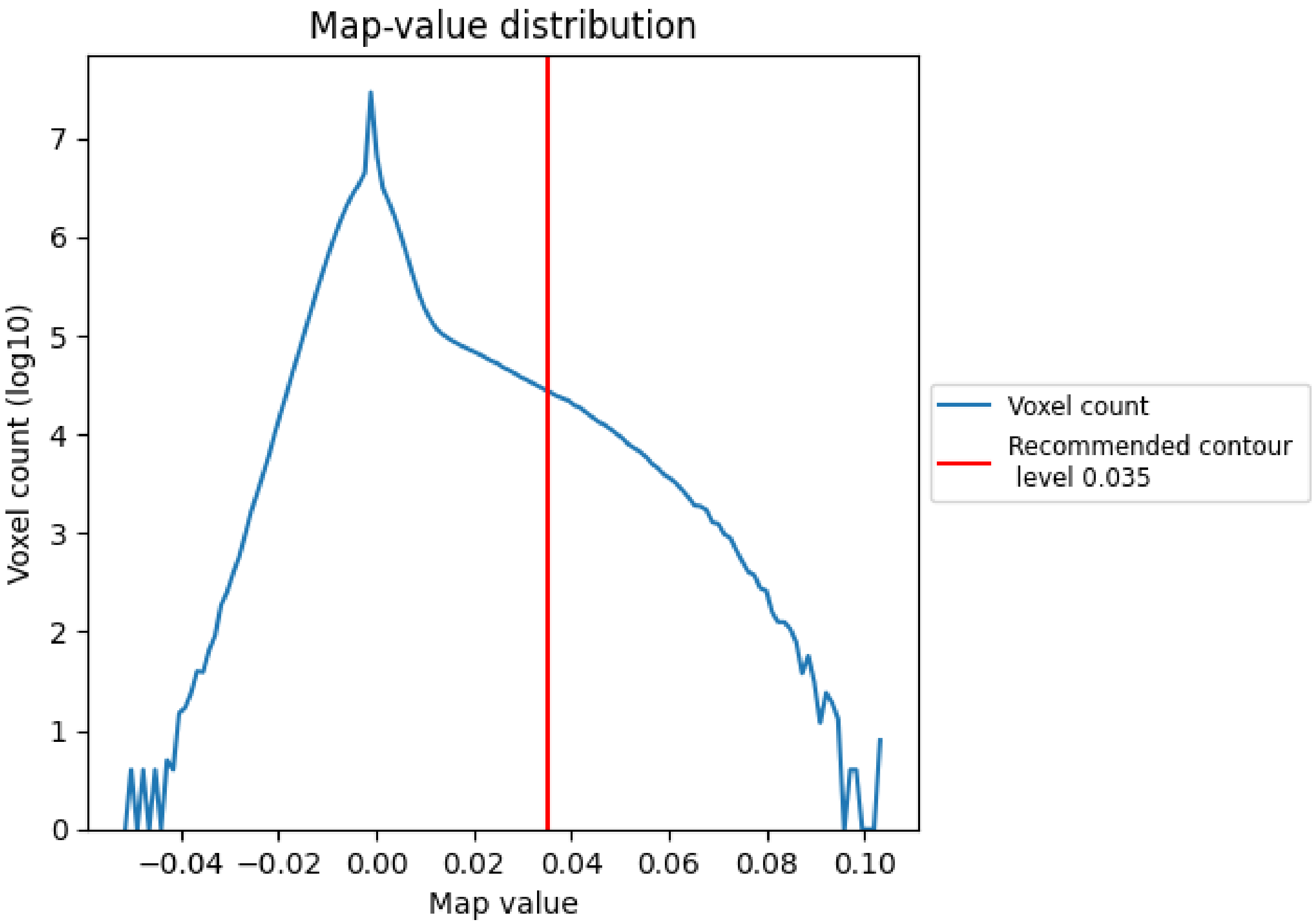
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

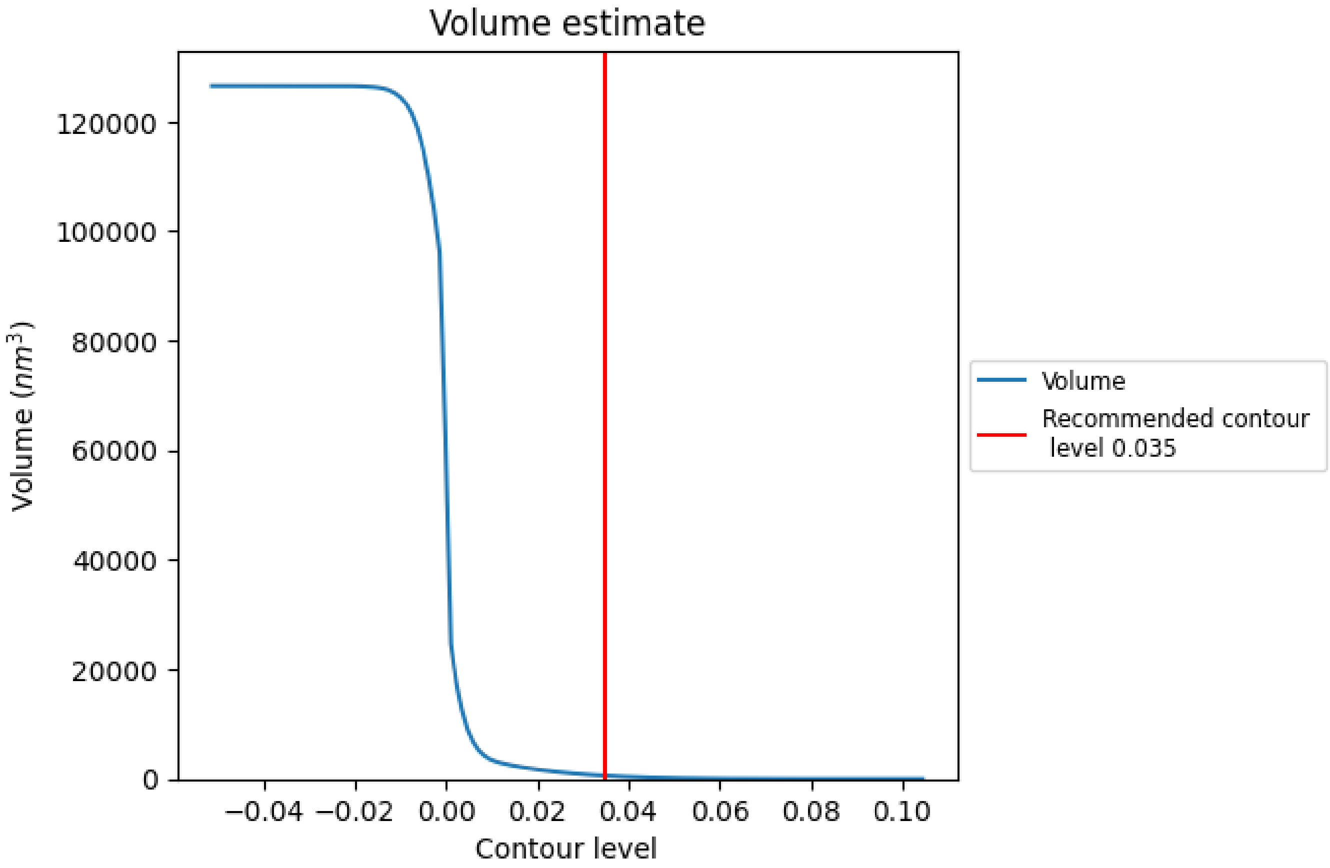
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

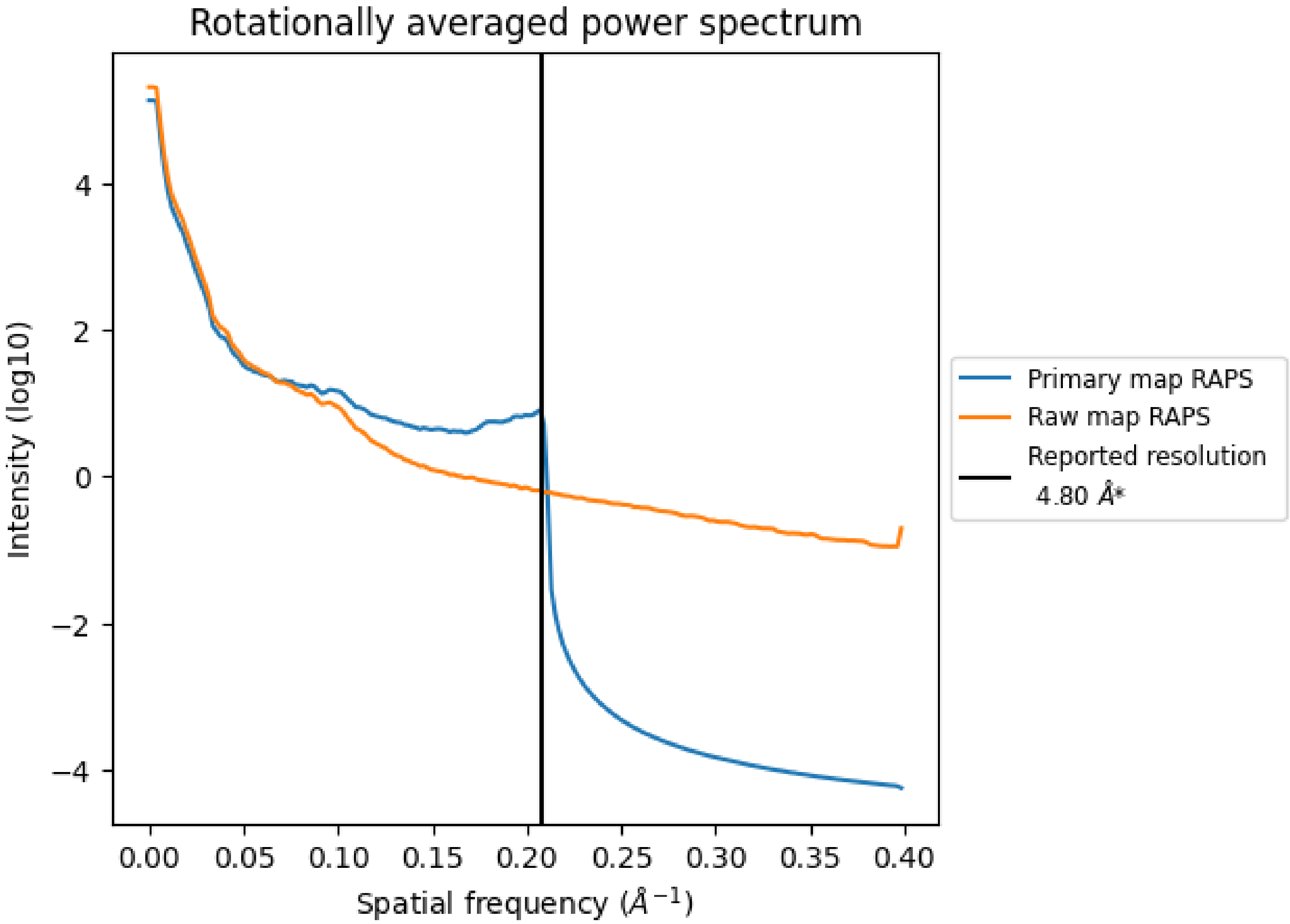
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 605 nm^3; this corresponds to an approximate mass of 547 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 ⓘ

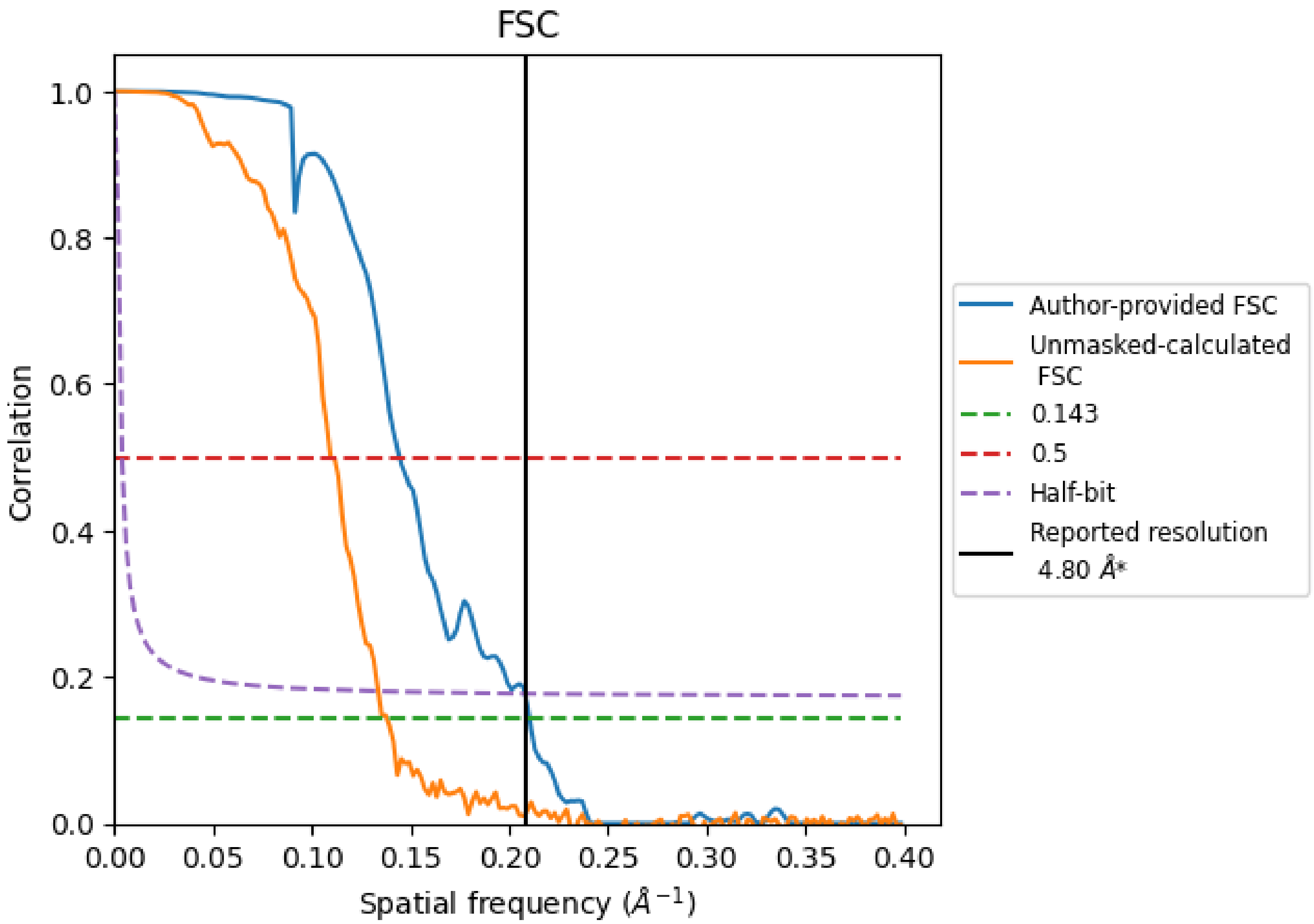


*Reported resolution corresponds to spatial frequency of 0.208 Å^{-1}

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 0.208 Å^{-1}

8.2 Resolution estimates ⓘ

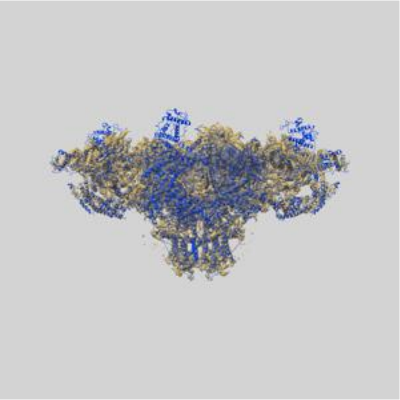
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.76	6.92	4.81
Unmasked-calculated*	7.24	9.13	7.48

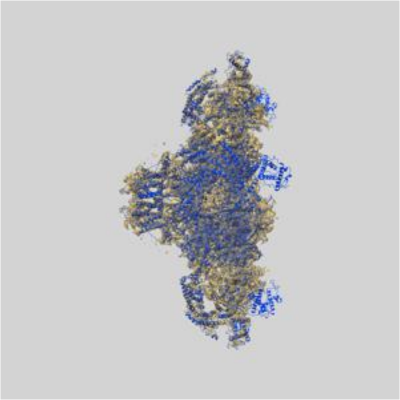
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.24 differs from the reported value 4.8 by more than 10 %

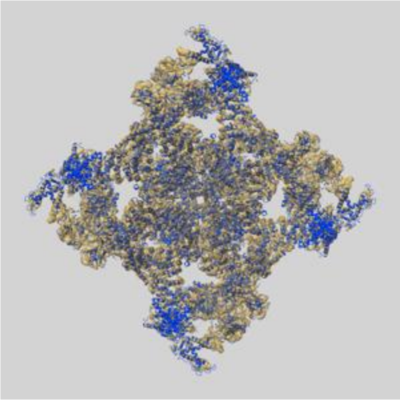
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8386 and PDB model 5TAV. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay

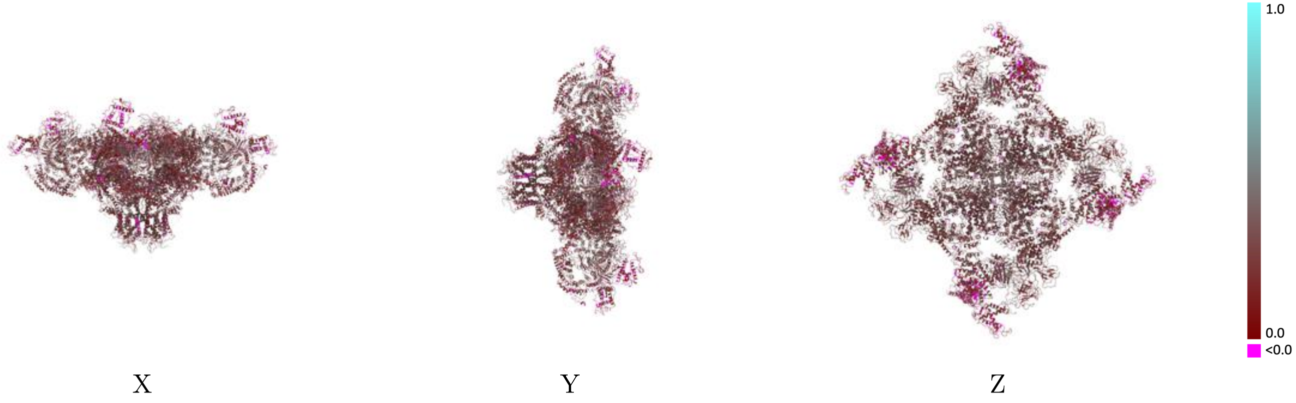

X


Y


Z

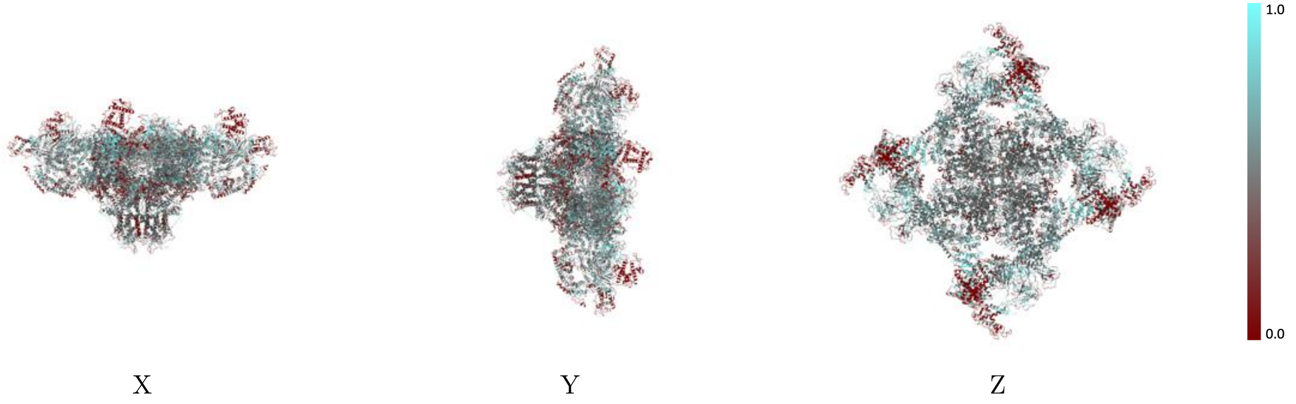
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ



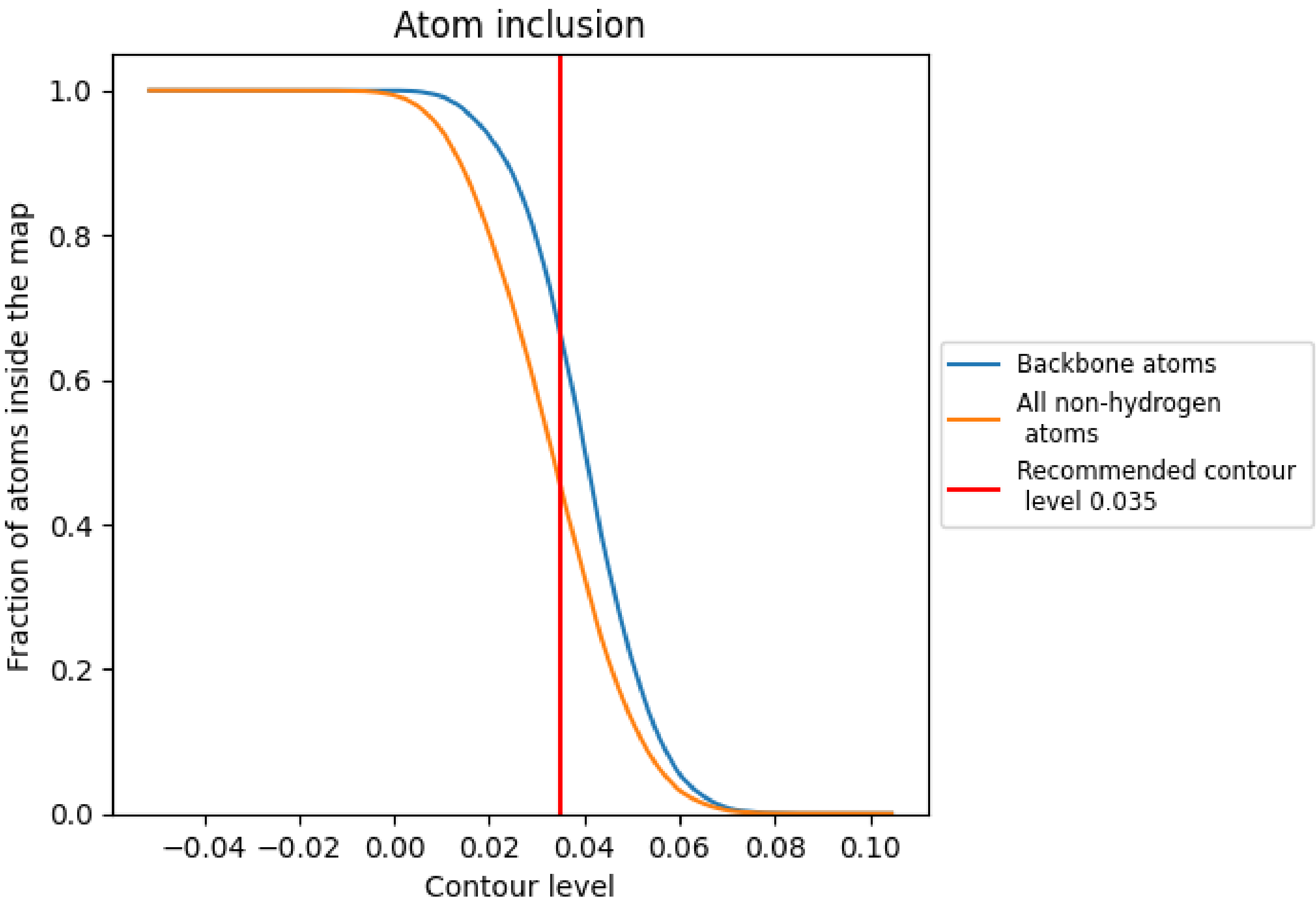
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 45% 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	■ 0.4527	■ 0.2520
A	■ 0.4628	■ 0.2710
B	■ 0.4525	■ 0.2520
E	■ 0.4524	■ 0.2520
F	■ 0.4653	■ 0.2720
G	■ 0.4521	■ 0.2510
H	■ 0.4615	■ 0.2720
I	■ 0.4525	■ 0.2520
J	■ 0.4615	■ 0.2720