Full wwPDB EM Validation Report ⓘ

Mar 2, 2024 – 03:52 PM EST

PDB ID	:	5T9N
EMDB ID	:	EMD-8373
Title	:	Structure of rabbit RyR1 (Ca2+-only dataset, class 2)
Authors	:	Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on	:	2016-09-09
Resolution	:	3.80 Å(reported)

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

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

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

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

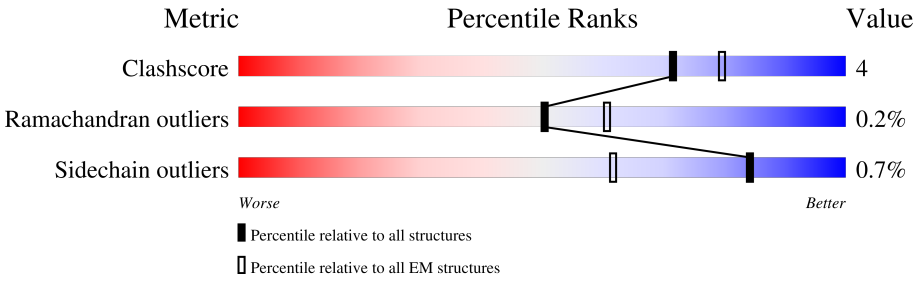
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	9% 88% 11%
1	F	108	7% 88% 11%
1	H	108	9% 88% 11%
1	J	108	9% 88% 11%
2	B	4676	18% 81% 8% 11%
2	E	4676	18% 81% 8% 11%
2	G	4676	18% 81% 8% 11%
2	I	4676	18% 81% 8% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 120756 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	E	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	I	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		
2	G	4168	Total	C	N	O	S	0	0
			29369	18608	5202	5402	157		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

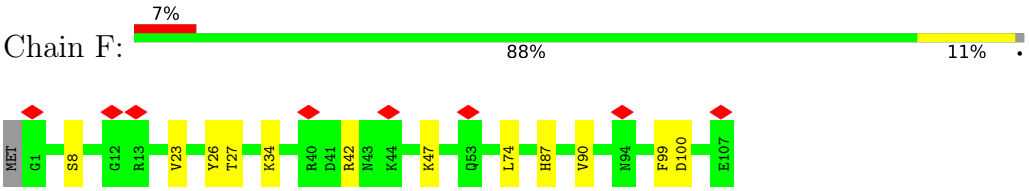
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0

3 Residue-property plots (i)

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

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



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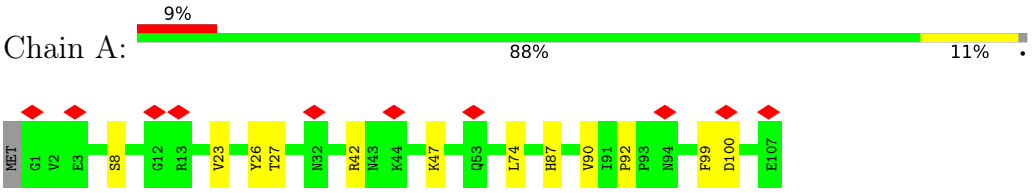
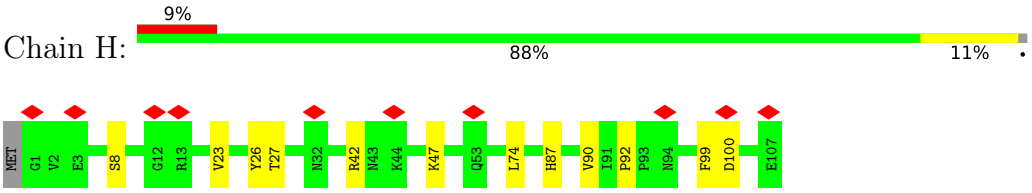
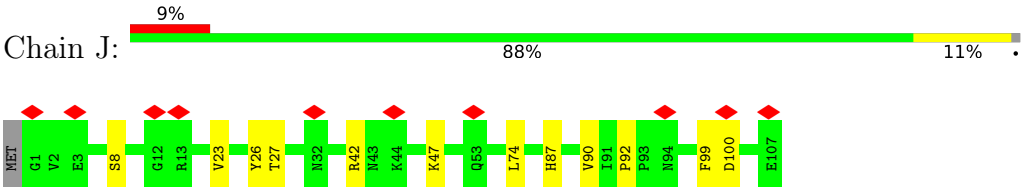


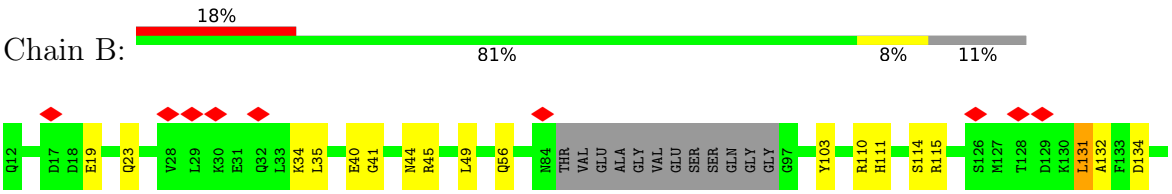
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



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



• Molecule 2: Ryanodine receptor 1

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A326 P327 K328 R329 D330 V331 E332 L357 T358 Y359 A360 A361 P362 D363 P364 K365 A366 L367 R368 L369 G370 V371 L372 K373 A376 H379 Q380 E381 G382 H383 M384 D385 D386 A387 R392 C393 Q394 Q395 G423 R426 G427 S428 G429 A432 G433 P434 A435 E439 P454 E458
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D619 L626 P627 G628 R629 Q634 T635 N636 L637 V641 P646 A653 F664 D669 E670 V671 T676 T689 S693 P694 E700 G703 G704 N705 G706 V707 S713 L719 G734 P740 E741 S745 C746 R758 L773 D774 F778 P779 K788
L793 R796 H797 Y808 H812 E813 A814 R835 G836 G841 C845 C854 D857 THR VAL GLN I861 V862 L863 P864 P865 H866 L867 E868 R869 I870 R871 E872 K873 L874 I878 R886 I887 E888 Q889 G890 W891 T892 Y893 G894 P895 V896 R897 D898 D899 N900 K901 R902
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GLN SER ARG TRP D1070 R1073 R1076 K1079 E1093 A1094 V1095 T1096 E1099 G1103 P1107 E1108 L1109 R1110 P1111 D1112 D1118 E1119 L1120 V1123 G1126 H1127 R1128 R1131 R1141 P1142 W1143 D1147 V1148 M1152 I1161 D1172 S1173 G1174 S1175 E1176 T1177 A1178 F1179 R1180
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ALA GLY E1622 C1630 Q1631 D1632 M1637 A1638 L1639 E1644 N1645 R1646 E1655 D1658 H1665 T1666 L1667 R1668 R1671 L1676 R1680 L1685 H1688 V1689 D1690 Q1691 L1698 E1699 L1707 R1708 A1709 G1710 Y1711 Y1712 D1713 I1718 H1719 L1720 E1721 R1725 R1728 S1729 M1730
E1733 E1741 T1742 R1743 F1748 P1749 P1750 G1751 R1752 K1753 G1754 G1755 N1756 A1757 R1758 R1759 H1760 G1766 V1767 R1772 L1786 P1787 A1788 ALA GLY VAL ALA E1793 A1794 P1795 A1796 R1797 I1802 R1808 L1812 L1815 D1828 V1839 P1840 L1844 V1845 S1846 T1847 I1853 F1854 Q1861
F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 L1931 P1932 V1935
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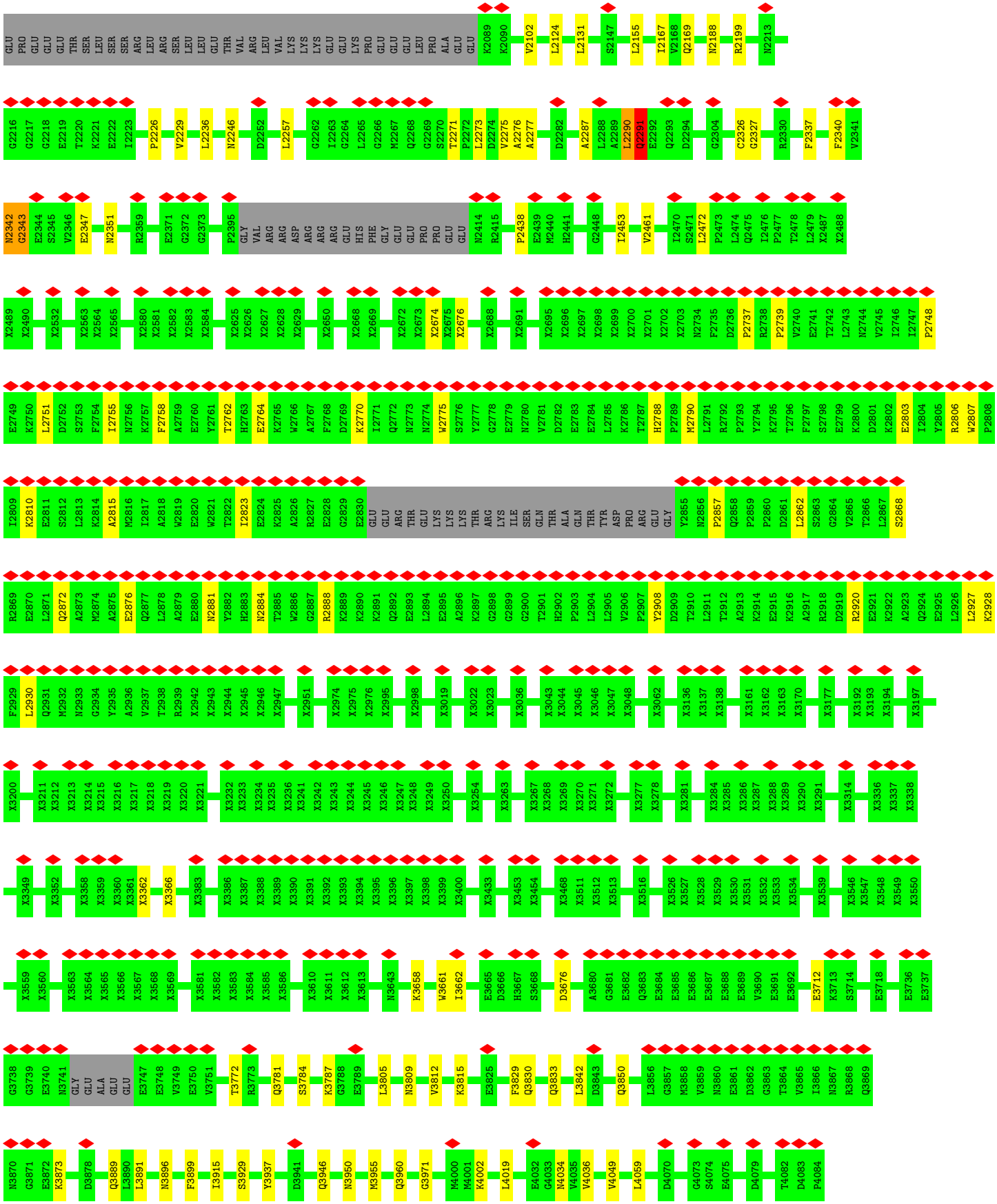
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X3200 X3211 X3212 X3213 X3214 X3215 X3216 X3217 X3218 X3219 X3220 X3221 X3232 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3254 X3263 X3267 X3268 X3269 X3270 X3271 X3272 X3277 X3278 X3281 X3284 X3285 X3286 X3287 X3288 X3289 X3290 X3291 X3314 X3336 X3337 X3338
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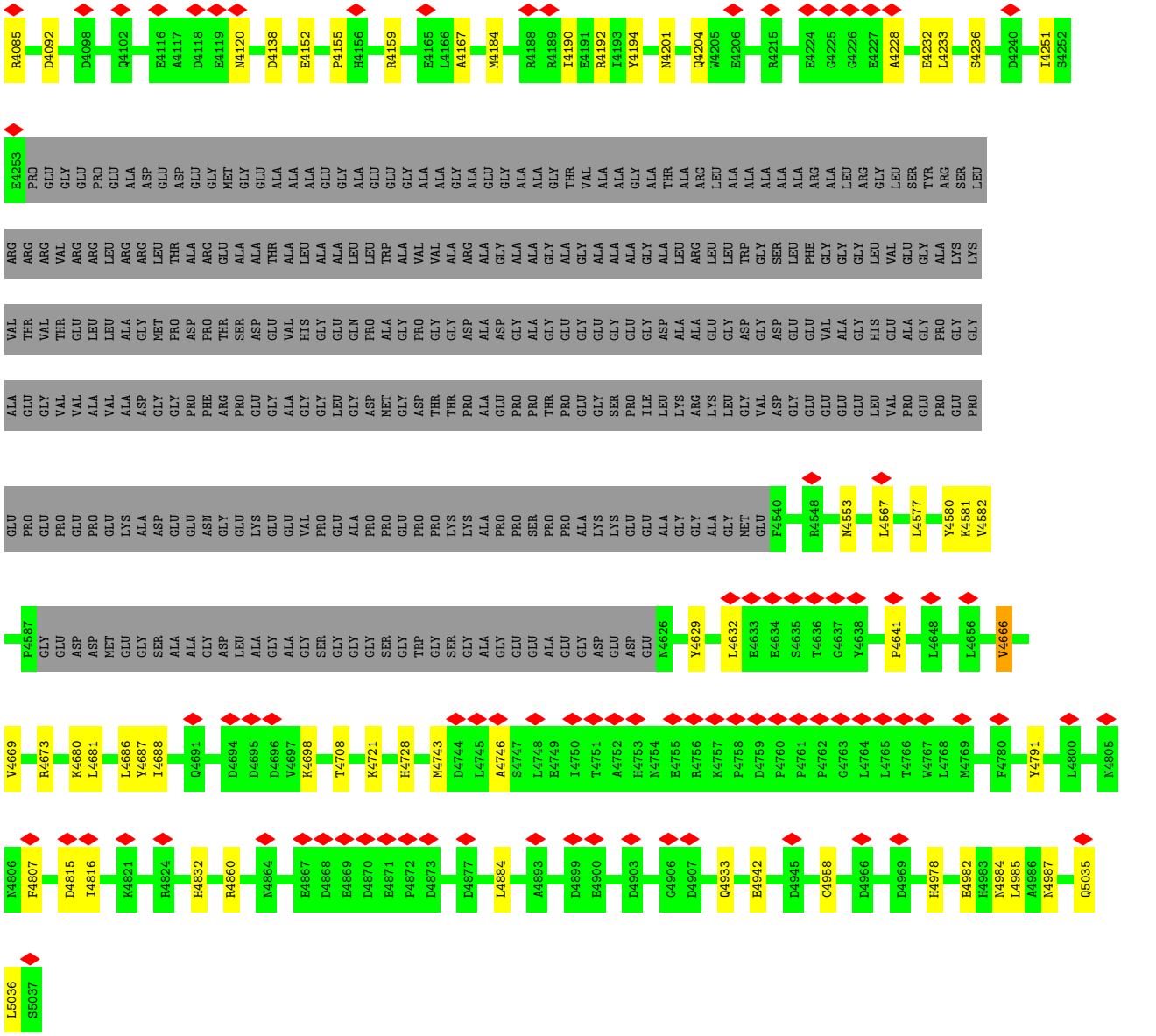
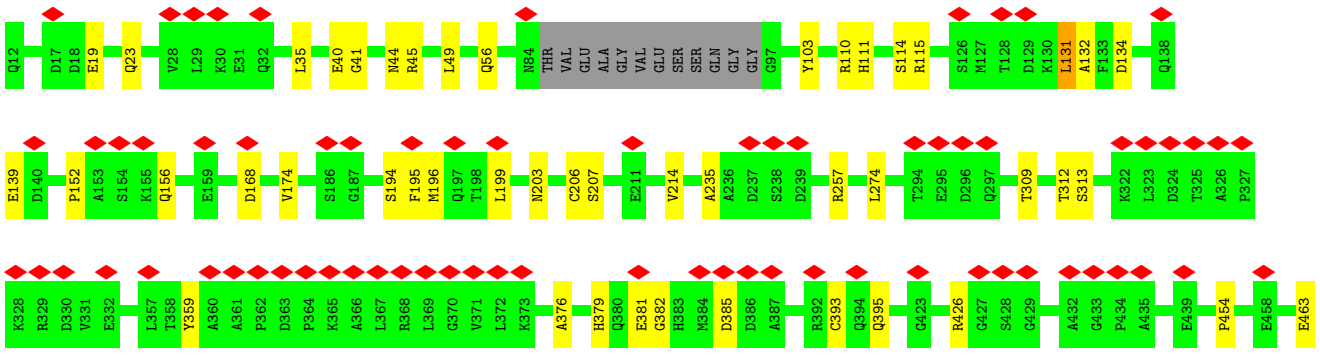
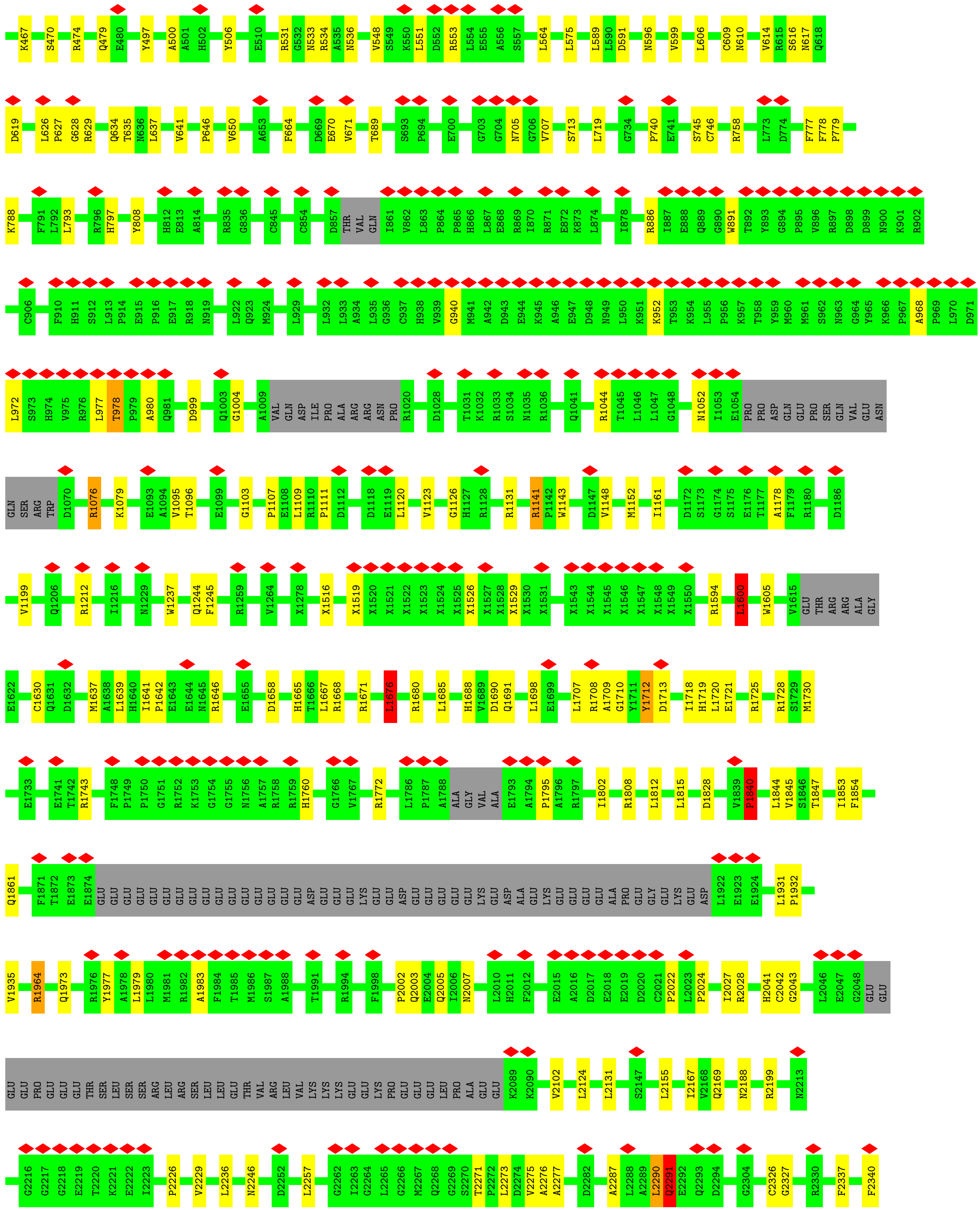
N3870 G3871 E3872 K3873 D3878 Q3889 L3890 L3891 N3896 F3899 I3915 S3929 Y3937 D3941 Q3946 N3950 M3955 Q3960 G3971 M4000 M4001 K4002 L4019 E4032 G4033 N4034 V4035 V4036 V4049 L4059 D4070 G4073 S4074 E4075 D4079 T4082 D4083 P4084



• Molecule 2: Ryanodine receptor 1

Chain E:

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Q1861 F1871 T1872 E1873 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA PRO GLU GLY GLU LYS GLU ASP L1922 E1923 E1924 L1931 P1932
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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 GLU K2089 K2090 V2102 L2124 L2131 S2147 L2155 I2167 V2168 Q2169 N2188 R2199 N2213
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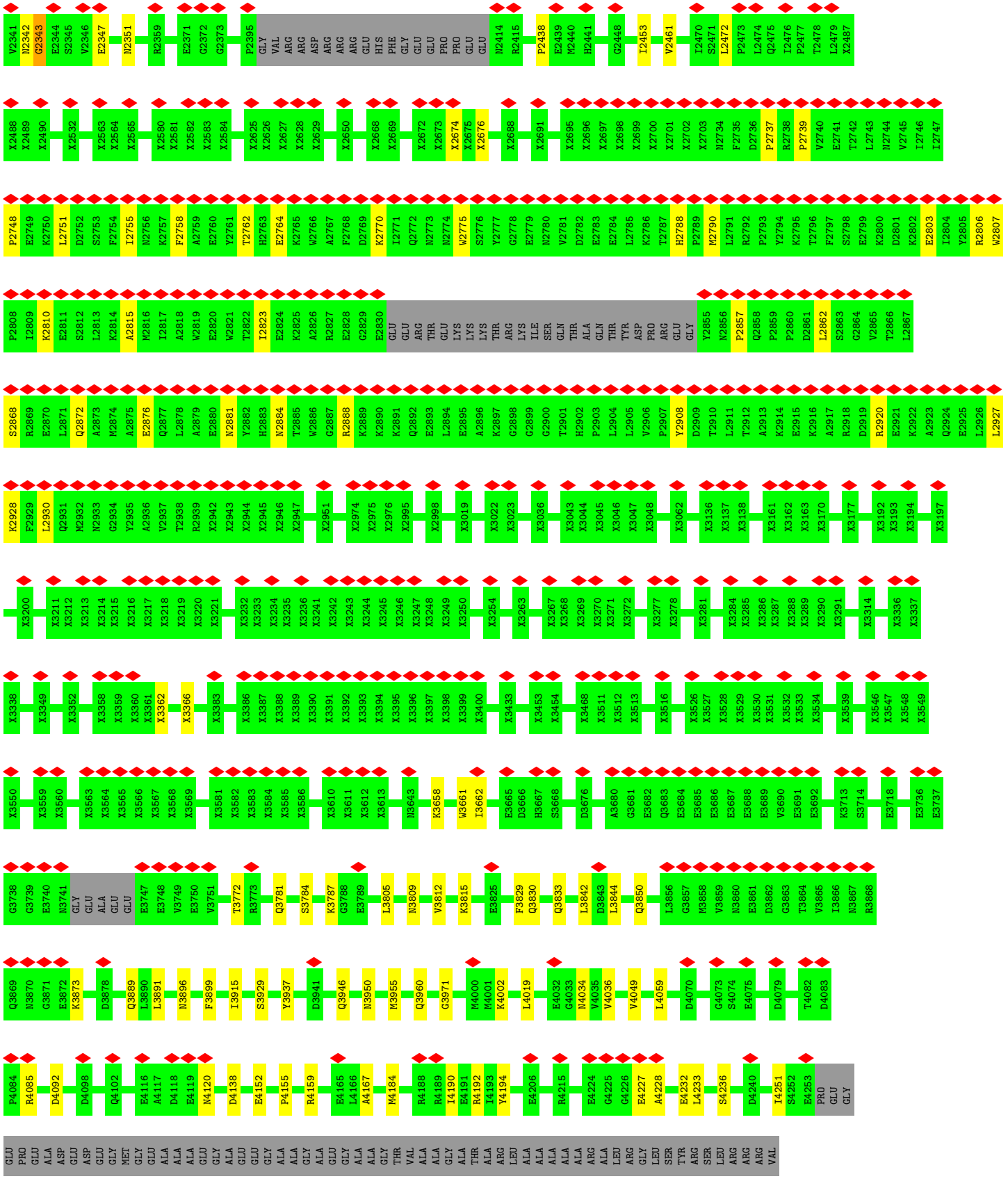
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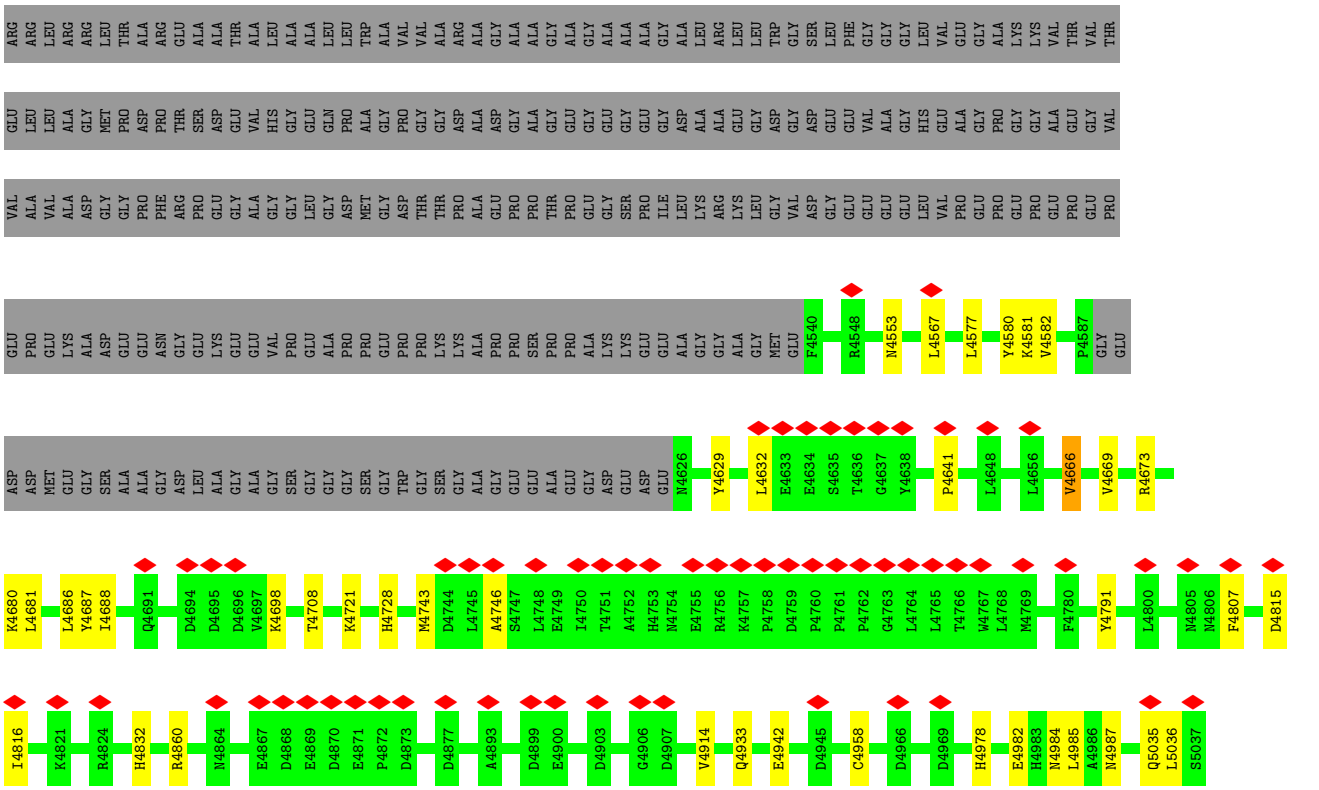
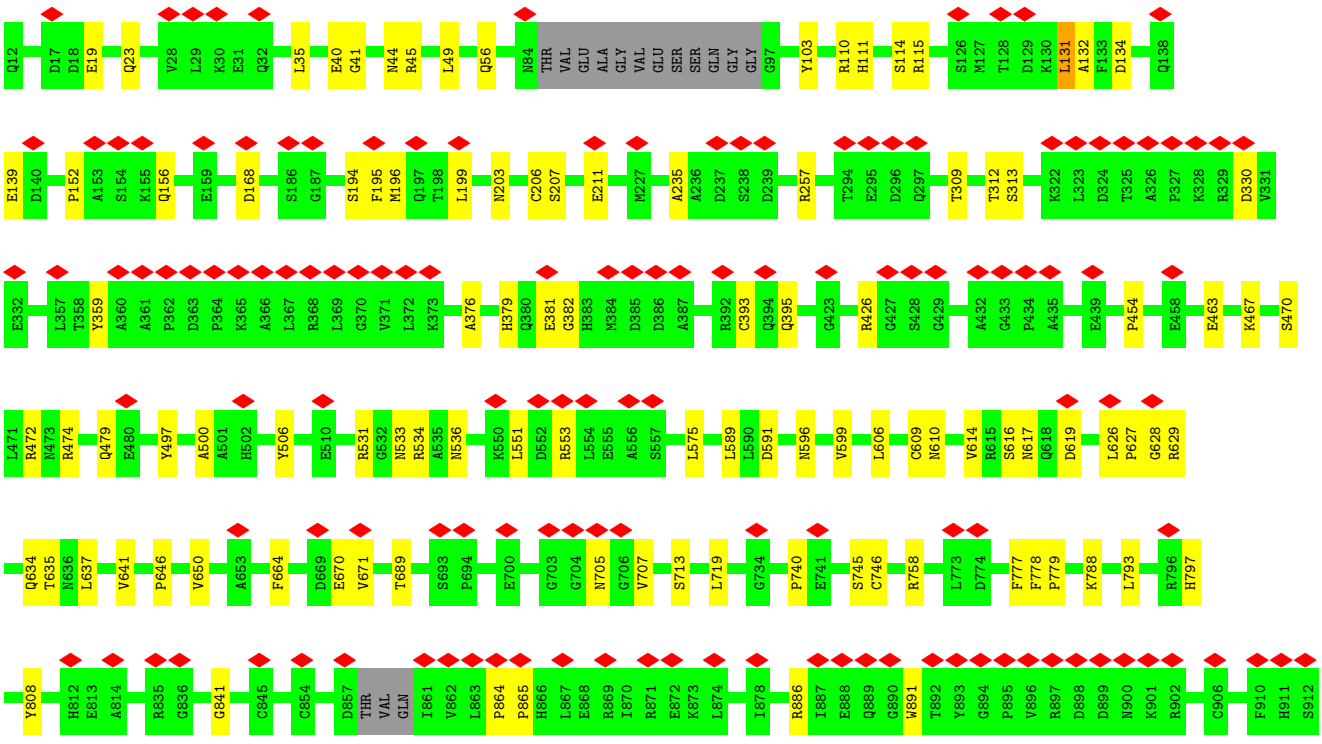
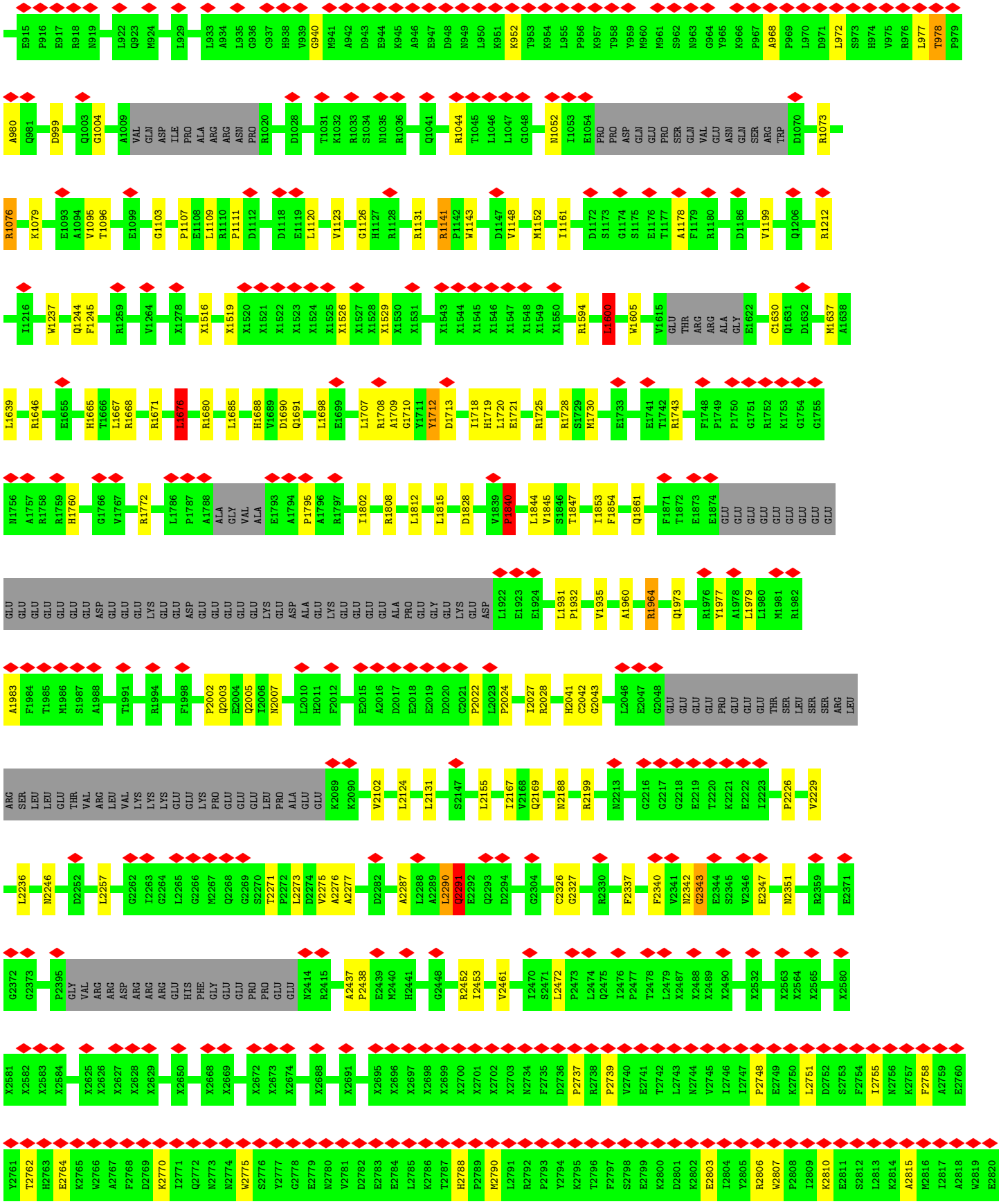


• Molecule 2: Ryanodine receptor 1

Chain I:

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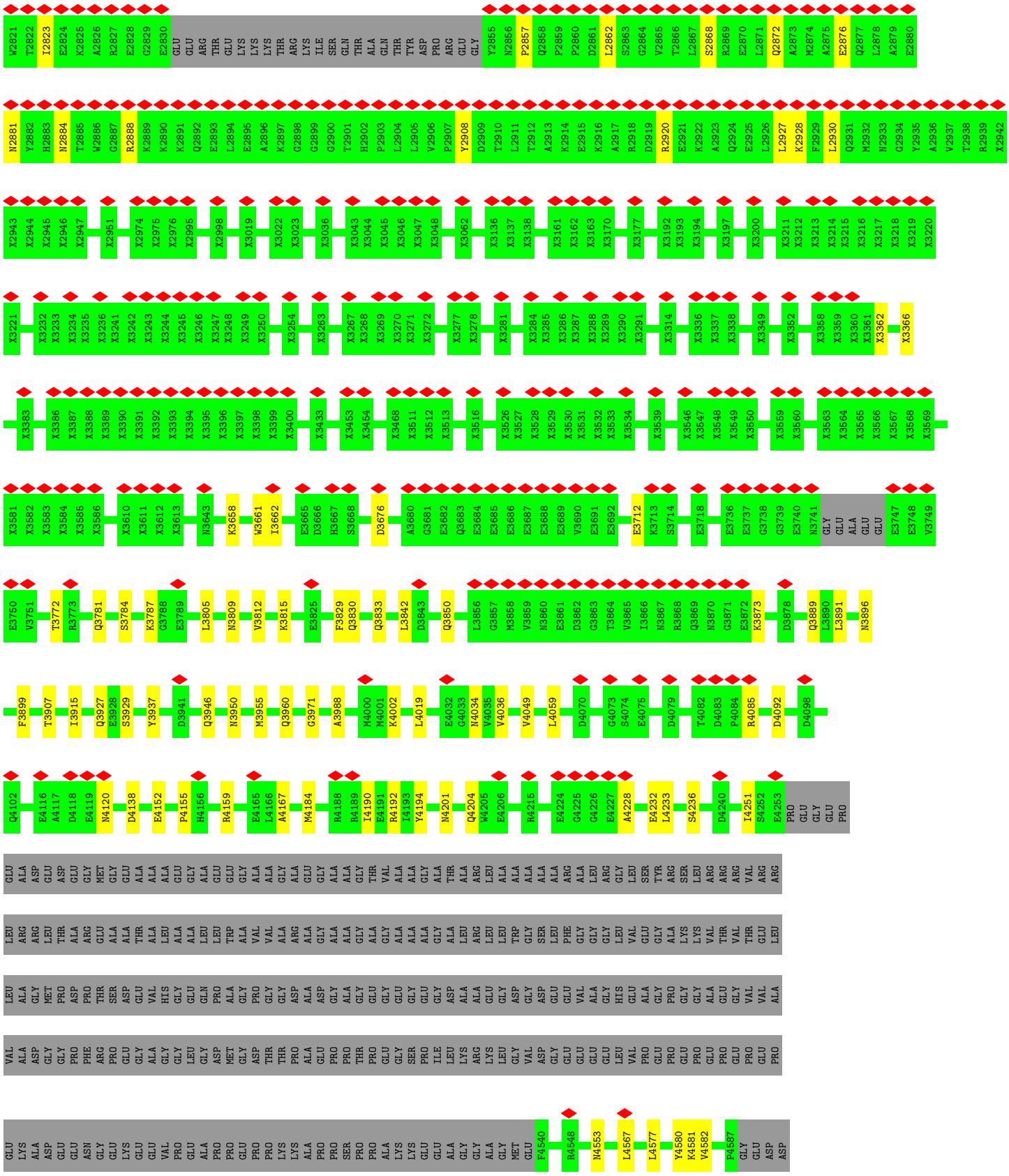
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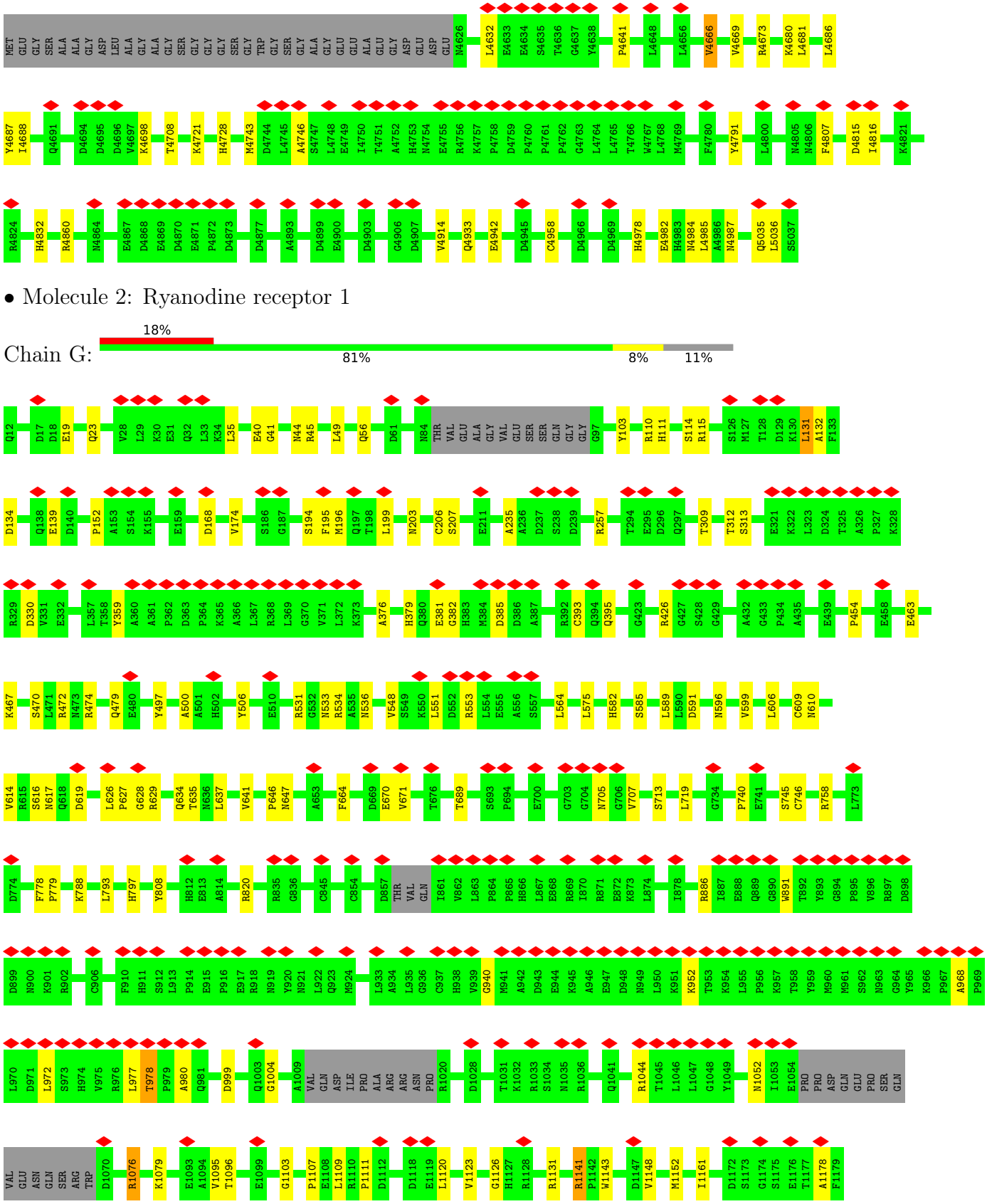
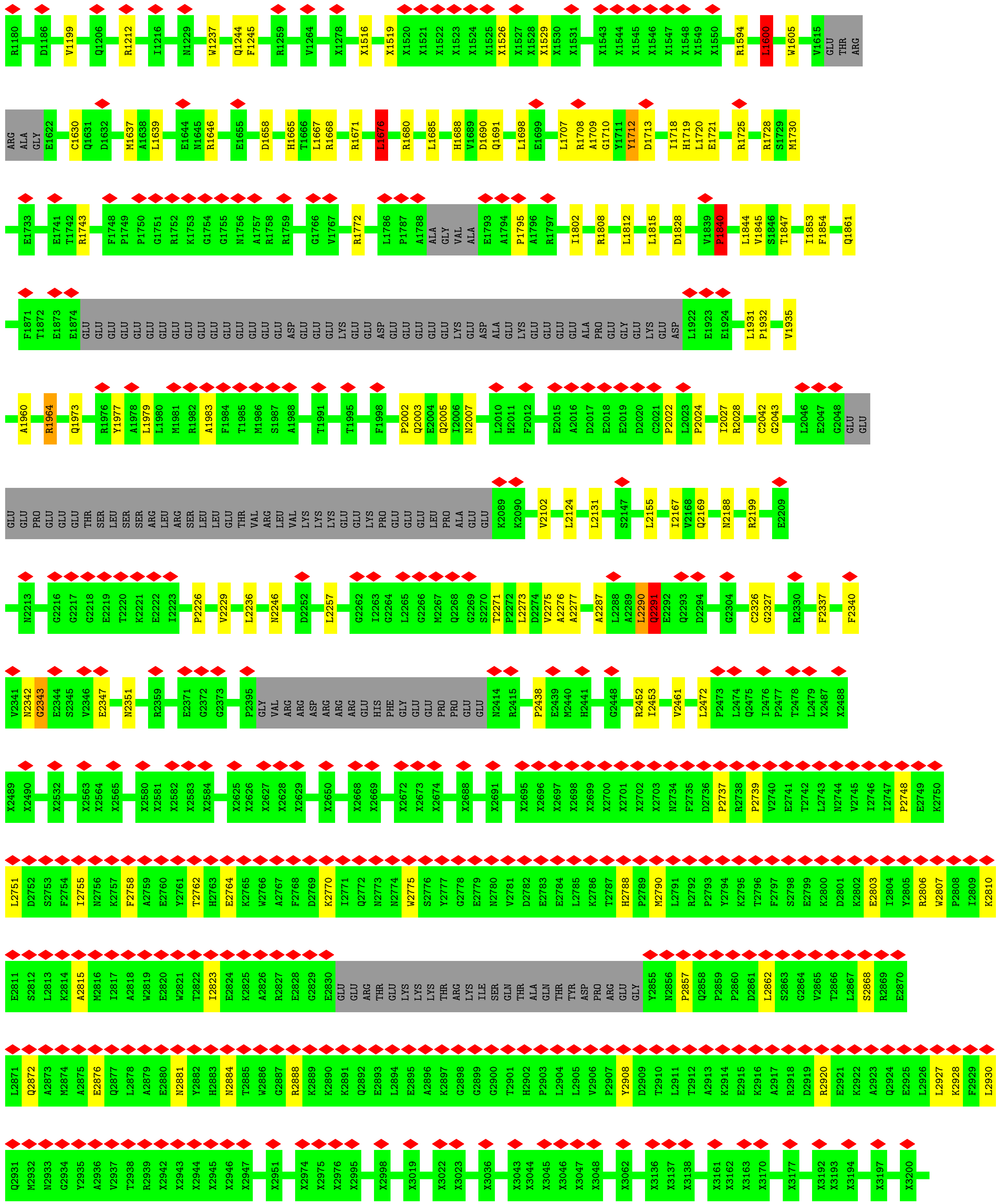


• Molecule 2: Ryanodine receptor 1

Chain G: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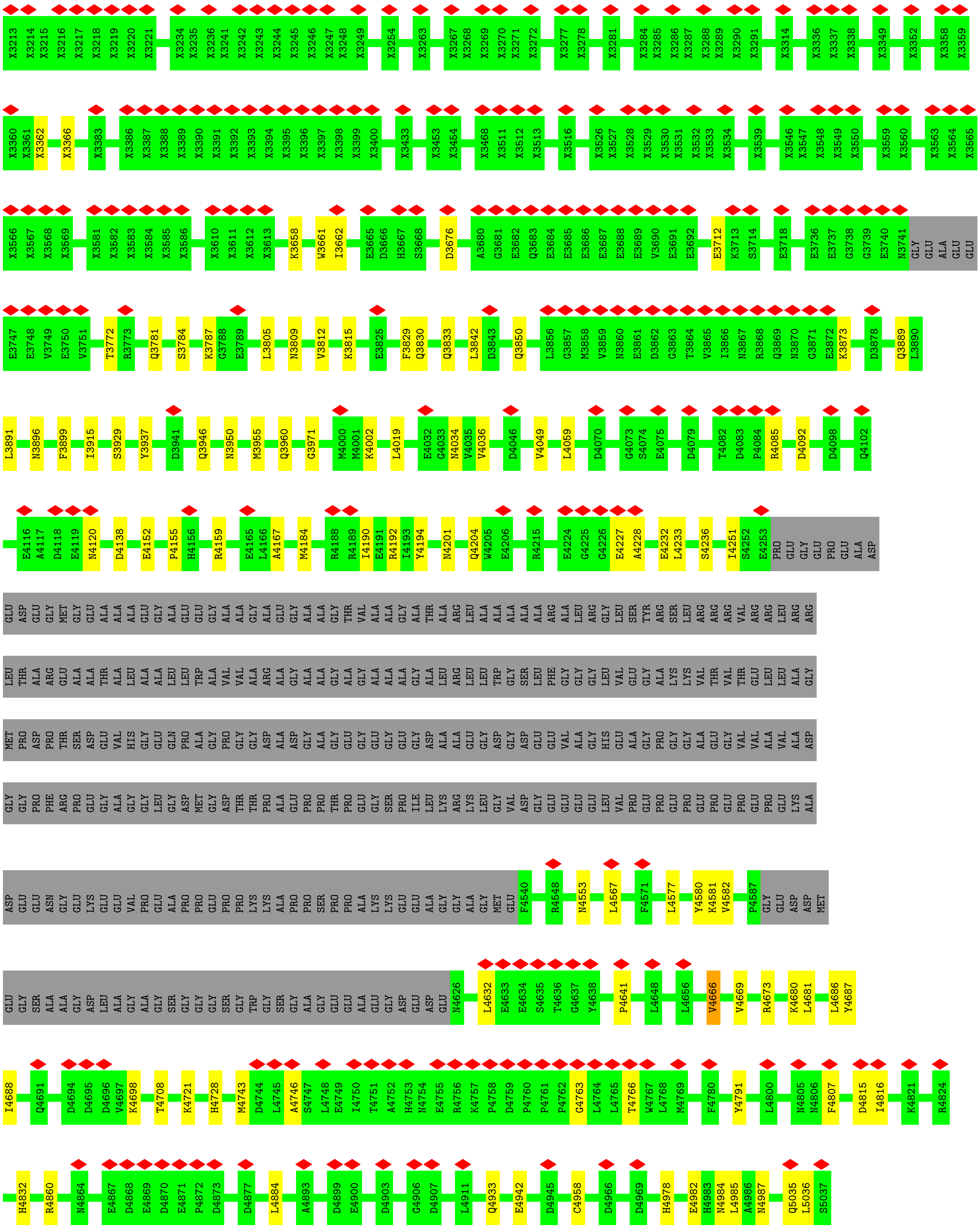
E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870
L2871 Q2872 A2873 M2874 A2875 E2876 Q2877 L2878 A2879 E2880 N2881 Y2882 H2883 N2884 T2885 W2886 G2887 R2888 K2889 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 D2909 T2910 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930
Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2951 X2974 X2975 X2976 X2995 X2998 X3019 X3022 X3023 X3036 X3043 X3044 X3045 X3046 X3047 X3048 X3062 X3136 X3137 X3138 X3161 X3162 X3163 X3170 X3177 X3192 X3193 X3194 X3197 X3200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X3360 X3361 X3362 X3366 X3383 X3386 X3387 X3388 X3389 X3390 X3391 X3392 X3393 X3394 X3395 X3396 X3397 X3398 X3399 X3400 X3433 X3453 X3454 X3468 X3511 X3512 X3513 X3516 X3526 X3527 X3528 X3529 X3530 X3531 X3532 X3533 X3534 X3539 X3546 X3547 X3548 X3549 X3550 X3559 X3560 X3563 X3564 X3565
X3566 X3567 X3568 X3569 X3581 X3582 X3583 X3584 X3585 X3586 X3610 X3611 X3612 X3613 K3658 W3661 I3662 E3665 D3666 H3667 S3668 D3676 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 E3712 K3713 S3714 E3718 E3736 E3737 G3738 G3739 E3740 N3741 GLY GLU ALA GLU GLU
E3747 E3748 V3749 E3750 V3751 T3772 R3773 Q3781 S3784 K3787 G3788 E3789 L3805 N3809 V3812 K3815 E3825 F3829 Q3830 Q3833 L3842 D3843 Q3850 L3856 G3857 M3858 V3859 N3860 E3861 D3862 G3863 T3864 V3865 I3866 N3867 R3868 Q3869 N3870 G3871 E3872 K3873 D3878 Q3889 L3890
L3891 N3896 F3899 I3915 S3929 Y3937 D3941 Q3946 N3950 M3955 Q3960 G3971 M4000 M4001 K4002 L4019 E4032 G4033 N4034 V4035 V4036 D4046 V4049 L4059 D4070 G4073 S4074 E4075 D4079 T4082 D4083 P4084 R4085 D4092 D4098 Q4102
E4116 A4117 D4118 E4119 N4120 D4138 E4152 P4155 H4156 R4159 E4165 L4166 A4167 M4184 R4188 R4189 I4190 E4191 R4192 I4193 Y4194 N4201 Q4204 W4205 E4206 R4215 E4224 G4225 G4226 E4227 A4228 E4232 L4233 S4236 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP
GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA GLU GLU GLY ALA ALA GLY ALA GLU GLY ALA ALA GLY THR VAL ALA ALA GLY ALA THR ALA ARG LEU ALA ALA ALA ALA ALA ARG ALA LEU ARG GLY LEU SER TYR ARG SER LEU ARG ARG ARG VAL ARG ARG LEU ARG ARG
LEU THR ALA ARG GLU ALA ALA THR ALA LEU ALA ALA LEU LEU TRP ALA VAL VAL ALA ARG ALA GLY ALA ALA GLY ALA GLY ALA ALA ALA GLY ALA LEU ARG LEU LEU TRP GLY SER LEU PHE GLY GLY GLY LEU VAL GLU GLY ALA LYS LYS VAL THR VAL THR GLU LEU LEU ALA GLY
MET PRO ASP PRO THR SER ASP GLU VAL HIS GLY GLU GLN PRO ALA GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLY ASP GLU GLU VAL ALA GLY HIS GLU ALA GLY PRO GLY GLY ALA GLU GLY VAL VAL ALA VAL ALA ASP
GLY GLY PRO PHE ARG PRO GLU GLY ALA GLY GLY LEU GLY ASP MET GLY ASP THR THR PRO ALA GLU PRO PRO THR PRO GLU GLY SER PRO ILE LEU LYS ARG LYS LEU GLY VAL ASP GLY GLU GLU GLU GLU LEU VAL PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU PRO GLU LYS ALA
ASP GLU GLU ASN GLY GLU LYS GLU GLU VAL PRO GLU ALA PRO PRO GLU PRO PRO LYS LYS ALA PRO PRO SER PRO PRO ALA LYS LYS GLU GLU ALA GLY GLY ALA GLY MET GLU F4540 R4548 N4553 L4567 F4571 L4577 Y4580 K4581 V4582 P4587 GLY GLU ASP ASP MET
GLU GLY SER ALA ALA GLY ASP LEU ALA GLY ALA GLY SER GLY GLY GLY SER GLY TRP GLY SER GLY ALA GLY GLU GLU ALA GLU GLY ASP GLU ASP GLU N4626 L4632 E4633 E4634 S4635 T4636 G4637 Y4638 P4641 L4648 L4656 V4666 V4669 R4673 K4680 L4681 L4686 Y4687
I4688 Q4691 D4694 D4695 D4696 V4697 K4698 T4708 K4721 H4728 M4743 D4744 L4745 A4746 S4747 L4748 E4749 I4750 T4751 A4752 H4753 N4754 E4755 R4756 K4757 P4758 D4759 P4760 P4761 P4762 G4763 L4764 L4765 T4766 W4767 L4768 M4769 F4780 Y4791 L4800 N4805 N4806 F4807 D4815 I4816 K4821 R4824
H4832 R4860 N4864 E4867 D4868 E4869 D4870 E4871 P4872 D4873 D4877 L4884 A4893 D4899 E4900 D4903 G4906 D4907 L4911 Q4933 E4942 D4945 C4958 D4966 D4969 H4978 E4982 H4983 N4984 L4985 A4986 N4987 Q5035 L5036 S5037

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	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: CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.31	0/834	0.52	0/1123
1	F	0.31	0/834	0.52	0/1123
1	H	0.31	0/834	0.52	0/1123
1	J	0.31	0/834	0.52	0/1123
2	B	0.31	0/25428	0.55	8/34534 (0.0%)
2	E	0.31	0/25428	0.55	8/34534 (0.0%)
2	G	0.31	0/25428	0.55	8/34534 (0.0%)
2	I	0.31	0/25428	0.55	8/34534 (0.0%)
All	All	0.31	0/105048	0.55	32/142628 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	17
2	E	0	17
2	G	0	17
2	I	0	17
All	All	0	72

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	131	LEU	CA-CB-CG	8.36	134.52	115.30
2	B	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	G	131	LEU	CA-CB-CG	8.34	134.49	115.30
2	I	1600	LEU	CA-CB-CG	6.97	131.32	115.30
2	G	1600	LEU	CA-CB-CG	6.96	131.30	115.30
2	E	1600	LEU	CA-CB-CG	6.95	131.29	115.30
2	B	1600	LEU	CA-CB-CG	6.94	131.27	115.30
2	G	1676	LEU	CA-CB-CG	6.52	130.29	115.30
2	I	1676	LEU	CA-CB-CG	6.49	130.24	115.30
2	E	1676	LEU	CA-CB-CG	6.49	130.23	115.30
2	B	1676	LEU	CA-CB-CG	6.49	130.22	115.30
2	B	977	LEU	CA-CB-CG	5.36	127.62	115.30
2	I	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	E	977	LEU	CA-CB-CG	5.34	127.59	115.30
2	G	977	LEU	CA-CB-CG	5.33	127.56	115.30
2	E	2290	LEU	CA-CB-CG	5.20	127.26	115.30
2	G	2290	LEU	CA-CB-CG	5.20	127.25	115.30
2	I	2290	LEU	CA-CB-CG	5.19	127.23	115.30
2	B	2290	LEU	CA-CB-CG	5.17	127.20	115.30
2	G	2291	GLN	C-N-CA	5.14	134.55	121.70
2	B	2291	GLN	C-N-CA	5.13	134.53	121.70
2	E	2291	GLN	C-N-CA	5.13	134.52	121.70
2	I	2291	GLN	C-N-CA	5.13	134.51	121.70
2	G	4985	LEU	CA-CB-CG	5.13	127.09	115.30
2	I	4985	LEU	CA-CB-CG	5.12	127.08	115.30
2	B	4985	LEU	CA-CB-CG	5.12	127.07	115.30
2	E	4985	LEU	CA-CB-CG	5.10	127.03	115.30
2	I	1667	LEU	CA-CB-CG	5.05	126.92	115.30
2	B	1667	LEU	CA-CB-CG	5.04	126.90	115.30
2	E	1667	LEU	CA-CB-CG	5.03	126.88	115.30
2	G	1667	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	808	TYR	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	808	TYR	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1795	PRO	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide

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Mol	Chain	Res	Type	Group
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	808	TYR	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	808	TYR	Peptide
1	J	8	SER	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	818	0	824	6	0
1	F	818	0	824	7	0
1	H	818	0	824	6	0
1	J	818	0	824	6	0
2	B	29369	0	24723	198	0
2	E	29369	0	24722	194	0
2	G	29369	0	24722	196	0
2	I	29369	0	24722	198	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
All	All	120756	0	102185	789	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (789) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4958:CYS:SG	2:I:4978:HIS:CD2	2.67	0.87
2:G:4958:CYS:SG	2:G:4978:HIS:CD2	2.67	0.87
2:E:4958:CYS:SG	2:E:4978:HIS:CD2	2.67	0.87
2:B:4958:CYS:SG	2:B:4978:HIS:CD2	2.67	0.87
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.75	0.68
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.75	0.68
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.27	0.68
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.27	0.67
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.75	0.67
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.77	0.67
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.77	0.67
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.27	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.77	0.66
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.78	0.66
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.27	0.66
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.77	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.78	0.66
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.78	0.65
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.77	0.65
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.79	0.65
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.79	0.65
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.79	0.64
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.79	0.64
2:I:4582:VAL:HG11	2:G:4860:ARG:HD2	1.81	0.62
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.82	0.62
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.82	0.62
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.34	0.61
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.65	0.61
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.33	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.33	0.61
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.33	0.61
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.82	0.61
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.65	0.61
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.34	0.61
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.65	0.61
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.65	0.60
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.34	0.60
2:E:670:GLU:HG3	2:E:788:LYS:H	1.66	0.60
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.33	0.60
2:G:670:GLU:HG3	2:G:788:LYS:H	1.66	0.60
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.34	0.60
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.34	0.60
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.34	0.60
2:B:670:GLU:HG3	2:B:788:LYS:H	1.66	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.34	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.34	0.60
2:I:670:GLU:HG3	2:I:788:LYS:H	1.66	0.59
2:E:2131:LEU:HB3	2:E:3662:ILE:HD13	1.85	0.59
2:G:2131:LEU:HB3	2:G:3662:ILE:HD13	1.85	0.59
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.83	0.59
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.84	0.59
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.84	0.59
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.85	0.59
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.85	0.59
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.85	0.59
2:I:2131:LEU:HB3	2:I:3662:ILE:HD13	1.85	0.59
2:B:2131:LEU:HB3	2:B:3662:ILE:HD13	1.85	0.58
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.85	0.58
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.85	0.58
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.85	0.58
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.85	0.58
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.85	0.58
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.69	0.58
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.68	0.58
2:B:609:CYS:SG	2:B:610:ASN:N	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LEU:O	2:B:617:ASN:ND2	2.37	0.58
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.85	0.58
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.85	0.58
2:I:41:GLY:O	2:I:45:ARG:NH1	2.37	0.57
2:I:609:CYS:SG	2:I:610:ASN:N	2.77	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.84	0.57
2:E:41:GLY:O	2:E:45:ARG:NH1	2.37	0.57
2:I:111:HIS:HD2	2:I:114:SER:H	1.51	0.57
2:G:111:HIS:HD2	2:G:114:SER:H	1.51	0.57
2:G:606:LEU:O	2:G:617:ASN:ND2	2.37	0.57
1:A:27:THR:HB	1:A:100:ASP:HB3	1.87	0.57
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.35	0.57
2:B:41:GLY:O	2:B:45:ARG:NH1	2.37	0.57
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.68	0.57
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.68	0.57
2:I:606:LEU:O	2:I:617:ASN:ND2	2.37	0.57
2:I:4832:HIS:NE2	2:I:4942:GLU:OE1	2.38	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.87	0.57
2:E:606:LEU:O	2:E:617:ASN:ND2	2.37	0.57
1:J:27:THR:HB	1:J:100:ASP:HB3	1.87	0.57
2:B:379:HIS:HD2	2:B:382:GLY:H	1.53	0.57
2:E:609:CYS:SG	2:E:610:ASN:N	2.77	0.57
2:B:4791:TYR:OH	2:B:4815:ASP:O	2.23	0.57
2:G:41:GLY:O	2:G:45:ARG:NH1	2.37	0.57
2:G:626:LEU:HG	2:G:628:GLY:H	1.70	0.57
2:I:626:LEU:HG	2:I:628:GLY:H	1.70	0.56
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.88	0.56
2:B:4832:HIS:NE2	2:B:4942:GLU:OE1	2.38	0.56
2:I:379:HIS:HD2	2:I:382:GLY:H	1.53	0.56
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.87	0.56
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.35	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.77	0.56
2:B:111:HIS:HD2	2:B:114:SER:H	1.51	0.56
2:I:4791:TYR:OH	2:I:4815:ASP:O	2.23	0.56
1:H:27:THR:HB	1:H:100:ASP:HB3	1.87	0.56
2:B:626:LEU:HG	2:B:628:GLY:H	1.70	0.56
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.87	0.56
2:E:4791:TYR:OH	2:E:4815:ASP:O	2.23	0.56
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.88	0.56
2:G:1730:MET:O	2:G:1772:ARG:NH1	2.39	0.56
2:E:111:HIS:HD2	2:E:114:SER:H	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.87	0.56
2:E:1730:MET:O	2:E:1772:ARG:NH1	2.39	0.56
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.87	0.56
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.88	0.56
2:E:626:LEU:HG	2:E:628:GLY:H	1.70	0.56
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.87	0.56
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.87	0.55
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.88	0.55
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.39	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:E:4049:VAL:HG21	2:E:4159:ARG:HD2	1.88	0.55
2:G:379:HIS:HD2	2:G:382:GLY:H	1.53	0.55
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.39	0.55
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.88	0.55
2:B:4049:VAL:HG21	2:B:4159:ARG:HD2	1.87	0.55
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.55
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.88	0.55
2:G:4791:TYR:OH	2:G:4815:ASP:O	2.23	0.55
2:B:2347:GLU:O	2:B:2351:ASN:N	2.40	0.55
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.89	0.55
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.88	0.55
2:B:1730:MET:O	2:B:1772:ARG:NH1	2.39	0.55
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.87	0.55
2:G:2347:GLU:O	2:G:2351:ASN:N	2.40	0.55
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.89	0.55
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.88	0.55
2:I:1730:MET:O	2:I:1772:ARG:NH1	2.39	0.55
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	1.88	0.55
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.39	0.55
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	1.88	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.54
2:E:379:HIS:HD2	2:E:382:GLY:H	1.53	0.54
2:G:4152:GLU:OE1	2:G:4192:ARG:NH2	2.41	0.54
2:E:4832:HIS:NE2	2:E:4942:GLU:OE1	2.38	0.54
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.89	0.54
2:E:56:GLN:O	2:E:309:THR:OG1	2.26	0.54
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.88	0.54
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.89	0.54
2:I:2758:PHE:O	2:I:2762:THR:N	2.40	0.54
2:E:4152:GLU:OE1	2:E:4192:ARG:NH2	2.41	0.54
2:I:2347:GLU:O	2:I:2351:ASN:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:56:GLN:O	2:G:309:THR:OG1	2.26	0.54
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.88	0.54
2:G:132:ALA:HA	2:G:194:SER:HB2	1.89	0.54
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.90	0.54
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.90	0.54
2:I:132:ALA:HA	2:I:194:SER:HB2	1.89	0.54
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.39	0.54
2:B:132:ALA:HA	2:B:194:SER:HB2	1.89	0.54
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.35	0.54
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.90	0.54
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.90	0.54
2:I:4152:GLU:OE1	2:I:4192:ARG:NH2	2.41	0.54
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.90	0.54
2:G:1148:VAL:HG21	2:G:1212:ARG:HG2	1.90	0.54
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.90	0.53
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.90	0.53
2:B:2876:GLU:OE1	2:B:2920:ARG:NH2	2.41	0.53
2:E:132:ALA:HA	2:E:194:SER:HB2	1.89	0.53
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.90	0.53
2:G:309:THR:O	2:G:313:SER:OG	2.26	0.53
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.89	0.53
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.39	0.53
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.90	0.53
2:I:309:THR:O	2:I:313:SER:OG	2.26	0.53
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.39	0.53
2:G:2758:PHE:O	2:G:2762:THR:N	2.40	0.53
2:B:4152:GLU:OE1	2:B:4192:ARG:NH2	2.41	0.53
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.90	0.53
2:I:2876:GLU:OE1	2:I:2920:ARG:NH2	2.41	0.53
2:E:1148:VAL:HG21	2:E:1212:ARG:HG2	1.90	0.53
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.90	0.53
2:B:1148:VAL:HG21	2:B:1212:ARG:HG2	1.90	0.53
2:E:2022:PRO:O	2:E:2028:ARG:NH2	2.41	0.53
2:E:2876:GLU:OE1	2:E:2920:ARG:NH2	2.41	0.53
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.90	0.53
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.90	0.53
2:I:454:PRO:HG2	2:I:531:ARG:HH12	1.74	0.53
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.39	0.53
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.90	0.52
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.35	0.52
2:I:56:GLN:O	2:I:309:THR:OG1	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.90	0.52
2:B:575:LEU:HD22	2:B:609:CYS:HB3	1.91	0.52
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.90	0.52
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.42	0.52
2:I:1148:VAL:HG21	2:I:1212:ARG:HG2	1.90	0.52
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.42	0.52
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.42	0.52
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.42	0.52
2:G:2876:GLU:OE1	2:G:2920:ARG:NH2	2.41	0.52
2:B:56:GLN:O	2:B:309:THR:OG1	2.26	0.52
2:I:575:LEU:HD22	2:I:609:CYS:HB3	1.91	0.52
2:I:4933:GLN:NE2	2:G:4933:GLN:OE1	2.43	0.52
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.75	0.52
2:G:40:GLU:HB3	2:G:44:ASN:HB3	1.91	0.52
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.39	0.52
2:B:4978:HIS:ND1	2:B:4982:GLU:OE1	2.39	0.52
2:E:309:THR:O	2:E:313:SER:OG	2.26	0.52
2:E:2758:PHE:O	2:E:2762:THR:N	2.40	0.52
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.42	0.52
2:B:40:GLU:HB3	2:B:44:ASN:HB3	1.91	0.52
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.42	0.52
2:G:575:LEU:HD22	2:G:609:CYS:HB3	1.91	0.52
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.52
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.42	0.52
2:E:575:LEU:HD22	2:E:609:CYS:HB3	1.91	0.52
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.83	0.52
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.43	0.52
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.42	0.52
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.92	0.52
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.42	0.52
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.43	0.52
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.75	0.52
2:G:454:PRO:HG2	2:G:531:ARG:HH12	1.74	0.52
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.43	0.52
2:G:4832:HIS:NE2	2:G:4942:GLU:OE1	2.38	0.52
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.43	0.51
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.43	0.51
2:E:40:GLU:HB3	2:E:44:ASN:HB3	1.91	0.51
2:E:454:PRO:HG2	2:E:531:ARG:HH12	1.74	0.51
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.39	0.51
2:G:689:THR:H	2:G:778:PHE:HE2	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.42	0.51
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.43	0.51
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.75	0.51
2:I:4567:LEU:HD12	2:I:4816:ILE:HD12	1.93	0.51
2:B:454:PRO:HG2	2:B:531:ARG:HH12	1.74	0.51
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.43	0.51
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.42	0.51
2:B:4567:LEU:HD12	2:B:4816:ILE:HD12	1.93	0.51
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.83	0.51
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.83	0.51
2:E:2347:GLU:O	2:E:2351:ASN:N	2.40	0.51
2:I:40:GLU:HB3	2:I:44:ASN:HB3	1.91	0.51
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.83	0.51
2:E:4567:LEU:HD12	2:E:4816:ILE:HD12	1.93	0.51
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.93	0.51
2:G:1245:PHE:HD1	2:G:1600:LEU:HB3	1.76	0.51
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.92	0.51
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.93	0.51
2:E:1245:PHE:HD1	2:E:1600:LEU:HB3	1.76	0.51
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.42	0.51
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.92	0.51
2:B:2758:PHE:O	2:B:2762:THR:N	2.40	0.51
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.93	0.51
2:B:309:THR:O	2:B:313:SER:OG	2.26	0.51
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.75	0.51
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.41	0.51
2:G:4567:LEU:HD12	2:G:4816:ILE:HD12	1.93	0.51
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.92	0.51
2:B:4933:GLN:OE1	2:E:4933:GLN:NE2	2.43	0.51
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.51
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.43	0.51
2:I:4581:LYS:HD2	2:I:4632:LEU:HD22	1.93	0.51
2:I:689:THR:H	2:I:778:PHE:HE2	1.58	0.50
2:G:2022:PRO:O	2:G:2028:ARG:NH2	2.41	0.50
1:A:92:PRO:HD3	2:B:627:PRO:HB2	1.92	0.50
2:B:689:THR:H	2:B:778:PHE:HE2	1.58	0.50
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.92	0.50
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.77	0.50
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.92	0.50
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.93	0.50
2:I:4984:ASN:ND2	2:I:4987:ASN:OD1	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.93	0.50
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.93	0.50
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.77	0.50
2:B:4933:GLN:NE2	2:I:4933:GLN:OE1	2.44	0.50
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.93	0.50
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.44	0.50
2:E:689:THR:H	2:E:778:PHE:HE2	1.58	0.50
2:E:4984:ASN:ND2	2:E:4987:ASN:OD1	2.38	0.50
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.94	0.50
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.94	0.50
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.77	0.50
2:E:4581:LYS:HD2	2:E:4632:LEU:HD22	1.94	0.50
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.77	0.49
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.46	0.49
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.93	0.49
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.94	0.49
2:B:4581:LYS:HD2	2:B:4632:LEU:HD22	1.94	0.49
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.92	0.49
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.94	0.49
2:G:627:PRO:O	2:G:629:ARG:NH1	2.46	0.49
2:I:1245:PHE:HD1	2:I:1600:LEU:HB3	1.76	0.49
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.92	0.49
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.39	0.49
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.77	0.49
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.94	0.49
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.94	0.49
2:I:627:PRO:O	2:I:629:ARG:NH1	2.46	0.49
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.49
2:G:4581:LYS:HD2	2:G:4632:LEU:HD22	1.93	0.49
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.95	0.49
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.77	0.49
2:B:1245:PHE:HD1	2:B:1600:LEU:HB3	1.76	0.49
2:G:3850:GLN:HB3	2:G:3873:LYS:HD3	1.95	0.49
2:B:627:PRO:O	2:B:629:ARG:NH1	2.46	0.48
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.46	0.48
2:E:3850:GLN:HB3	2:E:3873:LYS:HD3	1.95	0.48
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.95	0.48
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.95	0.48
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.95	0.48
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.94	0.48
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.77	0.48
2:E:4978:HIS:ND1	2:E:4982:GLU:OE1	2.39	0.48
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.95	0.48
2:G:2438:PRO:HB3	2:G:2453:ILE:HB	1.96	0.48
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.94	0.48
1:F:26:TYR:OH	1:F:42:ARG:NH2	2.47	0.48
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.39	0.48
2:B:2438:PRO:HB3	2:B:2453:ILE:HB	1.96	0.48
2:G:999:ASP:O	2:G:1004:GLY:N	2.47	0.48
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.47	0.48
2:I:2438:PRO:HB3	2:I:2453:ILE:HB	1.96	0.48
1:J:92:PRO:HD3	2:I:627:PRO:HB2	1.95	0.48
2:B:940:GLY:O	2:B:1052:ASN:N	2.47	0.48
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	1.95	0.48
2:I:940:GLY:O	2:I:1052:ASN:N	2.47	0.48
2:I:999:ASP:O	2:I:1004:GLY:N	2.47	0.48
2:I:1131:ARG:NH1	2:I:1178:ALA:O	2.47	0.48
2:G:4984:ASN:ND2	2:G:4987:ASN:OD1	2.38	0.48
2:B:1131:ARG:NH1	2:B:1178:ALA:O	2.47	0.48
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.96	0.48
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.48
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.87	0.48
2:B:999:ASP:O	2:B:1004:GLY:N	2.47	0.48
2:E:627:PRO:O	2:E:629:ARG:NH1	2.46	0.48
2:E:940:GLY:O	2:E:1052:ASN:N	2.47	0.48
2:E:1131:ARG:NH1	2:E:1178:ALA:O	2.47	0.48
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.47	0.48
2:E:1516:UNK:N	2:E:1529:UNK:O	2.47	0.48
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.47	0.48
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.96	0.48
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.95	0.48
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.47	0.48
2:B:1516:UNK:N	2:B:1529:UNK:O	2.47	0.48
2:B:3850:GLN:HB3	2:B:3873:LYS:HD3	1.95	0.48
2:I:1516:UNK:N	2:I:1529:UNK:O	2.47	0.48
2:G:614:VAL:HA	2:G:2169:GLN:HB3	1.96	0.48
2:G:1131:ARG:NH1	2:G:1178:ALA:O	2.47	0.48
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	1.95	0.48
2:E:359:TYR:HA	2:E:376:ALA:HA	1.96	0.47
2:E:999:ASP:O	2:E:1004:GLY:N	2.47	0.47
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.80	0.47
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.47	0.47
2:E:614:VAL:HA	2:E:2169:GLN:HB3	1.96	0.47
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.96	0.47
2:I:359:TYR:HA	2:I:376:ALA:HA	1.96	0.47
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	1.95	0.47
2:I:3850:GLN:HB3	2:I:3873:LYS:HD3	1.95	0.47
2:G:2868:SER:O	2:G:2872:GLN:N	2.45	0.47
1:H:26:TYR:OH	1:H:42:ARG:NH2	2.47	0.47
2:I:1720:LEU:HD12	2:I:1847:THR:HG23	1.97	0.47
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.87	0.47
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.97	0.47
2:I:2868:SER:O	2:I:2872:GLN:N	2.45	0.47
2:G:359:TYR:HA	2:G:376:ALA:HA	1.96	0.47
2:B:359:TYR:HA	2:B:376:ALA:HA	1.96	0.47
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.95	0.47
2:G:793:LEU:HD12	2:G:797:HIS:H	1.80	0.47
2:G:1720:LEU:HD12	2:G:1847:THR:HG23	1.97	0.47
1:H:92:PRO:HD3	2:G:627:PRO:HB2	1.95	0.47
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.96	0.47
2:B:1126:GLY:HA3	2:B:1143:TRP:CE2	2.49	0.47
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.96	0.47
2:I:1815:LEU:HD22	2:I:1845:VAL:HG21	1.97	0.47
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.47	0.47
2:G:1973:GLN:O	2:G:1977:TYR:N	2.47	0.47
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.96	0.47
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.97	0.47
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.96	0.47
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.80	0.47
2:E:1126:GLY:HA3	2:E:1143:TRP:CE2	2.49	0.47
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	1.95	0.47
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.77	0.47
2:E:2438:PRO:HB3	2:E:2453:ILE:HB	1.96	0.47
2:E:4138:ASP:OD1	2:E:4138:ASP:N	2.44	0.47
2:E:4933:GLN:OE1	2:G:4933:GLN:NE2	2.46	0.47
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.96	0.47
2:G:940:GLY:O	2:G:1052:ASN:N	2.47	0.47
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.95	0.47
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.87	0.47
2:E:1720:LEU:HD12	2:E:1847:THR:HG23	1.97	0.47
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1126:GLY:HA3	2:I:1143:TRP:CE2	2.49	0.47
2:B:1815:LEU:HD22	2:B:1845:VAL:HG21	1.97	0.47
2:B:1973:GLN:O	2:B:1977:TYR:N	2.47	0.47
2:E:793:LEU:HD12	2:E:797:HIS:H	1.80	0.47
2:G:1126:GLY:HA3	2:G:1143:TRP:CE2	2.49	0.47
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.97	0.47
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.96	0.47
2:G:4152:GLU:OE1	2:G:4194:TYR:OH	2.33	0.47
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.79	0.47
2:I:2908:TYR:OH	2:I:2920:ARG:NE	2.44	0.47
2:G:470:SER:O	2:G:474:ARG:NE	2.46	0.47
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.96	0.47
2:B:4152:GLU:OE1	2:B:4194:TYR:OH	2.33	0.47
2:B:1720:LEU:HD12	2:B:1847:THR:HG23	1.97	0.46
2:E:4152:GLU:OE1	2:E:4194:TYR:OH	2.33	0.46
2:G:614:VAL:HG22	2:G:616:SER:H	1.79	0.46
2:G:2155:LEU:HD13	2:G:2188:ASN:HD21	1.81	0.46
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.41	0.46
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.96	0.46
2:E:1973:GLN:O	2:E:1977:TYR:N	2.47	0.46
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.97	0.46
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.80	0.46
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.81	0.46
2:B:614:VAL:HA	2:B:2169:GLN:HB3	1.96	0.46
2:B:793:LEU:HD12	2:B:797:HIS:H	1.80	0.46
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.49	0.46
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.97	0.46
2:I:614:VAL:HG22	2:I:616:SER:H	1.79	0.46
2:I:4152:GLU:OE1	2:I:4194:TYR:OH	2.33	0.46
2:B:614:VAL:HG22	2:B:616:SER:H	1.79	0.46
2:G:1815:LEU:HD22	2:G:1845:VAL:HG21	1.97	0.46
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.44	0.46
2:I:2155:LEU:HD13	2:I:2188:ASN:HD21	1.81	0.46
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.81	0.46
2:B:2155:LEU:HD13	2:B:2188:ASN:HD21	1.81	0.46
2:E:1815:LEU:HD22	2:E:1845:VAL:HG21	1.97	0.46
2:E:2155:LEU:HD13	2:E:2188:ASN:HD21	1.80	0.46
2:G:1840:PRO:O	2:G:1844:LEU:N	2.48	0.46
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.81	0.46
2:B:470:SER:O	2:B:474:ARG:NE	2.45	0.46
2:E:1808:ARG:HD2	2:E:1854:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:793:LEU:HD12	2:I:797:HIS:H	1.80	0.46
2:E:614:VAL:HG22	2:E:616:SER:H	1.79	0.46
2:E:1840:PRO:O	2:E:1844:LEU:N	2.48	0.46
2:I:614:VAL:HA	2:I:2169:GLN:HB3	1.96	0.46
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.51	0.46
2:I:1840:PRO:O	2:I:1844:LEU:N	2.48	0.46
2:G:1808:ARG:HD2	2:G:1854:PHE:HA	1.98	0.46
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.51	0.45
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.49	0.45
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.97	0.45
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.98	0.45
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.49	0.45
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.98	0.45
2:I:4708:THR:O	2:I:4721:LYS:NZ	2.48	0.45
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.97	0.45
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.45
2:I:1808:ARG:HD2	2:I:1854:PHE:HA	1.98	0.45
2:I:4978:HIS:ND1	2:I:4982:GLU:OE1	2.39	0.45
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.49	0.45
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.51	0.45
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.99	0.45
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.98	0.45
2:E:2868:SER:O	2:E:2872:GLN:N	2.45	0.45
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.99	0.45
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.98	0.45
2:I:1973:GLN:O	2:I:1977:TYR:N	2.47	0.45
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.51	0.45
2:I:3842:LEU:O	2:I:3929:SER:OG	2.35	0.45
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.45
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.98	0.45
2:B:134:ASP:OD1	2:B:134:ASP:N	2.49	0.45
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.45
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.51	0.45
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.44	0.45
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.99	0.45
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.98	0.45
2:G:4978:HIS:ND1	2:G:4982:GLU:OE1	2.39	0.45
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.99	0.45
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.51	0.45
2:B:1808:ARG:HD2	2:B:1854:PHE:HA	1.98	0.45
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3946:GLN:OE1	2:B:3950:ASN:ND2	2.50	0.45
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.99	0.45
2:I:4036:VAL:HG11	2:I:5035:GLN:HB3	1.99	0.45
2:G:3946:GLN:OE1	2:G:3950:ASN:ND2	2.50	0.45
2:G:4036:VAL:HG11	2:G:5035:GLN:HB3	1.99	0.45
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.81	0.44
2:B:1840:PRO:O	2:B:1844:LEU:N	2.48	0.44
2:E:3946:GLN:OE1	2:E:3950:ASN:ND2	2.50	0.44
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.99	0.44
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.99	0.44
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.51	0.44
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.97	0.44
2:G:3842:LEU:O	2:G:3929:SER:OG	2.35	0.44
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	1.99	0.44
2:B:4036:VAL:HG11	2:B:5035:GLN:HB3	1.99	0.44
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.99	0.44
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.99	0.44
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	1.99	0.44
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.99	0.44
2:I:4681:LEU:HD21	2:I:4687:TYR:HD2	1.82	0.44
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.83	0.44
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.99	0.44
2:E:134:ASP:N	2:E:134:ASP:OD1	2.49	0.44
2:E:4036:VAL:HG11	2:E:5035:GLN:HB3	1.99	0.44
2:E:4681:LEU:HD21	2:E:4687:TYR:HD2	1.82	0.44
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.99	0.44
2:G:134:ASP:OD1	2:G:134:ASP:N	2.49	0.44
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.98	0.44
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.99	0.44
2:B:3842:LEU:O	2:B:3929:SER:OG	2.35	0.44
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.98	0.44
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	1.99	0.44
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	2.00	0.44
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.44
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.98	0.44
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.44
2:B:4629:TYR:OH	2:I:4860:ARG:NH2	2.49	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.82	0.44
2:I:3946:GLN:OE1	2:I:3950:ASN:ND2	2.50	0.44
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	2.00	0.44
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:ASP:HB2	2:I:156:GLN:HE21	1.83	0.44
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.99	0.44
2:B:4681:LEU:HD21	2:B:4687:TYR:HD2	1.82	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.99	0.44
2:I:4228:ALA:O	2:I:4232:GLU:N	2.51	0.44
2:G:1096:THR:HG23	2:G:1199:VAL:HG22	2.00	0.44
2:G:4092:ASP:OD1	2:G:4092:ASP:N	2.51	0.44
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.99	0.44
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.99	0.44
2:B:1096:THR:HG23	2:B:1199:VAL:HG22	2.00	0.44
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.00	0.44
2:B:4228:ALA:O	2:B:4232:GLU:N	2.51	0.44
2:B:4708:THR:O	2:B:4721:LYS:NZ	2.48	0.44
2:E:4233:LEU:HA	2:E:4236:SER:HB3	2.00	0.44
2:I:470:SER:O	2:I:474:ARG:NE	2.46	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.82	0.44
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.99	0.43
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.00	0.43
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	2.00	0.43
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.83	0.43
2:G:2024:PRO:O	2:G:2028:ARG:NE	2.47	0.43
2:G:4681:LEU:HD21	2:G:4687:TYR:HD2	1.82	0.43
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.83	0.43
2:E:3842:LEU:O	2:E:3929:SER:OG	2.35	0.43
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.01	0.43
2:B:978:THR:HB	2:B:980:ALA:H	1.82	0.43
2:B:4233:LEU:HA	2:B:4236:SER:HB3	2.00	0.43
2:E:1096:THR:HG23	2:E:1199:VAL:HG22	2.00	0.43
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	2.00	0.43
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.99	0.43
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.00	0.43
2:I:2024:PRO:O	2:I:2028:ARG:NE	2.47	0.43
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.00	0.43
2:G:4228:ALA:O	2:G:4232:GLU:N	2.51	0.43
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.00	0.43
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.43
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	2.01	0.43
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.00	0.43
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.43
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ASP:OD1	2:I:134:ASP:N	2.49	0.43
2:I:1096:THR:HG23	2:I:1199:VAL:HG22	2.00	0.43
2:I:1979:LEU:HA	2:I:1983:ALA:HB3	2.01	0.43
2:E:426:ARG:HB2	2:E:506:TYR:HA	2.01	0.43
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.00	0.43
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	1.99	0.43
2:B:426:ARG:HB2	2:B:506:TYR:HA	2.01	0.43
2:E:4251:ILE:HG22	2:E:4553:ASN:HD22	1.84	0.43
2:I:637:LEU:HD23	2:I:1637:MET:HB3	2.01	0.43
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.01	0.43
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.00	0.43
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.00	0.43
2:B:206:CYS:SG	2:B:207:SER:N	2.92	0.43
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.99	0.43
2:B:1979:LEU:HA	2:B:1983:ALA:HB3	2.01	0.43
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.52	0.43
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	2.01	0.43
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.99	0.43
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.83	0.43
2:E:4914:VAL:HG21	2:G:4884:LEU:HD11	2.01	0.43
2:G:637:LEU:HD23	2:G:1637:MET:HB3	2.01	0.43
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.01	0.43
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.99	0.43
2:G:4708:THR:O	2:G:4721:LYS:NZ	2.48	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:I:551:LEU:HD21	2:I:589:LEU:HD13	2.01	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.01	0.43
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.00	0.43
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.48	0.43
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.48	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.43
2:E:156:GLN:HE21	2:G:385:ASP:HB2	1.84	0.43
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.00	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.84	0.43
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.00	0.43
2:G:1707:LEU:O	2:G:1709:ALA:N	2.52	0.43
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.99	0.42
2:E:174:VAL:O	2:G:2452:ARG:NH1	2.52	0.42
2:E:206:CYS:SG	2:E:207:SER:N	2.92	0.42
2:I:4092:ASP:OD1	2:I:4092:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4233:LEU:HA	2:I:4236:SER:HB3	2.00	0.42
2:G:206:CYS:SG	2:G:207:SER:N	2.92	0.42
2:G:629:ARG:HD3	2:G:634:GLN:HG2	2.01	0.42
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.99	0.42
2:B:1076:ARG:HD3	2:B:1237:TRP:HB2	2.00	0.42
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.00	0.42
2:E:1979:LEU:HA	2:E:1983:ALA:HB3	2.00	0.42
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.52	0.42
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.42
2:E:4092:ASP:N	2:E:4092:ASP:OD1	2.51	0.42
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.53	0.42
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.00	0.42
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.51	0.42
2:I:4251:ILE:HG22	2:I:4553:ASN:HD22	1.84	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.01	0.42
2:G:3362:UNK:O	2:G:3366:UNK:N	2.53	0.42
2:B:637:LEU:HD23	2:B:1637:MET:HB3	2.01	0.42
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.41	0.42
2:B:4984:ASN:ND2	2:B:4987:ASN:OD1	2.38	0.42
2:E:3362:UNK:O	2:E:3366:UNK:N	2.53	0.42
2:G:4251:ILE:HG22	2:G:4553:ASN:HD22	1.84	0.42
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	2.01	0.42
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.84	0.42
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.53	0.42
2:I:206:CYS:SG	2:I:207:SER:N	2.92	0.42
2:I:978:THR:HB	2:I:980:ALA:H	1.82	0.42
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.52	0.42
2:I:3362:UNK:O	2:I:3366:UNK:N	2.53	0.42
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.52	0.42
2:G:4233:LEU:HA	2:G:4236:SER:HB3	2.00	0.42
2:B:19:GLU:HB2	2:B:206:CYS:HB3	2.01	0.42
2:B:629:ARG:HD3	2:B:634:GLN:HG2	2.01	0.42
2:B:1760:HIS:HE1	2:B:2041:HIS:HA	1.85	0.42
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.01	0.42
2:E:1707:LEU:O	2:E:1709:ALA:N	2.52	0.42
2:E:4228:ALA:O	2:E:4232:GLU:N	2.51	0.42
2:E:4708:THR:O	2:E:4721:LYS:NZ	2.48	0.42
2:G:479:GLN:HE21	2:G:536:ASN:ND2	2.18	0.42
2:G:1685:LEU:HA	2:G:1688:HIS:HD2	1.85	0.42
2:B:551:LEU:HD21	2:B:589:LEU:HD13	2.01	0.42
2:B:1707:LEU:O	2:B:1709:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD21	2:E:589:LEU:HD13	2.01	0.42
2:I:1707:LEU:O	2:I:1709:ALA:N	2.52	0.42
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.53	0.42
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.42
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	2.01	0.42
2:G:19:GLU:HB2	2:G:206:CYS:HB3	2.01	0.42
2:G:3662:ILE:H	2:G:3662:ILE:HG13	1.73	0.42
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.01	0.42
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.35	0.42
2:E:168:ASP:HB3	2:E:199:LEU:HD22	2.02	0.42
2:E:479:GLN:HE21	2:E:536:ASN:ND2	2.18	0.42
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.42
2:I:479:GLN:HE21	2:I:536:ASN:ND2	2.18	0.42
2:I:1685:LEU:HA	2:I:1688:HIS:HD2	1.85	0.42
2:I:3891:LEU:HB3	2:I:3899:PHE:CE2	2.55	0.42
2:G:1979:LEU:HA	2:G:1983:ALA:HB3	2.00	0.42
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.01	0.42
2:B:479:GLN:HE21	2:B:536:ASN:ND2	2.18	0.41
2:B:864:PRO:HA	2:B:865:PRO:HD3	1.92	0.41
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.53	0.41
2:B:4092:ASP:OD1	2:B:4092:ASP:N	2.51	0.41
2:E:637:LEU:HD23	2:E:1637:MET:HB3	2.01	0.41
2:I:19:GLU:HB2	2:I:206:CYS:HB3	2.01	0.41
2:G:551:LEU:HD21	2:G:589:LEU:HD13	2.01	0.41
2:G:4763:GLY:O	2:G:4766:THR:OG1	2.32	0.41
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.84	0.41
2:B:1685:LEU:HA	2:B:1688:HIS:HD2	1.85	0.41
2:B:3362:UNK:O	2:B:3366:UNK:N	2.53	0.41
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.00	0.41
2:G:168:ASP:HB3	2:G:199:LEU:HD22	2.02	0.41
2:G:426:ARG:HB2	2:G:506:TYR:HA	2.01	0.41
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.35	0.41
2:G:4815:ASP:OD1	2:G:4815:ASP:N	2.53	0.41
2:B:4860:ARG:NH2	2:E:4629:TYR:OH	2.50	0.41
2:E:629:ARG:HD3	2:E:634:GLN:HG2	2.01	0.41
2:E:2788:HIS:CE1	2:E:2790:MET:HB2	2.56	0.41
2:B:156:GLN:HE21	2:E:385:ASP:HB2	1.85	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:3891:LEU:HB3	2:B:3899:PHE:CE2	2.55	0.41
2:B:4884:LEU:HD11	2:I:4914:VAL:HG21	2.03	0.41
2:E:19:GLU:HB2	2:E:206:CYS:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2337:PHE:HA	2:E:2340:PHE:HB2	2.02	0.41
2:E:3891:LEU:HB3	2:E:3899:PHE:CE2	2.55	0.41
2:I:426:ARG:HB2	2:I:506:TYR:HA	2.01	0.41
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.84	0.41
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	2.01	0.41
2:I:1760:HIS:HE1	2:I:2041:HIS:HA	1.85	0.41
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.85	0.41
2:B:2024:PRO:HB2	2:B:2027:ILE:HG12	2.02	0.41
2:B:2788:HIS:CE1	2:B:2790:MET:HB2	2.56	0.41
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.41
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.01	0.41
2:G:582:HIS:O	2:G:585:SER:OG	2.29	0.41
2:G:2024:PRO:HB2	2:G:2027:ILE:HG12	2.02	0.41
2:G:2337:PHE:HA	2:G:2340:PHE:HB2	2.03	0.41
2:G:4201:ASN:HA	2:G:4204:GLN:HB3	2.03	0.41
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.41
2:B:3829:PHE:HD1	2:B:3915:ILE:HD11	1.86	0.41
2:E:2290:LEU:HG	2:E:2291:GLN:H	1.85	0.41
2:E:2815:ALA:HB3	2:E:2881:ASN:HD21	1.86	0.41
2:I:330:ASP:OD1	2:I:330:ASP:N	2.54	0.41
2:I:2290:LEU:HG	2:I:2291:GLN:H	1.86	0.41
2:I:3829:PHE:HD1	2:I:3915:ILE:HD11	1.86	0.41
2:I:3927:GLN:NE2	2:I:3988:ALA:O	2.50	0.41
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	2.02	0.41
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.53	0.41
2:B:2868:SER:O	2:B:2872:GLN:N	2.45	0.41
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	2.02	0.41
2:E:1658:ASP:N	2:E:1658:ASP:OD1	2.54	0.41
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.85	0.41
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.41
2:I:2788:HIS:CE1	2:I:2790:MET:HB2	2.56	0.41
2:B:214:VAL:HG12	2:B:274:LEU:HD12	2.03	0.41
2:B:4251:ILE:HG22	2:B:4553:ASN:HD22	1.84	0.41
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.35	0.41
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	2.01	0.41
2:G:3891:LEU:HB3	2:G:3899:PHE:CE2	2.55	0.41
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	2.02	0.41
2:B:2024:PRO:O	2:B:2028:ARG:NE	2.47	0.41
2:B:2188:ASN:OD1	2:B:2188:ASN:N	2.54	0.41
2:B:2290:LEU:HG	2:B:2291:GLN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2815:ALA:HB3	2:B:2881:ASN:HD21	1.86	0.41
2:E:470:SER:O	2:E:474:ARG:NE	2.46	0.41
2:E:1641:ILE:HA	2:E:1642:PRO:HD3	1.96	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	0.41
2:E:1760:HIS:HE1	2:E:2041:HIS:HA	1.85	0.41
2:E:2024:PRO:O	2:E:2028:ARG:NE	2.47	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:I:629:ARG:HD3	2:I:634:GLN:HG2	2.01	0.41
2:I:1141:ARG:H	2:I:1141:ARG:HD2	1.86	0.41
2:I:2024:PRO:HB2	2:I:2027:ILE:HG12	2.02	0.41
2:I:4201:ASN:HA	2:I:4204:GLN:HB3	2.03	0.41
2:G:330:ASP:OD1	2:G:330:ASP:N	2.54	0.41
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	2.02	0.41
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.03	0.41
2:G:2788:HIS:CE1	2:G:2790:MET:HB2	2.55	0.41
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.52	0.41
2:B:2337:PHE:HA	2:B:2340:PHE:HB2	2.02	0.41
2:E:1685:LEU:HA	2:E:1688:HIS:HD2	1.85	0.41
2:E:1725:ARG:HA	2:E:1728:ARG:HG2	2.03	0.41
2:I:1725:ARG:HH21	2:I:1725:ARG:HD2	1.71	0.41
2:I:2452:ARG:NH1	2:G:174:VAL:O	2.54	0.41
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.53	0.41
2:G:2815:ALA:HB3	2:G:2881:ASN:HD21	1.86	0.41
2:B:330:ASP:OD1	2:B:330:ASP:N	2.54	0.40
2:B:1141:ARG:HD2	2:B:1141:ARG:H	1.86	0.40
2:E:214:VAL:HG12	2:E:274:LEU:HD12	2.03	0.40
2:E:2024:PRO:HB2	2:E:2027:ILE:HG12	2.02	0.40
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.40
2:G:1658:ASP:N	2:G:1658:ASP:OD1	2.54	0.40
2:G:3829:PHE:HD1	2:G:3915:ILE:HD11	1.86	0.40
2:B:1131:ARG:HH12	2:B:1178:ALA:HB3	1.86	0.40
2:B:1658:ASP:N	2:B:1658:ASP:OD1	2.54	0.40
2:E:1141:ARG:HD2	2:E:1141:ARG:H	1.86	0.40
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.92	0.40
2:I:168:ASP:HB3	2:I:199:LEU:HD22	2.02	0.40
2:I:2815:ALA:HB3	2:I:2881:ASN:HD21	1.86	0.40
2:I:3662:ILE:H	2:I:3662:ILE:HG13	1.73	0.40
2:G:1141:ARG:H	2:G:1141:ARG:HD2	1.86	0.40
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.51	0.40
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1725:ARG:HA	2:B:1728:ARG:HG2	2.03	0.40
2:E:3829:PHE:HD1	2:E:3915:ILE:HD11	1.86	0.40
2:I:211:GLU:OE2	2:I:3907:THR:OG1	2.31	0.40
2:I:650:VAL:HB	2:I:777:PHE:HB2	2.04	0.40
2:I:1131:ARG:HH12	2:I:1178:ALA:HB3	1.86	0.40
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.54	0.40
2:G:2290:LEU:HG	2:G:2291:GLN:H	1.86	0.40
2:B:23:GLN:HE21	2:B:34:LYS:HB3	1.87	0.40
2:B:841:GLY:HA2	2:B:1073:ARG:HD2	2.04	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:E:548:VAL:HG12	2:E:564:LEU:HD22	2.04	0.40
2:E:650:VAL:HB	2:E:777:PHE:HB2	2.04	0.40
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.48	0.40
2:I:841:GLY:HA2	2:I:1073:ARG:HD2	2.04	0.40
2:I:2337:PHE:HA	2:I:2340:PHE:HB2	2.02	0.40
2:I:2437:ALA:HA	2:I:2438:PRO:HD3	1.93	0.40
2:G:1725:ARG:HA	2:G:1728:ARG:HG2	2.03	0.40
2:B:4201:ASN:HA	2:B:4204:GLN:HB3	2.03	0.40
2:E:2674:UNK:O	2:E:2676:UNK:N	2.54	0.40
2:I:864:PRO:HA	2:I:865:PRO:HD3	1.92	0.40
2:I:1725:ARG:HA	2:I:1728:ARG:HG2	2.02	0.40
2:G:548:VAL:HG12	2:G:564:LEU:HD22	2.04	0.40
2:G:647:ASN:ND2	2:G:820:ARG:O	2.46	0.40
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.40
2:G:3676:ASP:N	2:G:3676:ASP:OD1	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/108 (97%)	93 (89%)	12 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	H	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
1	J	105/108 (97%)	93 (89%)	12 (11%)	0	100	100
2	B	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	47	79
2	E	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	47	79
2	G	3235/4676 (69%)	2898 (90%)	331 (10%)	6 (0%)	47	79
2	I	3235/4676 (69%)	2899 (90%)	330 (10%)	6 (0%)	47	79
All	All	13360/19136 (70%)	11967 (90%)	1369 (10%)	24 (0%)	50	79

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	G	1708	ARG
2	B	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	G	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	E	2291	GLN
2	I	2291	GLN
2	G	2291	GLN
2	B	2291	GLN
2	B	2343	GLY
2	E	2343	GLY
2	I	2343	GLY
2	G	2343	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/89 (99%)	88 (100%)	0	100 100
1	F	88/89 (99%)	88 (100%)	0	100 100
1	H	88/89 (99%)	88 (100%)	0	100 100
1	J	88/89 (99%)	88 (100%)	0	100 100
2	B	2493/3202 (78%)	2476 (99%)	17 (1%)	84 91
2	E	2493/3202 (78%)	2476 (99%)	17 (1%)	84 91
2	G	2493/3202 (78%)	2476 (99%)	17 (1%)	84 91
2	I	2493/3202 (78%)	2476 (99%)	17 (1%)	84 91
All	All	10324/13164 (78%)	10256 (99%)	68 (1%)	84 91

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	719	LEU
2	B	978	THR
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	2461	VAL
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	E	131	LEU
2	E	534	ARG

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Mol	Chain	Res	Type
2	E	553	ARG
2	E	719	LEU
2	E	978	THR
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	2461	VAL
2	E	3787	LYS
2	E	3805	LEU
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	I	131	LEU
2	I	534	ARG
2	I	553	ARG
2	I	719	LEU
2	I	978	THR
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	2461	VAL
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	G	131	LEU
2	G	534	ARG
2	G	553	ARG
2	G	719	LEU
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG

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Mol	Chain	Res	Type
2	G	2461	VAL
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) 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	23	GLN
2	B	57	ASN
2	B	105	HIS
2	B	111	HIS
2	B	156	GLN
2	B	203	ASN
2	B	273	HIS
2	B	379	HIS
2	B	383	HIS
2	B	479	GLN
2	B	582	HIS
2	B	1158	ASN
2	B	1598	GLN
2	B	1691	GLN
2	B	1693	GLN
2	B	1719	HIS
2	B	2005	GLN
2	B	2127	GLN
2	B	3771	HIS
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4806	ASN
2	E	23	GLN

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Mol	Chain	Res	Type
2	E	57	ASN
2	E	105	HIS
2	E	111	HIS
2	E	156	GLN
2	E	203	ASN
2	E	273	HIS
2	E	379	HIS
2	E	383	HIS
2	E	479	GLN
2	E	582	HIS
2	E	1158	ASN
2	E	1598	GLN
2	E	1688	HIS
2	E	1691	GLN
2	E	1693	GLN
2	E	1719	HIS
2	E	2005	GLN
2	E	2127	GLN
2	E	3771	HIS
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	4034	ASN
2	E	4120	ASN
2	E	4553	ASN
2	I	23	GLN
2	I	57	ASN
2	I	105	HIS
2	I	111	HIS
2	I	156	GLN
2	I	203	ASN
2	I	273	HIS
2	I	379	HIS
2	I	383	HIS
2	I	479	GLN
2	I	582	HIS
2	I	1158	ASN
2	I	1598	GLN
2	I	1691	GLN
2	I	1693	GLN
2	I	1719	HIS
2	I	2005	GLN

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Mol	Chain	Res	Type
2	I	2127	GLN
2	I	3771	HIS
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	4034	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	5003	HIS
2	G	23	GLN
2	G	57	ASN
2	G	105	HIS
2	G	111	HIS
2	G	156	GLN
2	G	203	ASN
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	479	GLN
2	G	582	HIS
2	G	1158	ASN
2	G	1598	GLN
2	G	1691	GLN
2	G	1693	GLN
2	G	1719	HIS
2	G	2005	GLN
2	G	2127	GLN
2	G	3771	HIS
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	4034	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	5003	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	12
2	B	12
2	E	12
2	G	12

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3613:UNK	C	3639:THR	N	43.02
1	B	3613:UNK	C	3639:THR	N	43.01
1	E	3613:UNK	C	3639:THR	N	43.01
1	G	3613:UNK	C	3639:THR	N	42.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3163:UNK	C	3170:UNK	N	16.39
1	E	3163:UNK	C	3170:UNK	N	16.39
1	I	3163:UNK	C	3170:UNK	N	16.39
1	G	3163:UNK	C	3170:UNK	N	16.39
1	B	3468:UNK	C	3511:UNK	N	15.14
1	E	3468:UNK	C	3511:UNK	N	15.14
1	I	3468:UNK	C	3511:UNK	N	15.14
1	G	3468:UNK	C	3511:UNK	N	15.14
1	E	3063:UNK	C	3134:UNK	N	14.90
1	B	3063:UNK	C	3134:UNK	N	14.89
1	I	3063:UNK	C	3134:UNK	N	14.89
1	G	3063:UNK	C	3134:UNK	N	14.89
1	G	2703:UNK	C	2734:ASN	N	14.64
1	B	2703:UNK	C	2734:ASN	N	14.61
1	E	2703:UNK	C	2734:ASN	N	14.59
1	I	2703:UNK	C	2734:ASN	N	14.59
1	B	3236:UNK	C	3241:UNK	N	13.53
1	E	3236:UNK	C	3241:UNK	N	13.53
1	I	3236:UNK	C	3241:UNK	N	13.53
1	G	3236:UNK	C	3241:UNK	N	13.53
1	G	1564:UNK	C	1573:MET	N	12.52
1	B	1564:UNK	C	1573:MET	N	12.51
1	I	1564:UNK	C	1573:MET	N	12.51
1	E	1564:UNK	C	1573:MET	N	12.49
1	B	2976:UNK	C	2995:UNK	N	12.26
1	E	2976:UNK	C	2995:UNK	N	12.26
1	I	2976:UNK	C	2995:UNK	N	12.26
1	G	2976:UNK	C	2995:UNK	N	12.26
1	E	3254:UNK	C	3261:UNK	N	8.39
1	I	3254:UNK	C	3261:UNK	N	8.39
1	B	3254:UNK	C	3261:UNK	N	8.38
1	G	3254:UNK	C	3261:UNK	N	8.38
1	B	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.79
1	G	1297:UNK	C	1430:UNK	N	5.79
1	E	1297:UNK	C	1430:UNK	N	5.77
1	G	2939:ARG	C	2942:UNK	N	3.40
1	B	2939:ARG	C	2942:UNK	N	3.37
1	E	2939:ARG	C	2942:UNK	N	3.36
1	I	2939:ARG	C	2942:UNK	N	3.36
1	E	2479:LEU	C	2487:UNK	N	3.29
1	I	2479:LEU	C	2487:UNK	N	3.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2479:LEU	C	2487:UNK	N	3.28
1	G	2479:LEU	C	2487:UNK	N	3.25

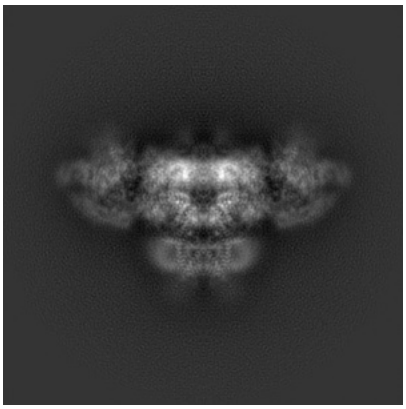
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8373. These allow visual inspection of the internal detail of the map and identification of artifacts.

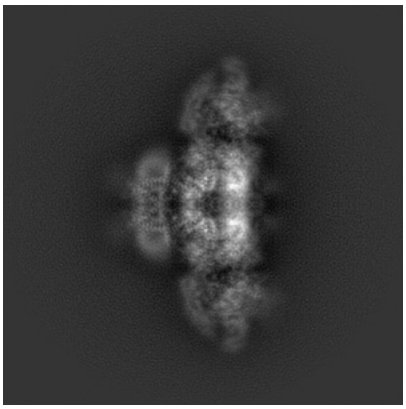
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

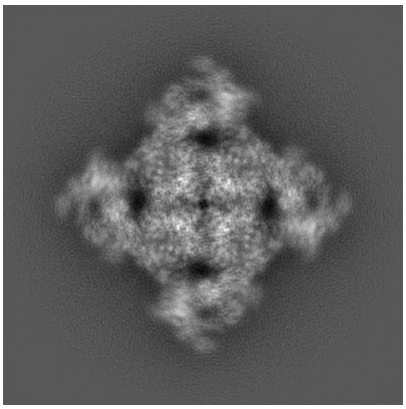
6.1.1 Primary map



X

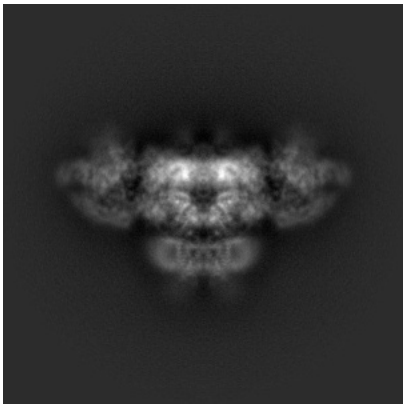


Y

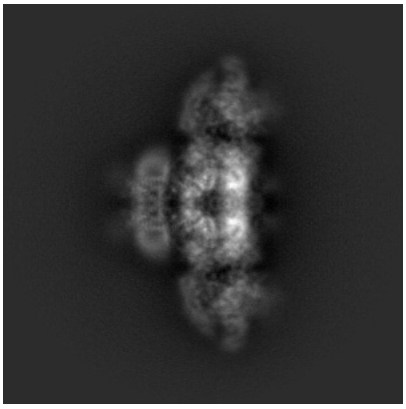


Z

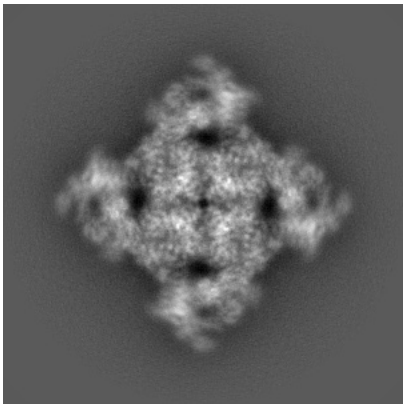
6.1.2 Raw map



X



Y

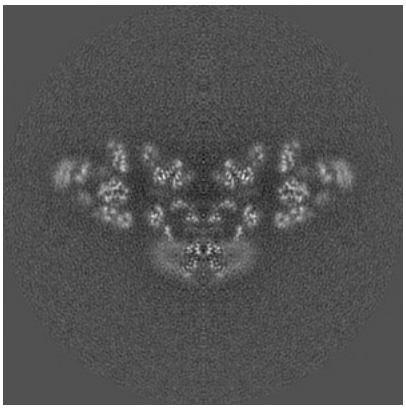


Z

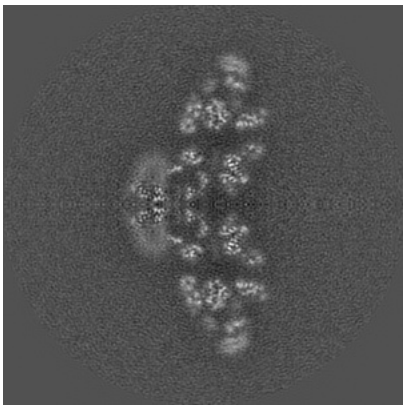
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

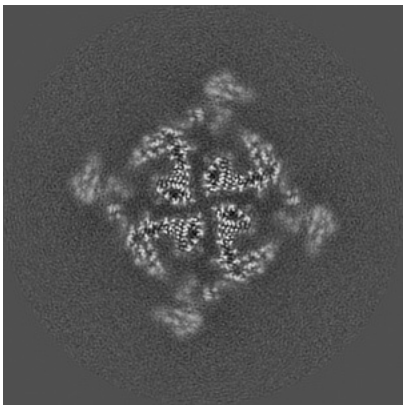
6.2.1 Primary map



X Index: 200

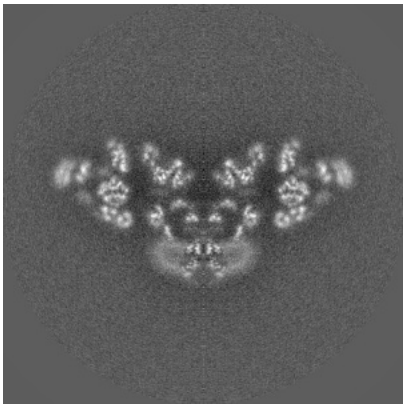


Y Index: 200

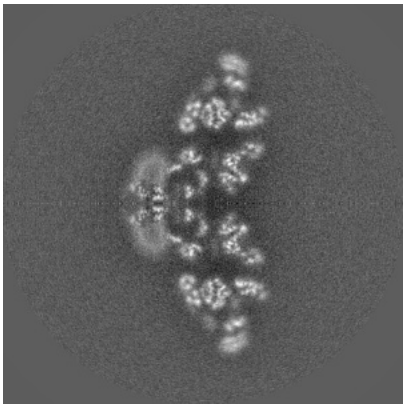


Z Index: 200

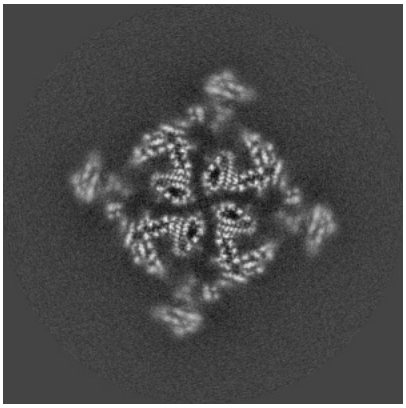
6.2.2 Raw map



X Index: 200



Y Index: 200

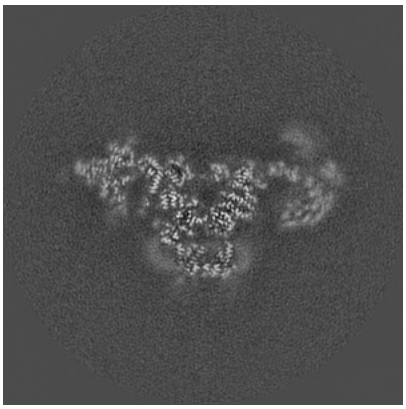


Z Index: 200

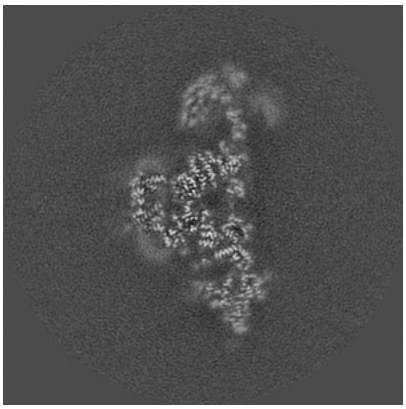
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

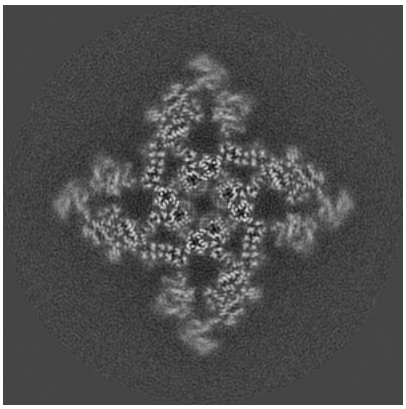
6.3.1 Primary map



X Index: 216

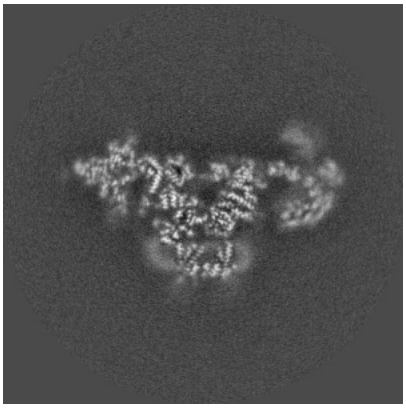


Y Index: 184

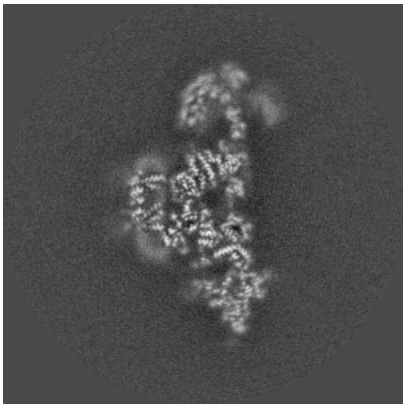


Z Index: 227

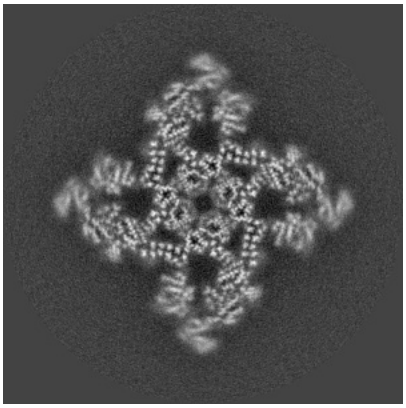
6.3.2 Raw map



X Index: 216



Y Index: 184

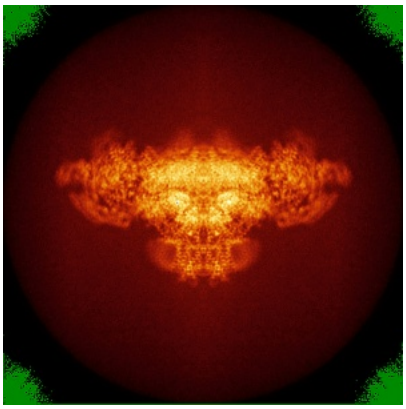


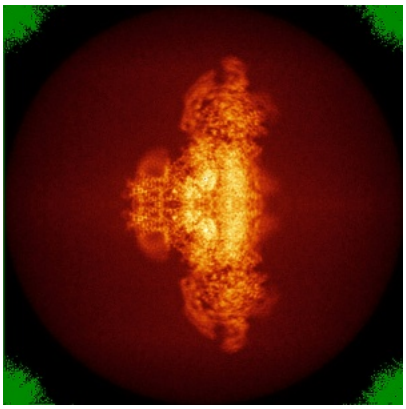
Z Index: 227

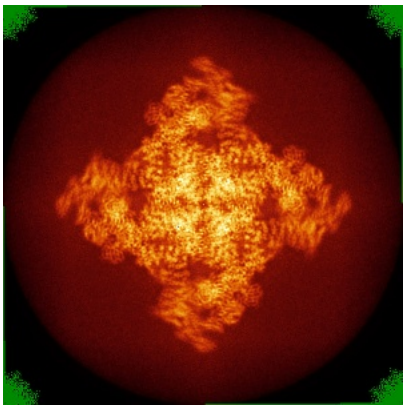
The images above show the largest variance slices of the map in three orthogonal directions.

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

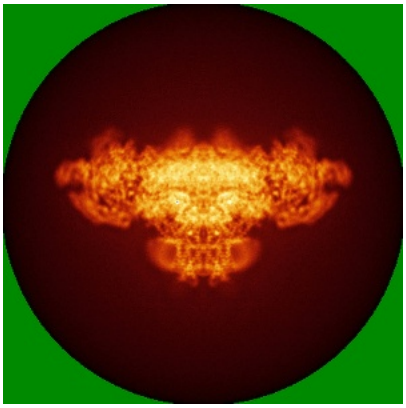
6.4.1 Primary map

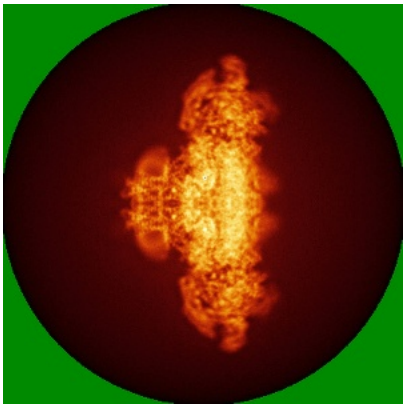

X

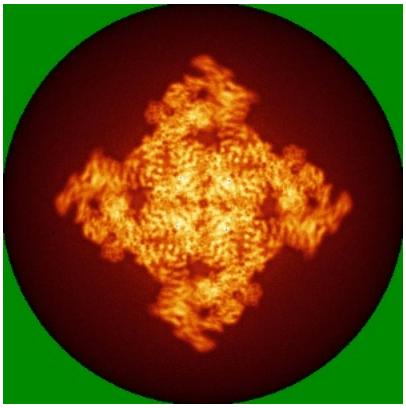

Y


Z

6.4.2 Raw map


X

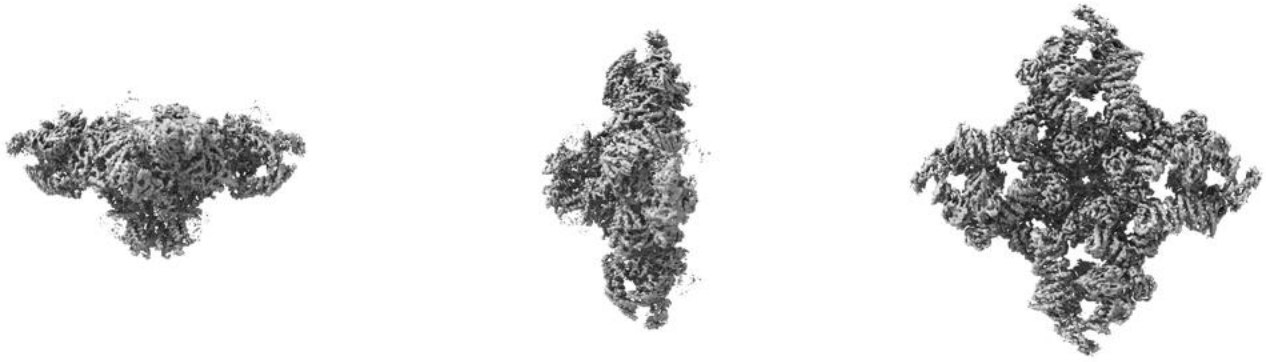

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

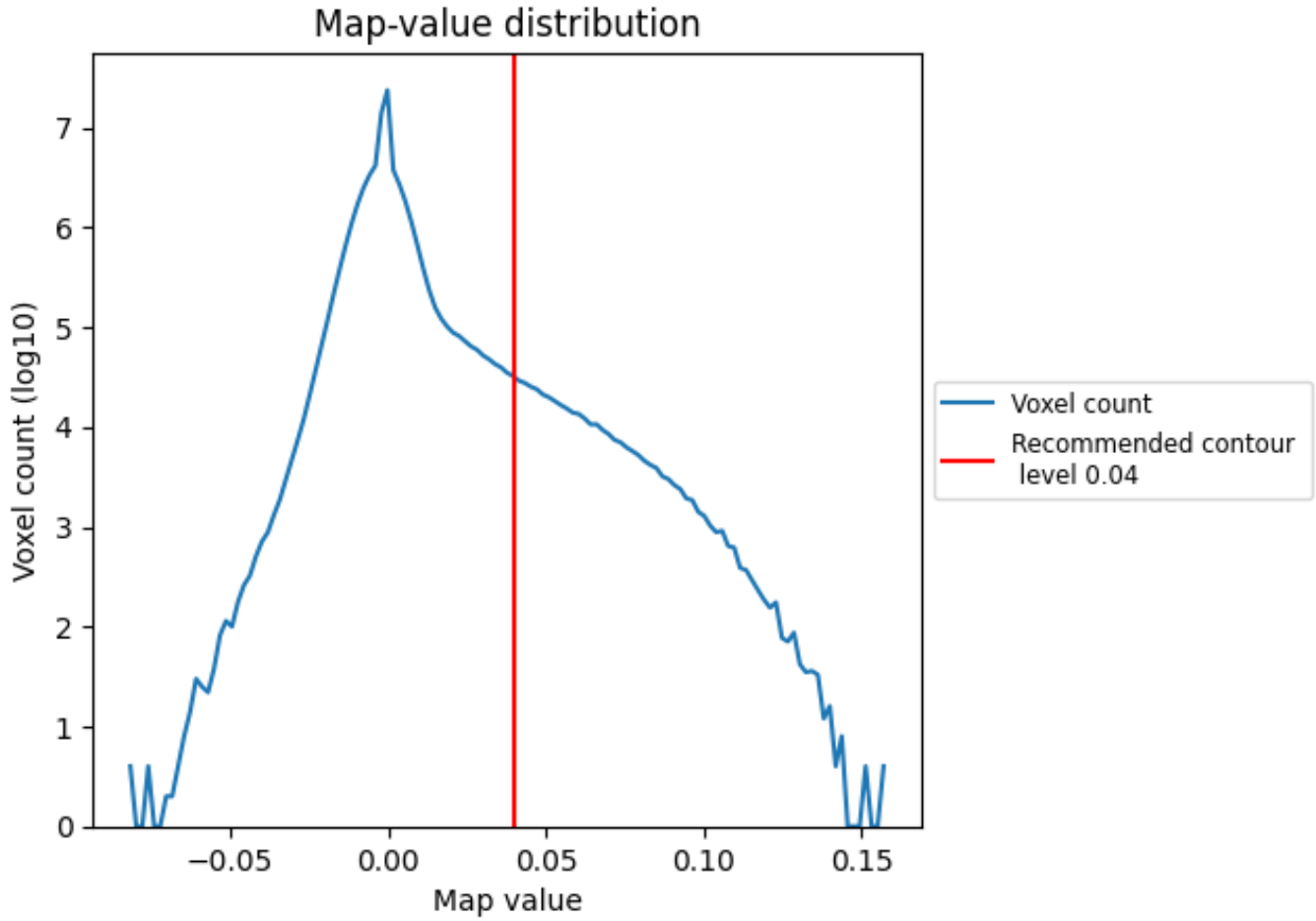
6.6 Mask visualisation (i)

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

7 Map analysis

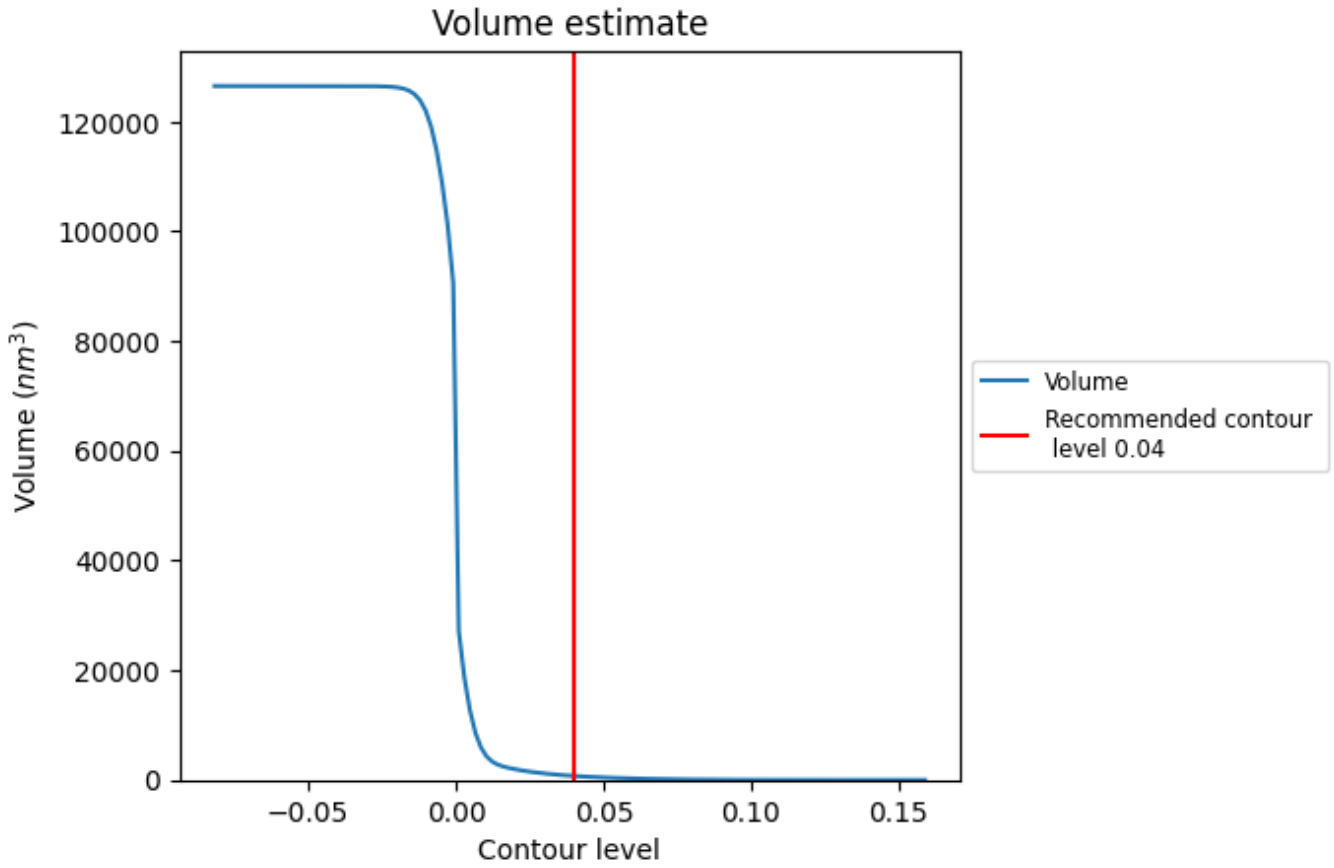
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

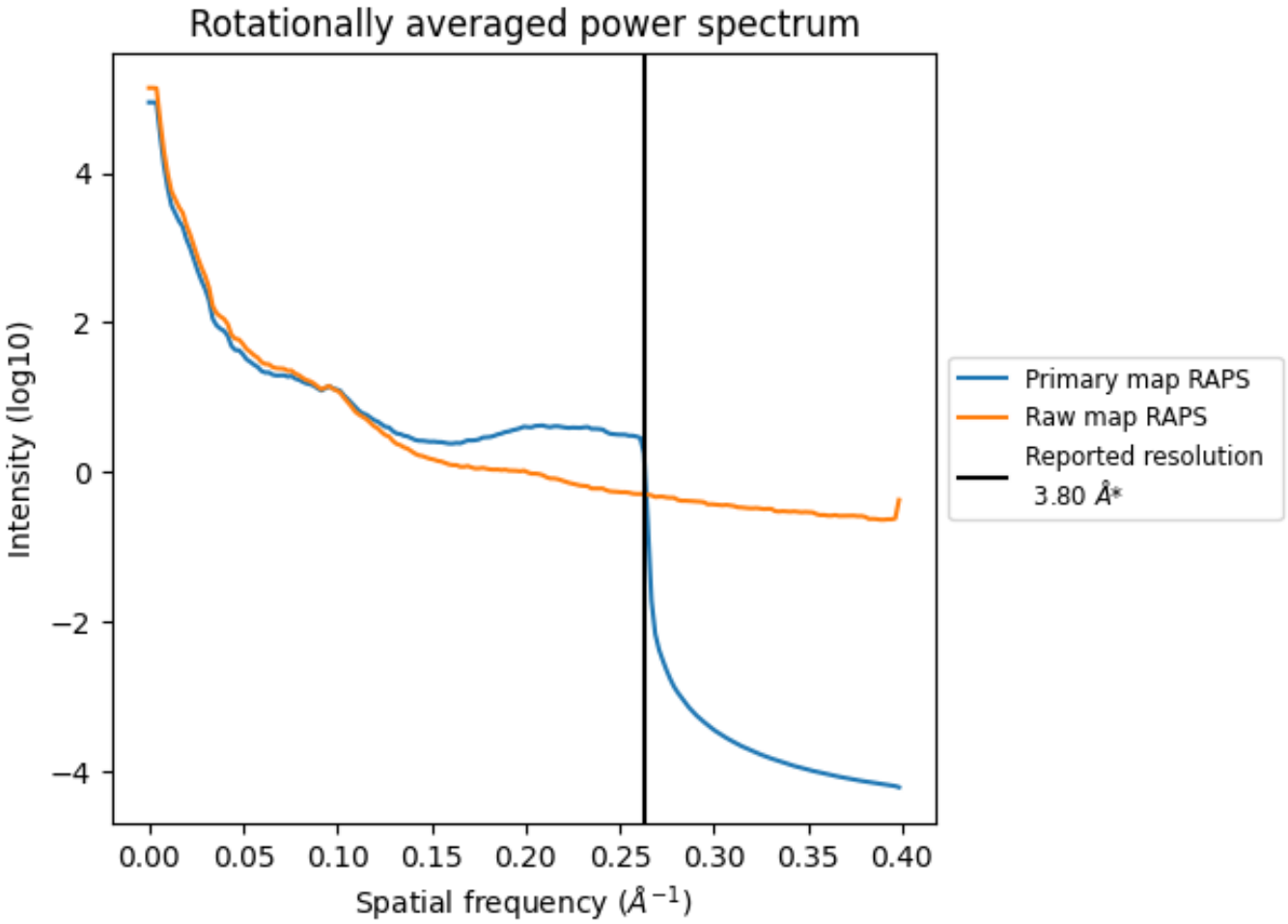
7.2 Volume estimate



The volume at the recommended contour level is 729 nm^3; this corresponds to an approximate mass of 658 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

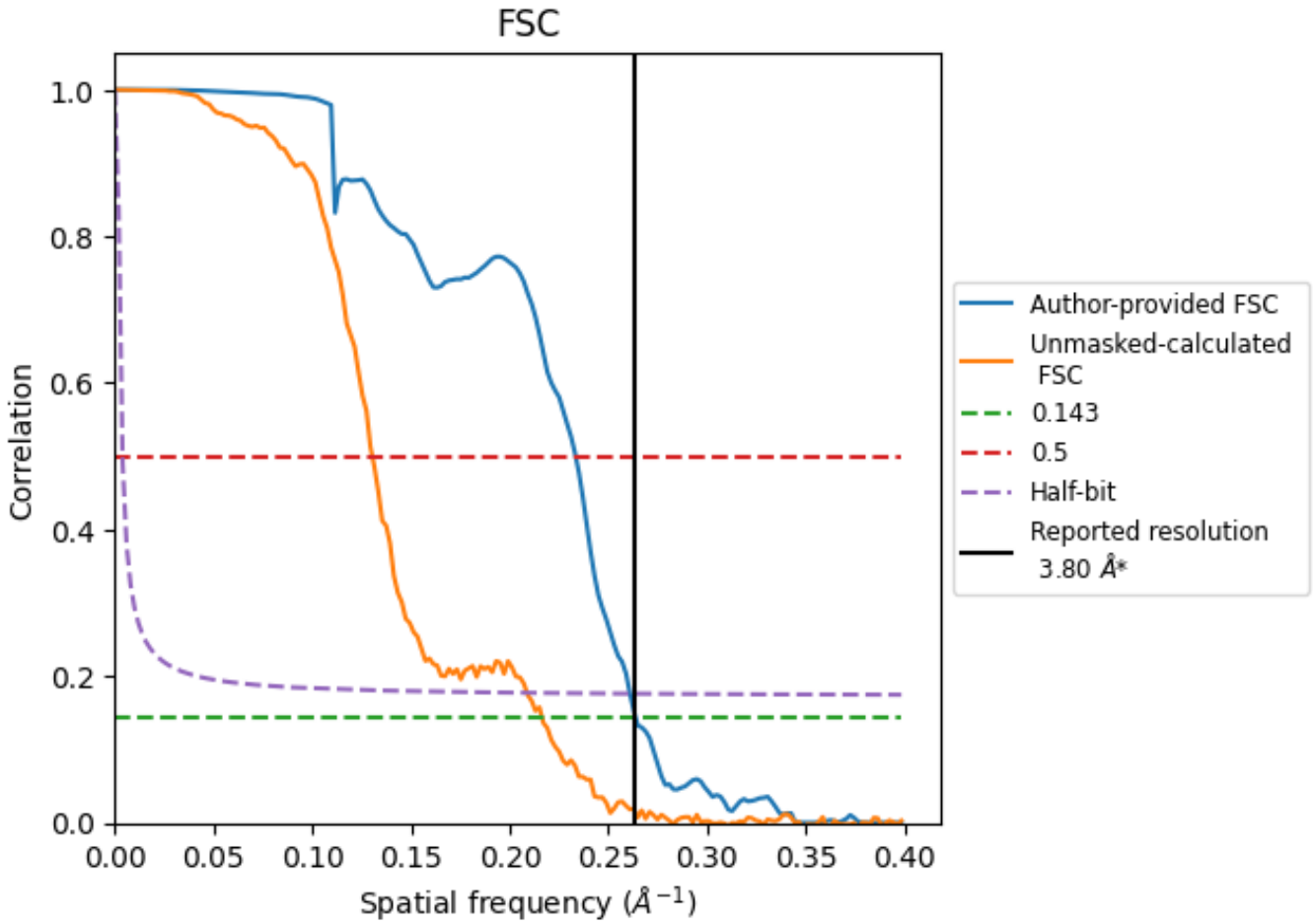


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

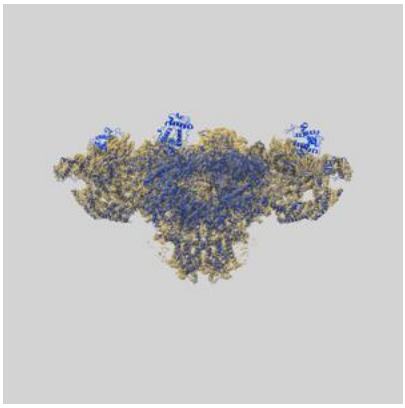
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.79	4.28	3.83
Unmasked-calculated*	4.62	7.67	4.79

*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 4.62 differs from the reported value 3.8 by more than 10 %

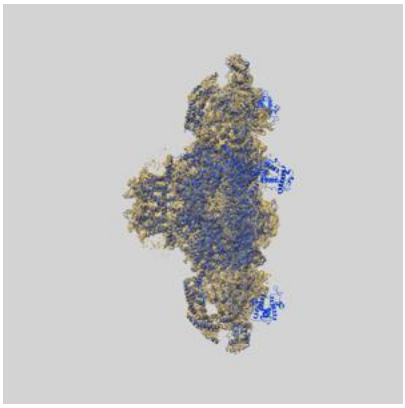
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8373 and PDB model 5T9N. Per-residue inclusion information can be found in section 3 on page 5.

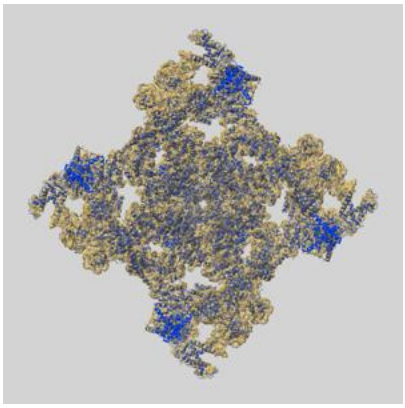
9.1 Map-model overlay



X



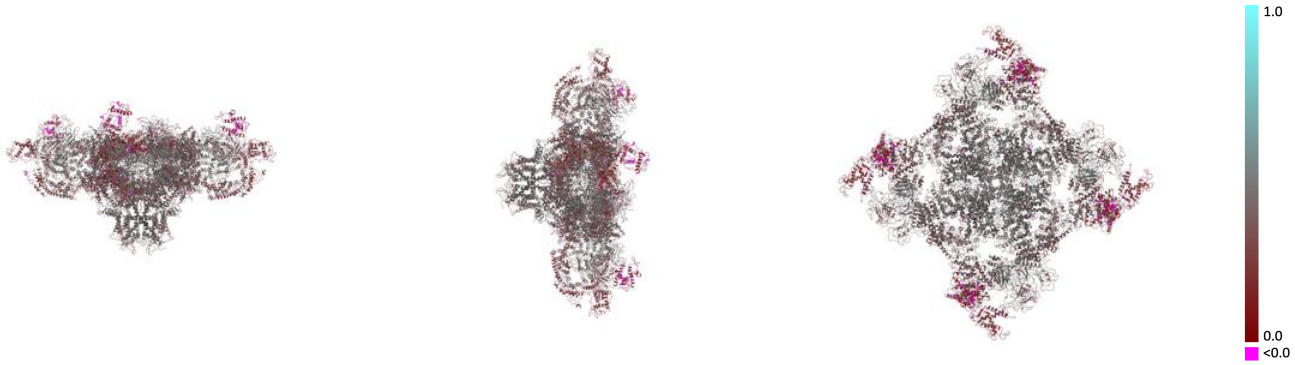
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

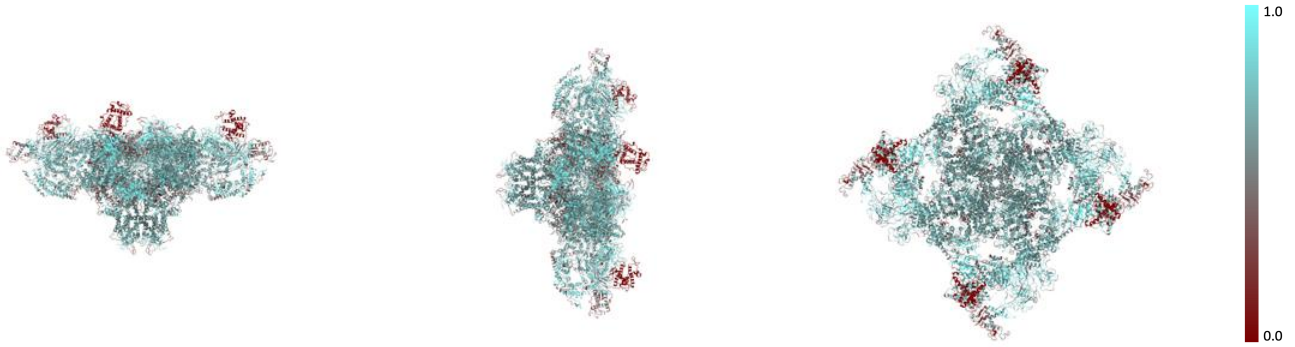
9.2 Q-score mapped to coordinate model



X Y Z

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

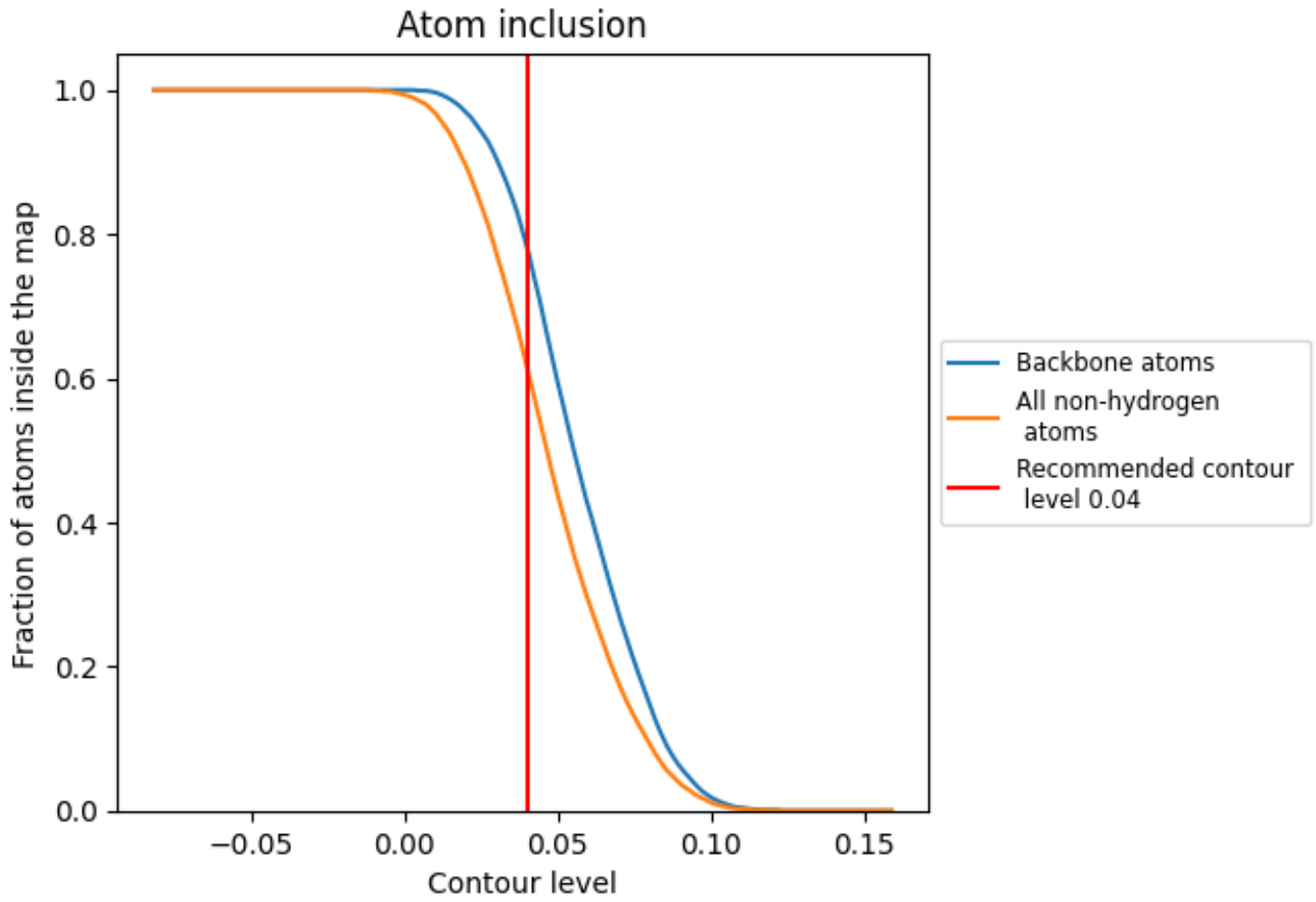
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 62% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.3680
A	0.6350	0.3810
B	0.6150	0.3680
E	0.6150	0.3670
F	0.6340	0.3870
G	0.6150	0.3680
H	0.6390	0.3850
I	0.6150	0.3680
J	0.6380	0.3820