Full wwPDB EM Validation Report

Feb 25, 2024 – 09:49 AM EST

PDB ID	:	7JMH
EMDB ID	:	EMD-22394
Title	:	Functional Pathways of Biomolecules Retrieved from Single-particle Snapshots - Frame 35 - State 4 (S4)
Authors	:	Dashti, A.; des Georges, A.; Frank, J.; Ourmazd, A.
Deposited on	:	2020-07-31
Resolution	:	4.50 Å(reported)
Based on initial model	:	5TB4

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 (i) 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 (i)) were used in the production of this report:

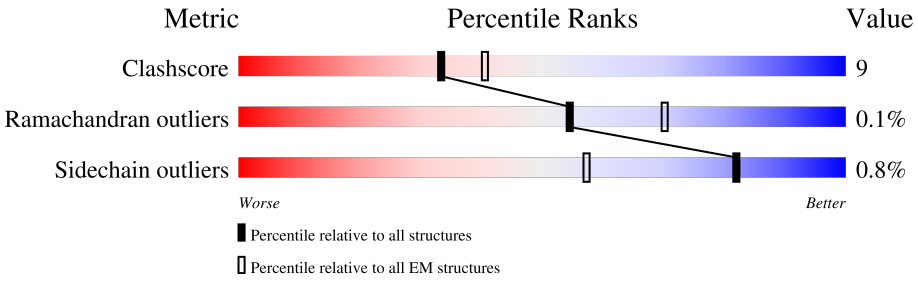
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.50 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	107	30% 69% 31%
1	F	107	44% 68% 32%
1	H	107	46% 70% 30%
1	J	107	43% 67% 33%
2	B	4687	34% 71% 18% 11%
2	E	4687	38% 71% 18% 11%
2	G	4687	44% 70% 18% 11%
2	I	4687	43% 71% 18% 11%

2 Entry composition

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	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	F	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 type 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	G	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		

- 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	G	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of

Interest" by depositor).

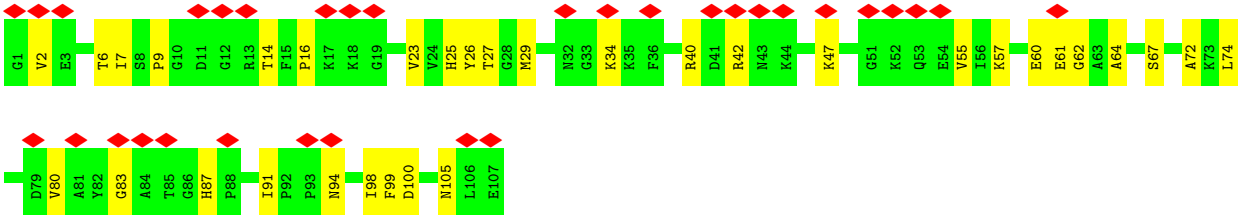
Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	E	1	Total Ca 1 1	0
4	G	1	Total Ca 1 1	0
4	I	1	Total Ca 1 1	0

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.

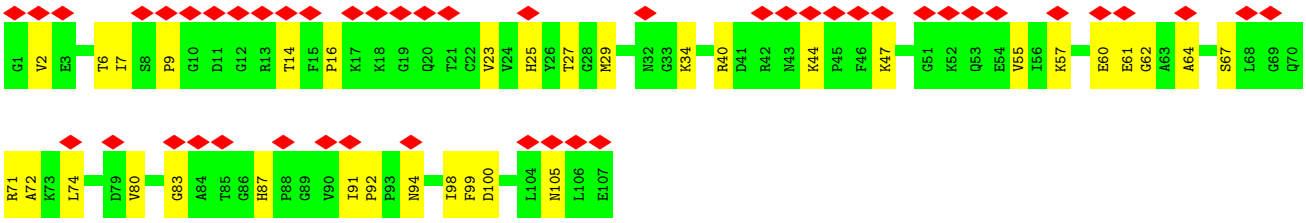
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A:



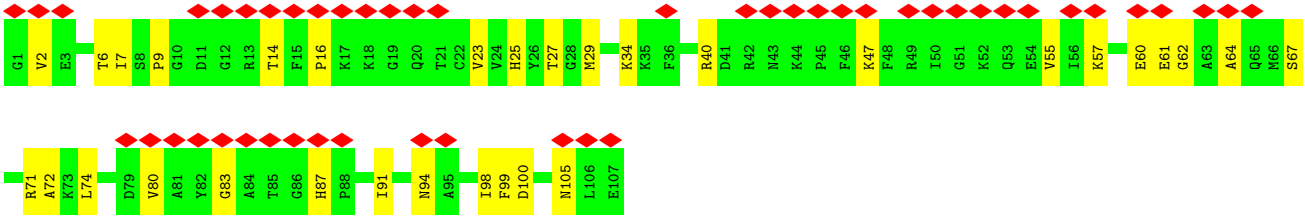
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



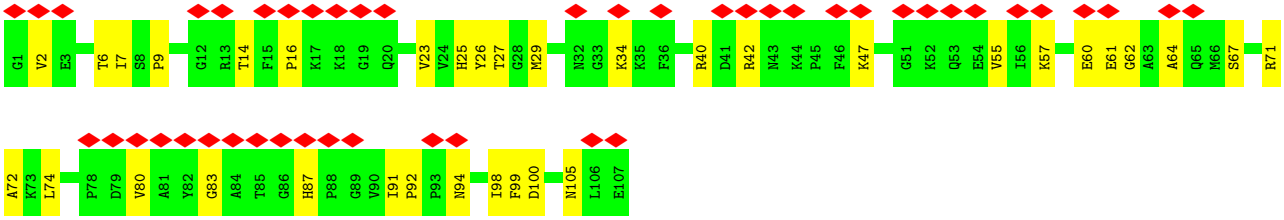
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H:



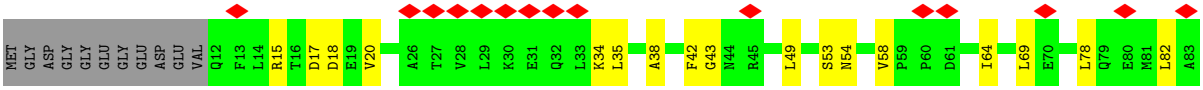
• Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

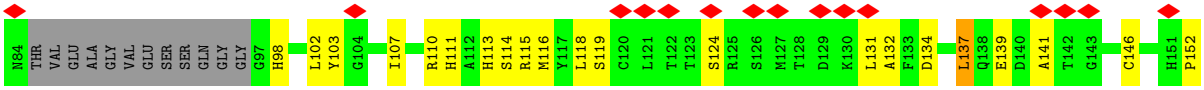
Chain J:

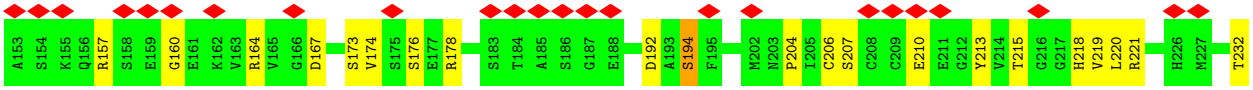


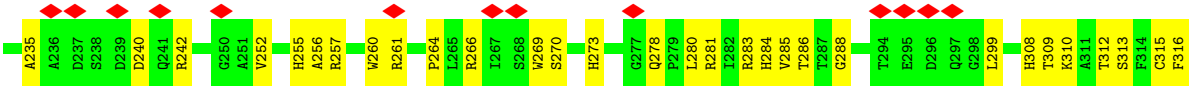
• Molecule 2: ryanodine receptor type 1

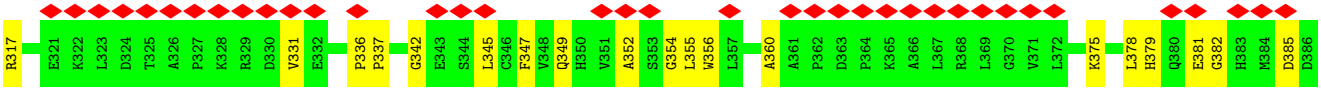
Chain B:

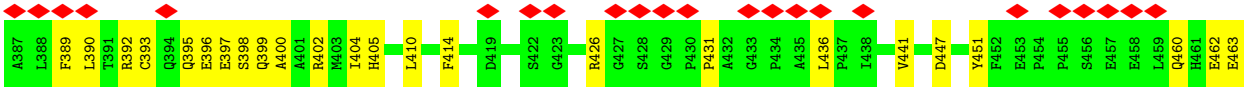


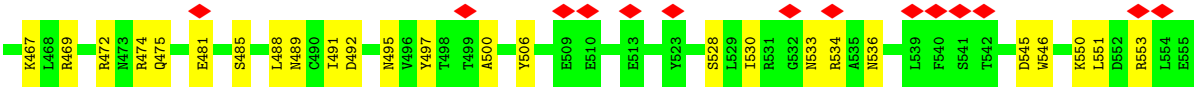


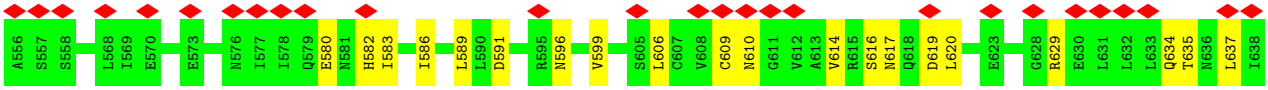


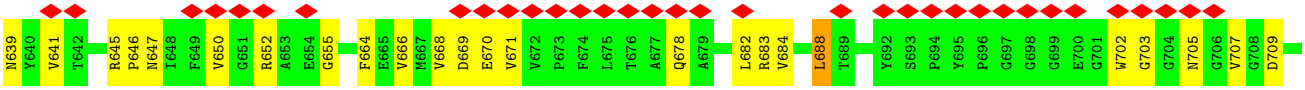


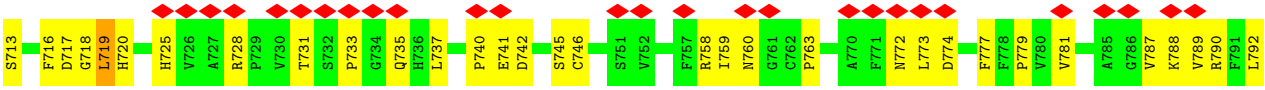


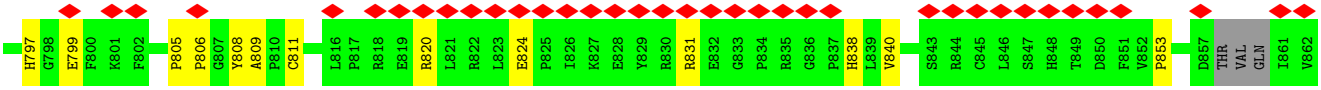










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E1583 R1584 K1585 N1586 P1587 Q1590 C1591 R1594 L1595 Q1598 M1599 L1600 V1603 S1604 W1605 P1609 N1610 H1611 F1612 L1613 Q1614 V1615 GLU THR ARG ARG ALA GLY E1622 R1623 L1624 G1625 W1626 A1627 V1628 Q1629 C1630 Q1631 D1632 P1633 L1634 T1635 M1636 M1637 A1638 L1639 E1643 E1644 N1645 R1646 C1647 M1648 D1649 I1650
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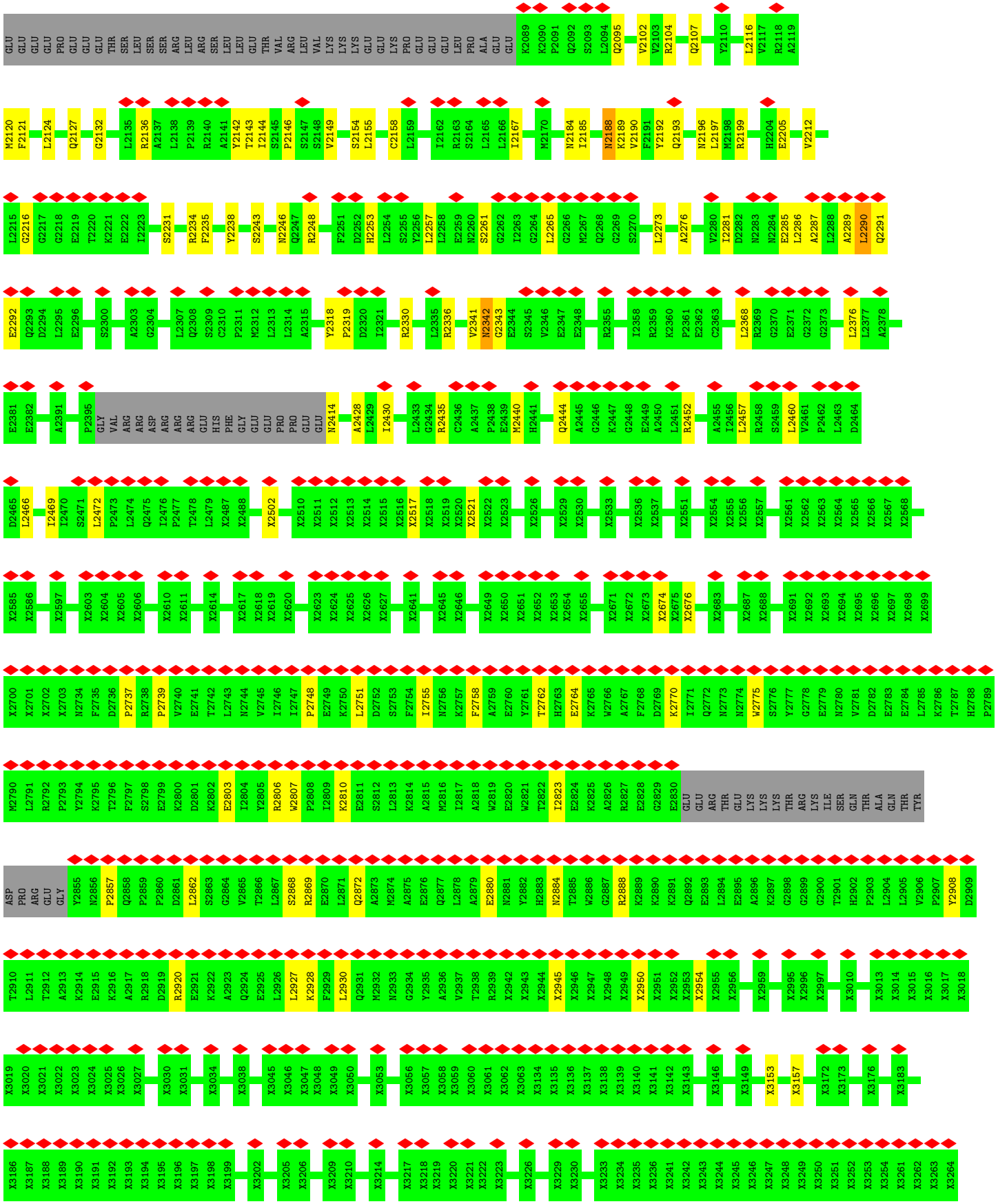
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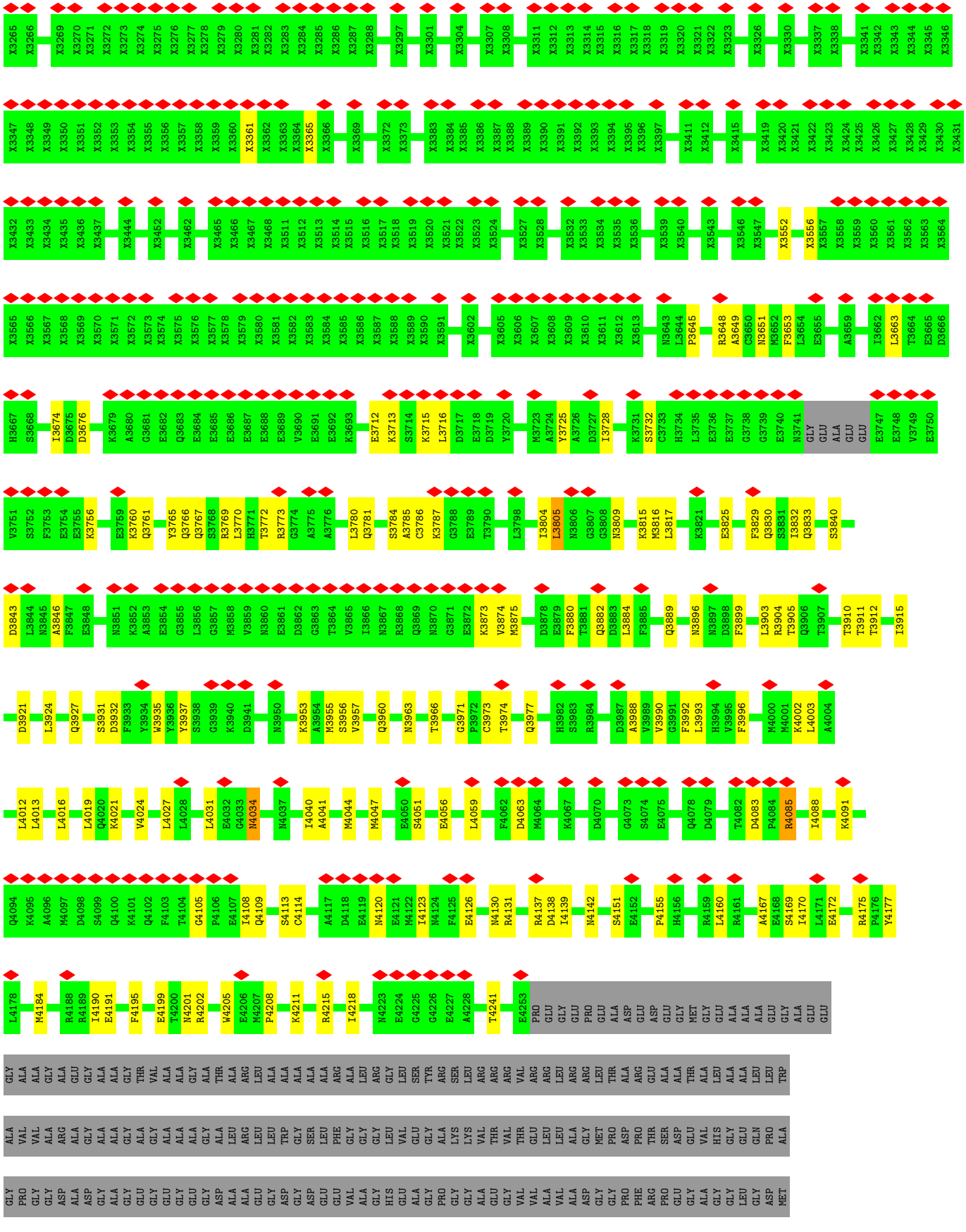
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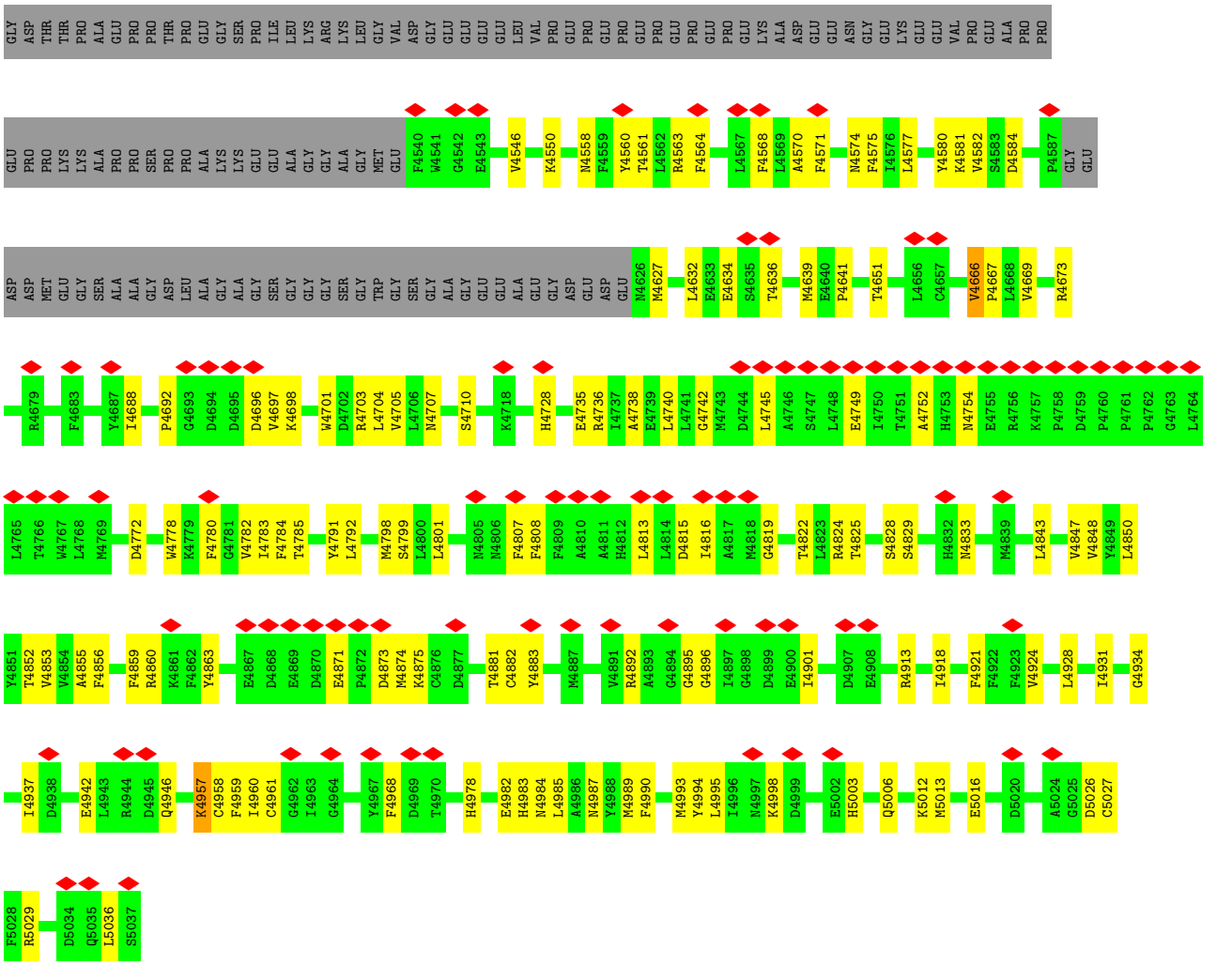
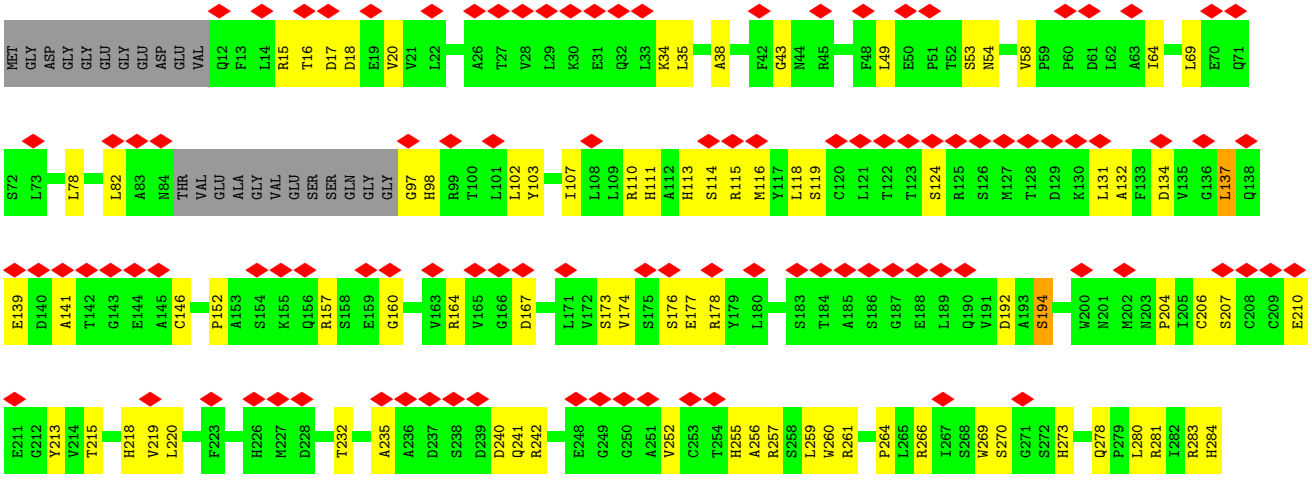
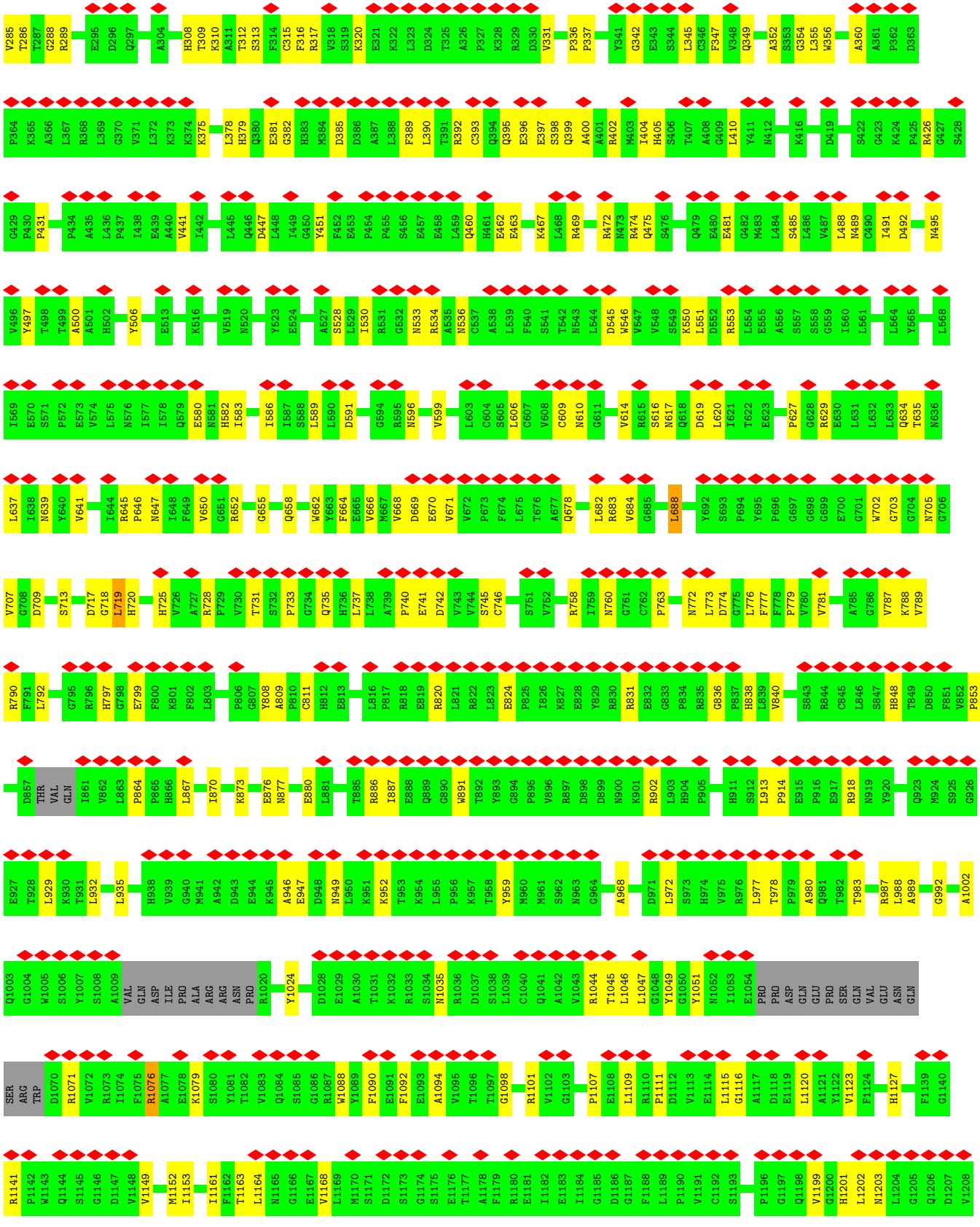
GLY PRO GLY GLY ASP ALA ASP GLY ALA GLY GLU GLY GLU GLY GLU GLY ASP ALA ALA GLU GLY ASP GLU GLU VAL GLU HIS GLU ALA GLY PRO GLY GLY ALA VAL VAL ALA VAL ALA ASP GLY GLY PRO PHE ARG PRO GLU GLU GLY ALA GLY GLY LEU GLY ASP MET



• Molecule 2: ryanodine receptor type 1

Chain E:

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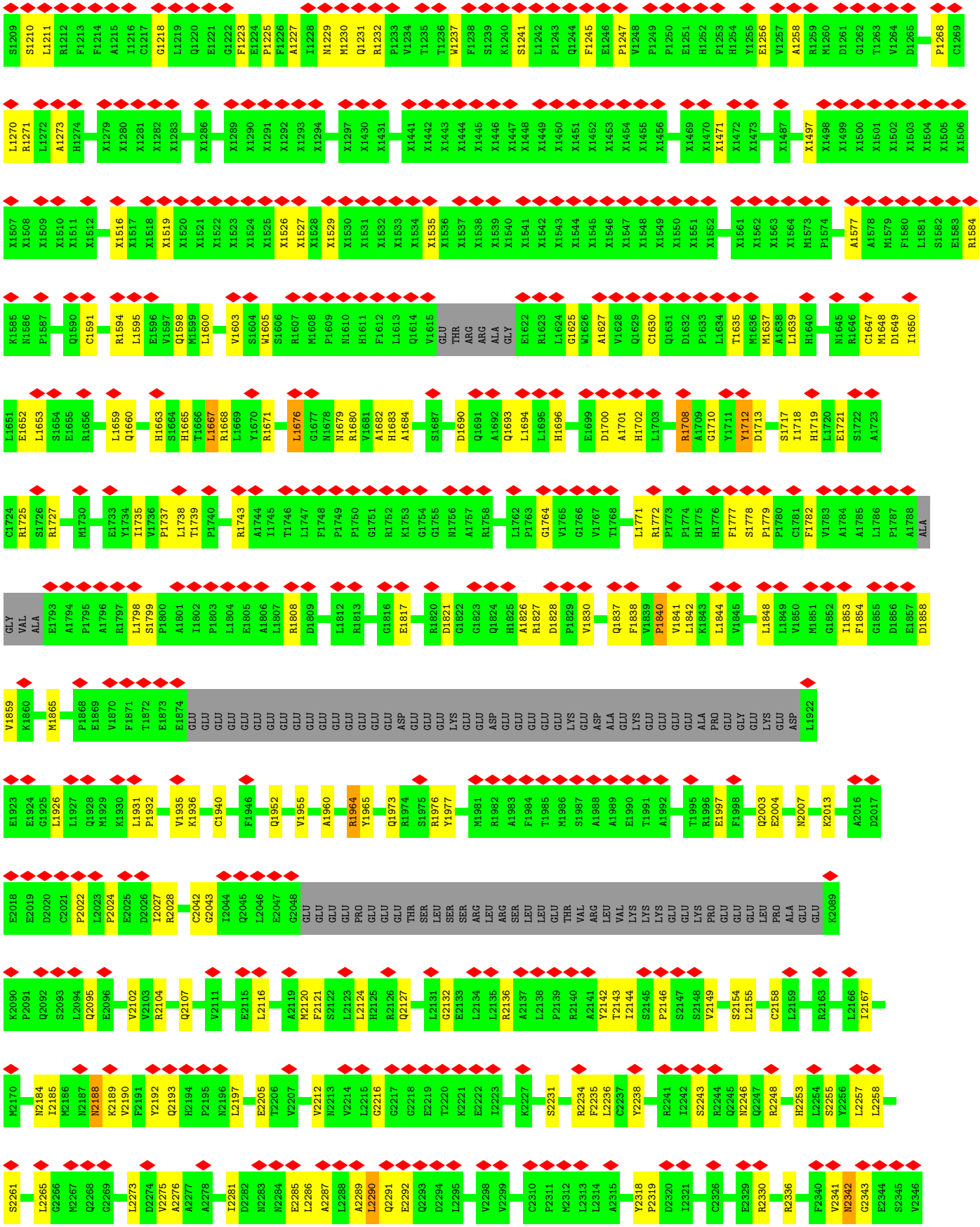

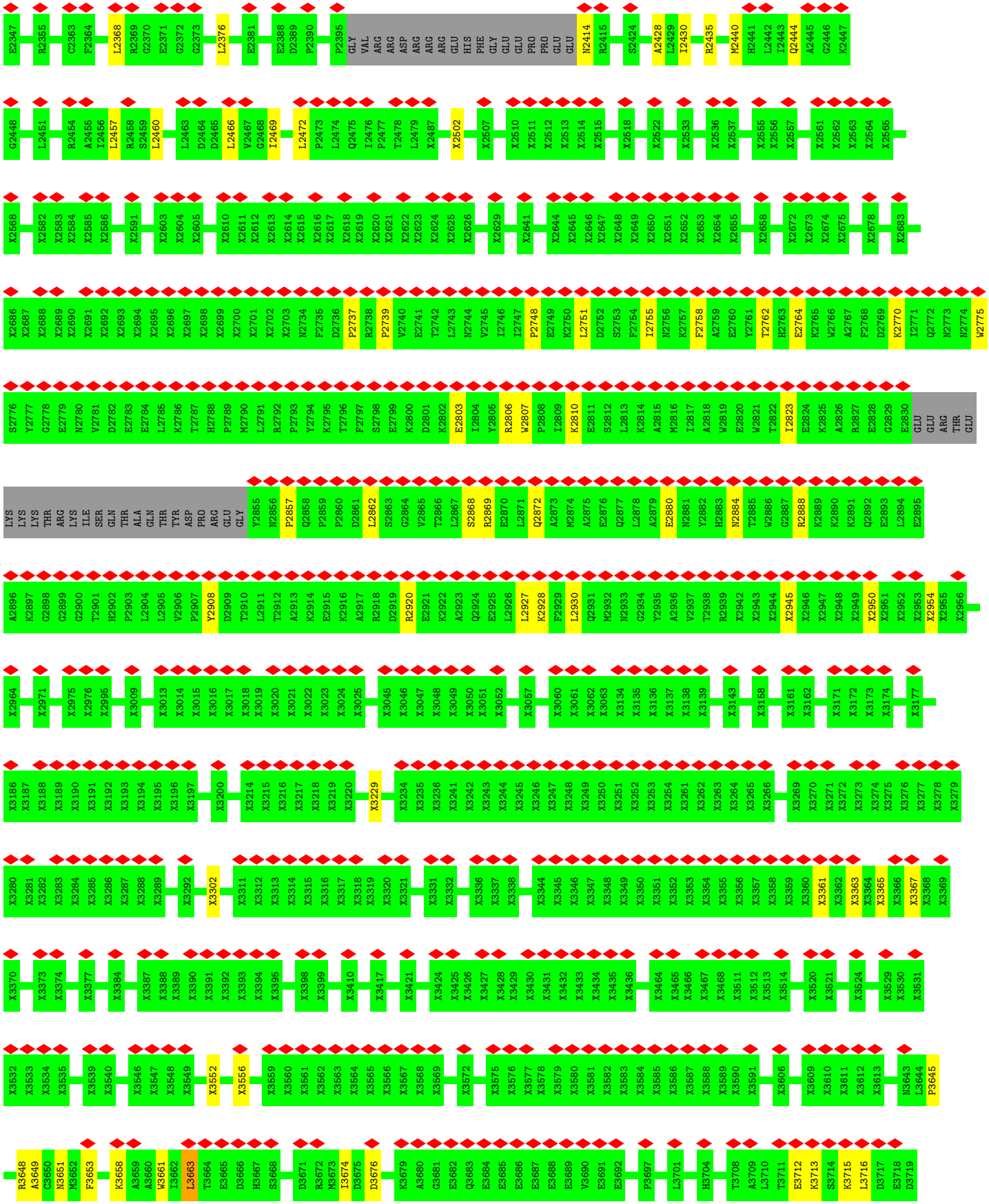
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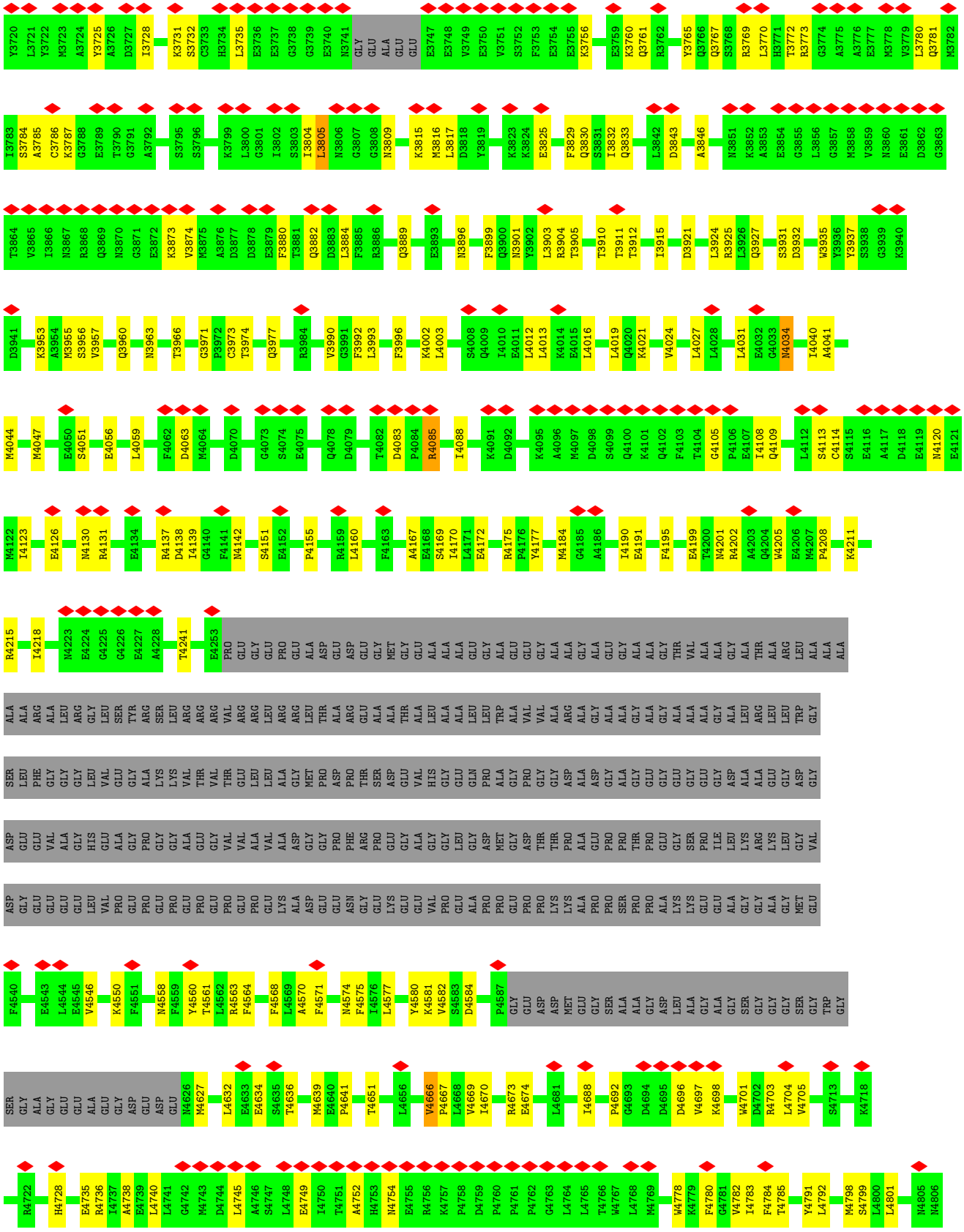
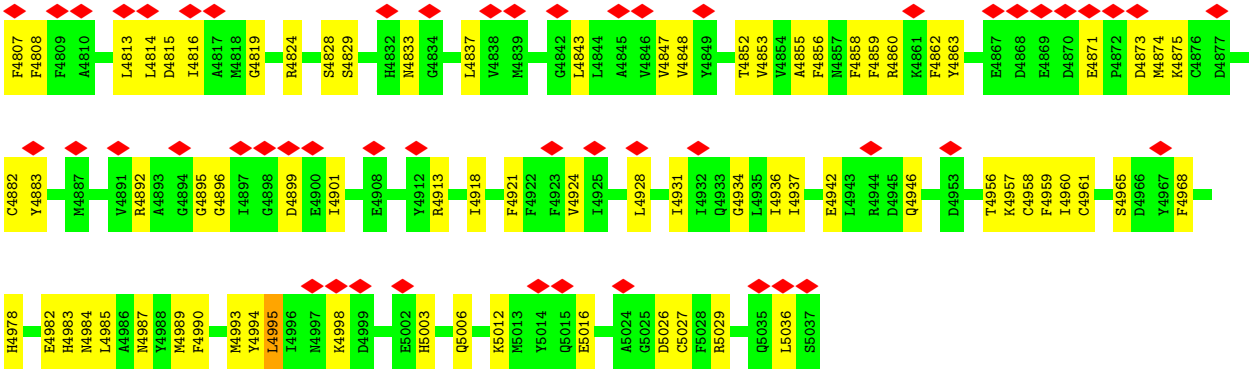
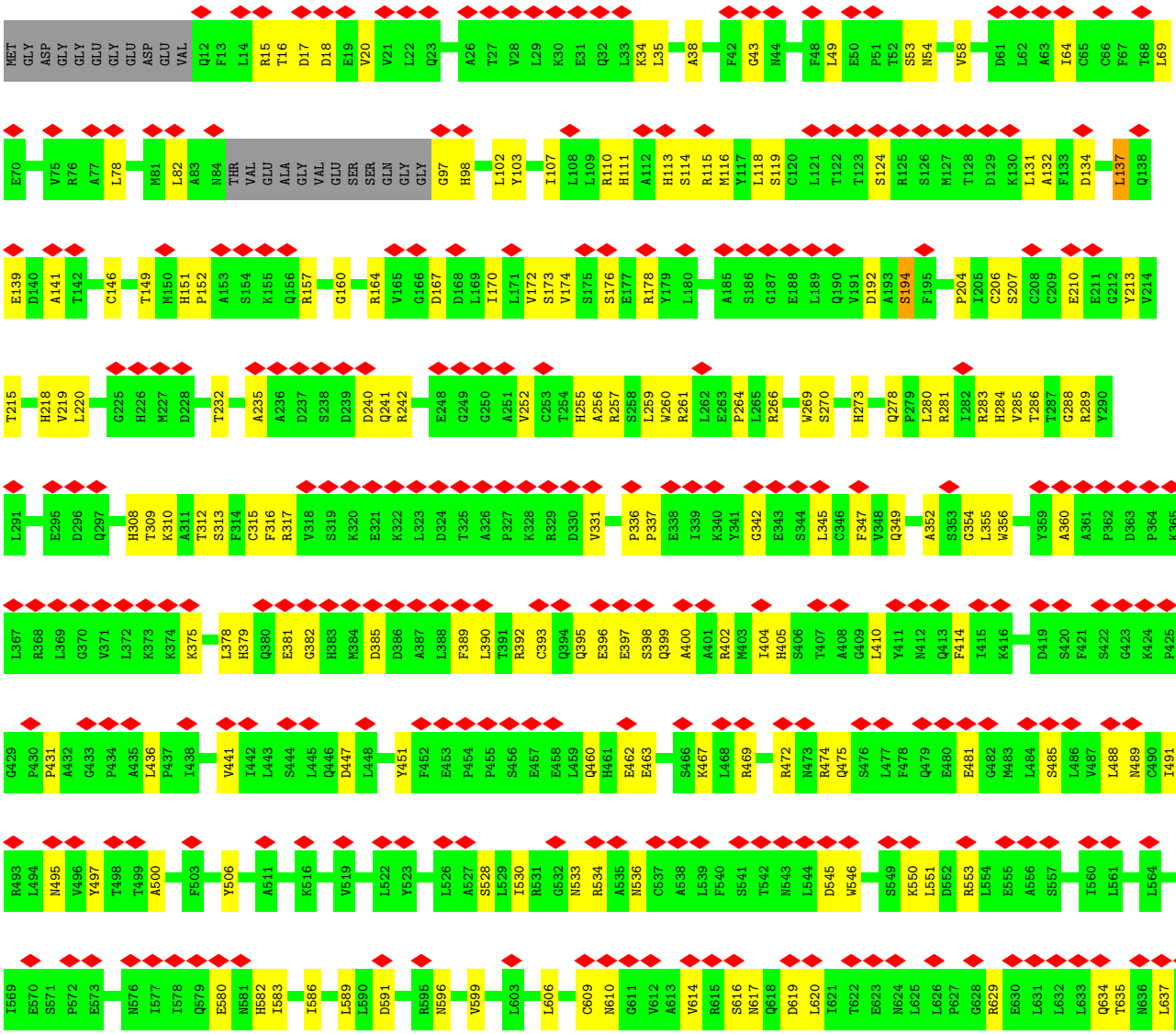
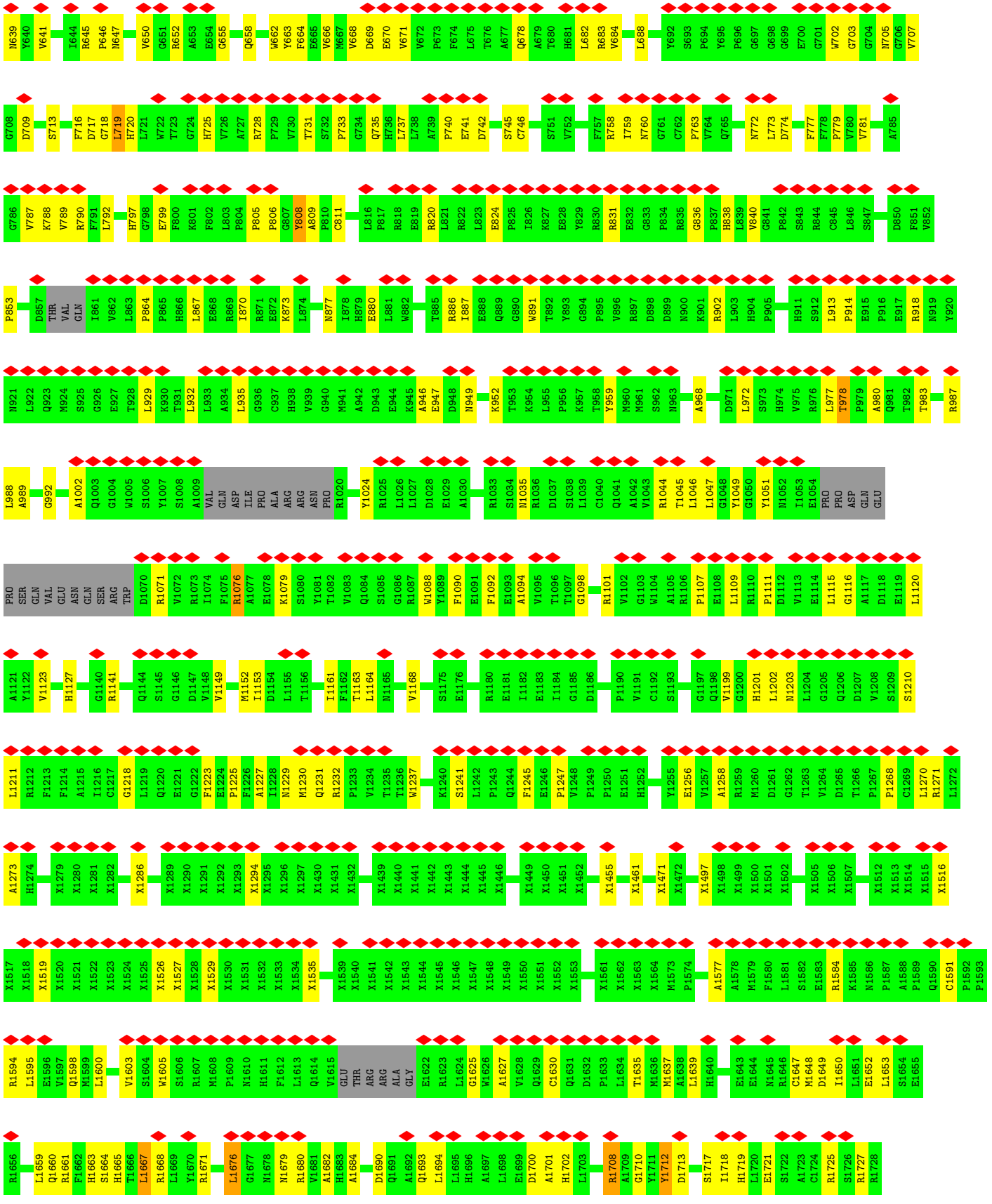




• Molecule 2: ryanodine receptor type 1

Chain G:

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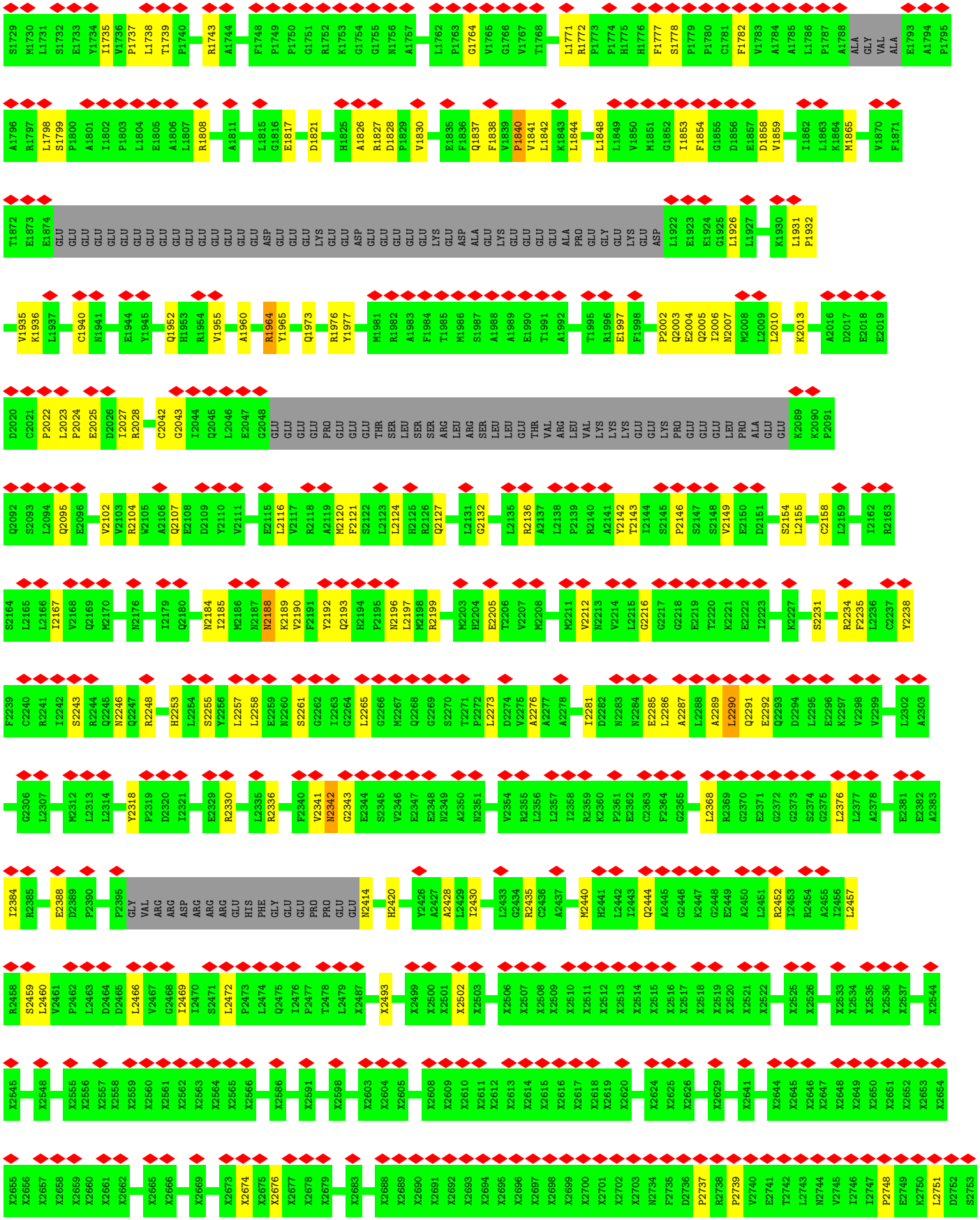

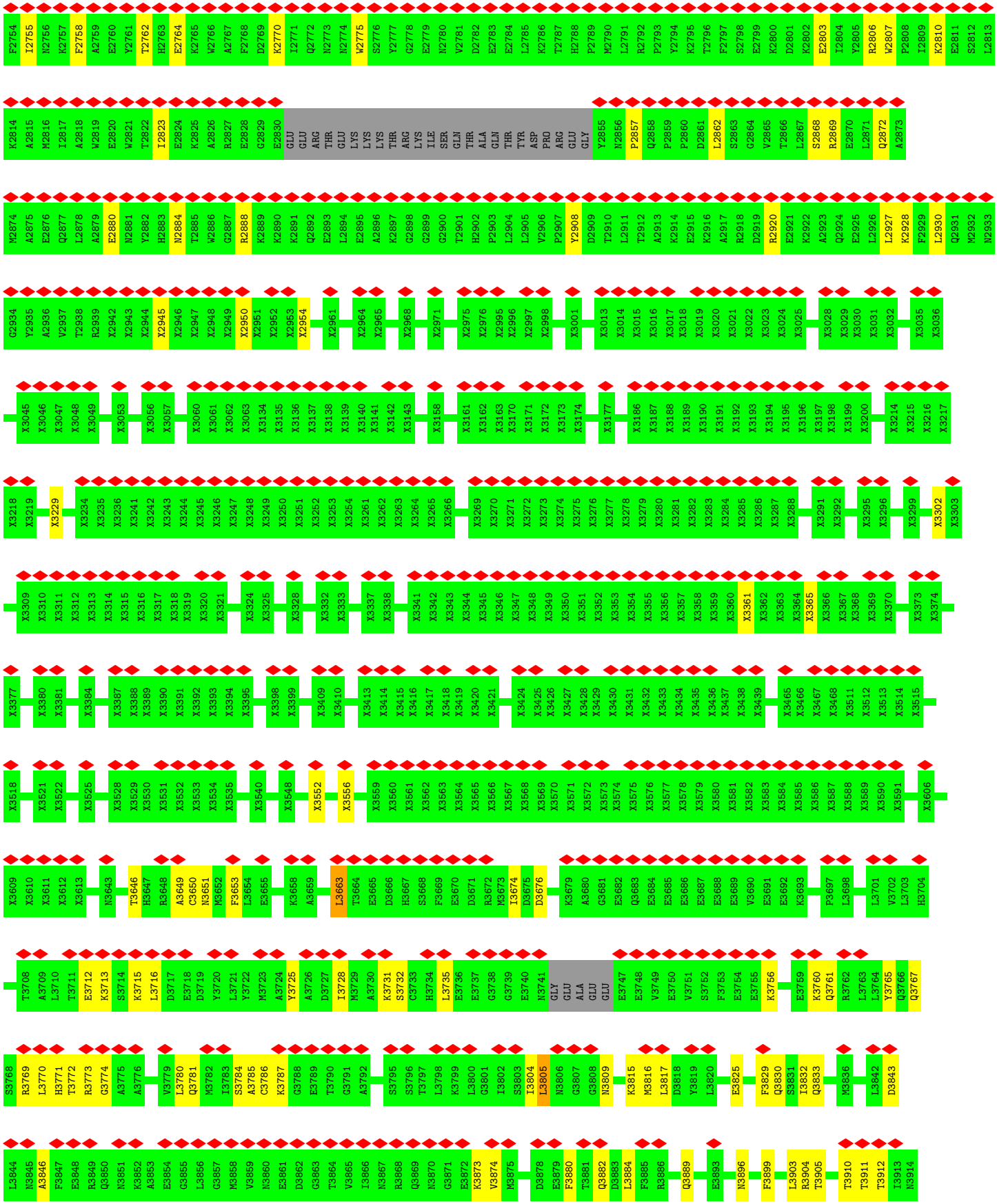
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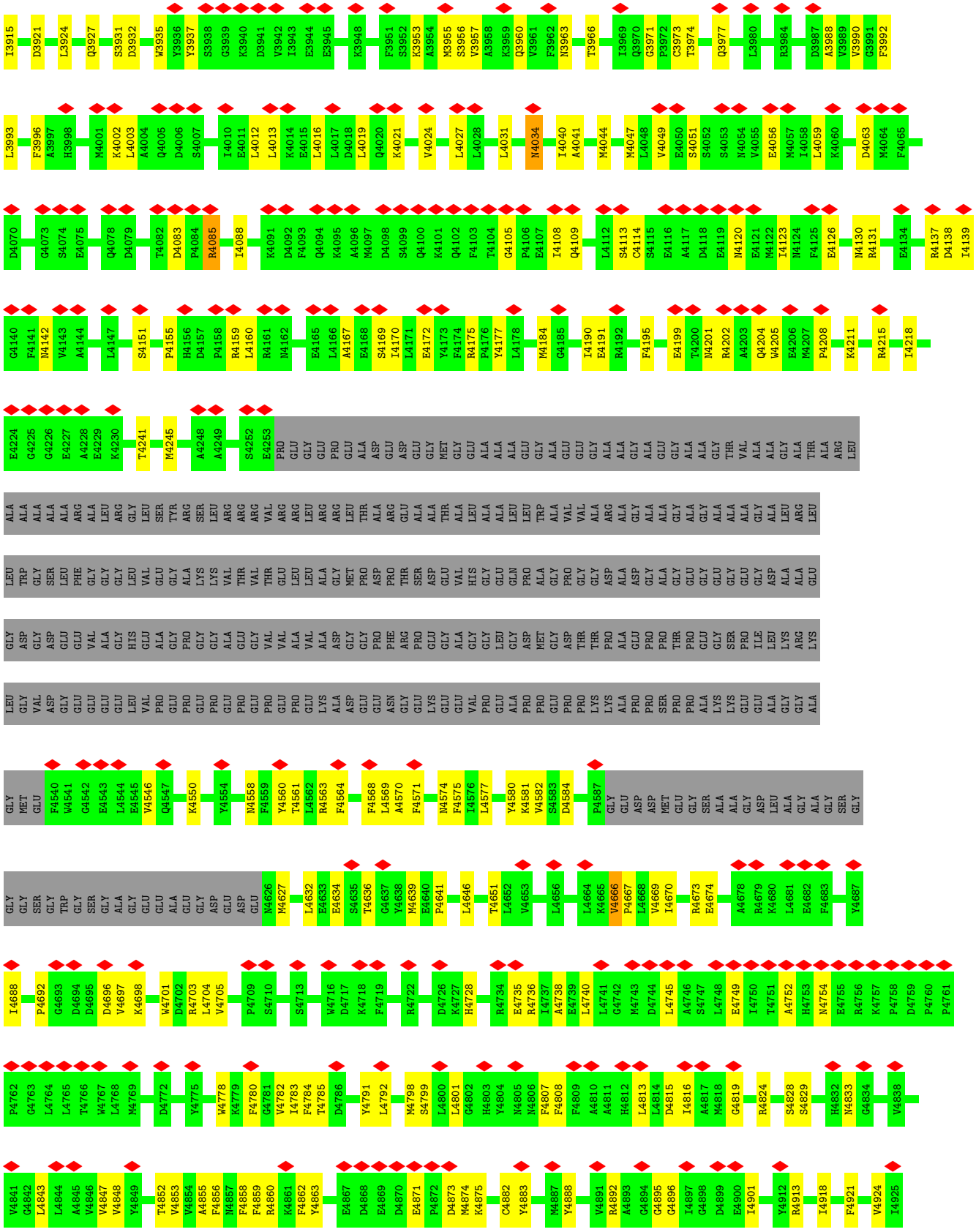
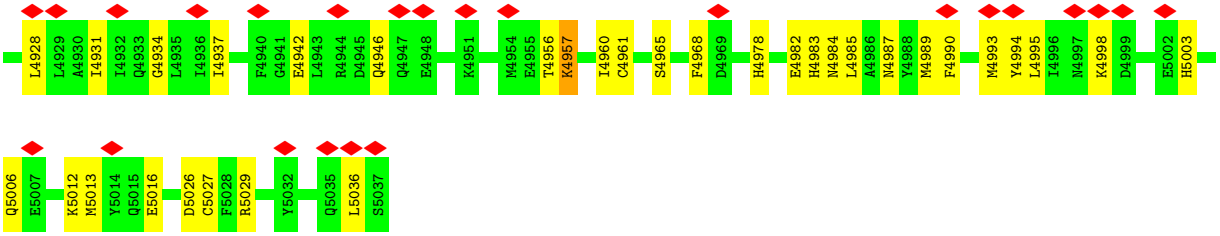
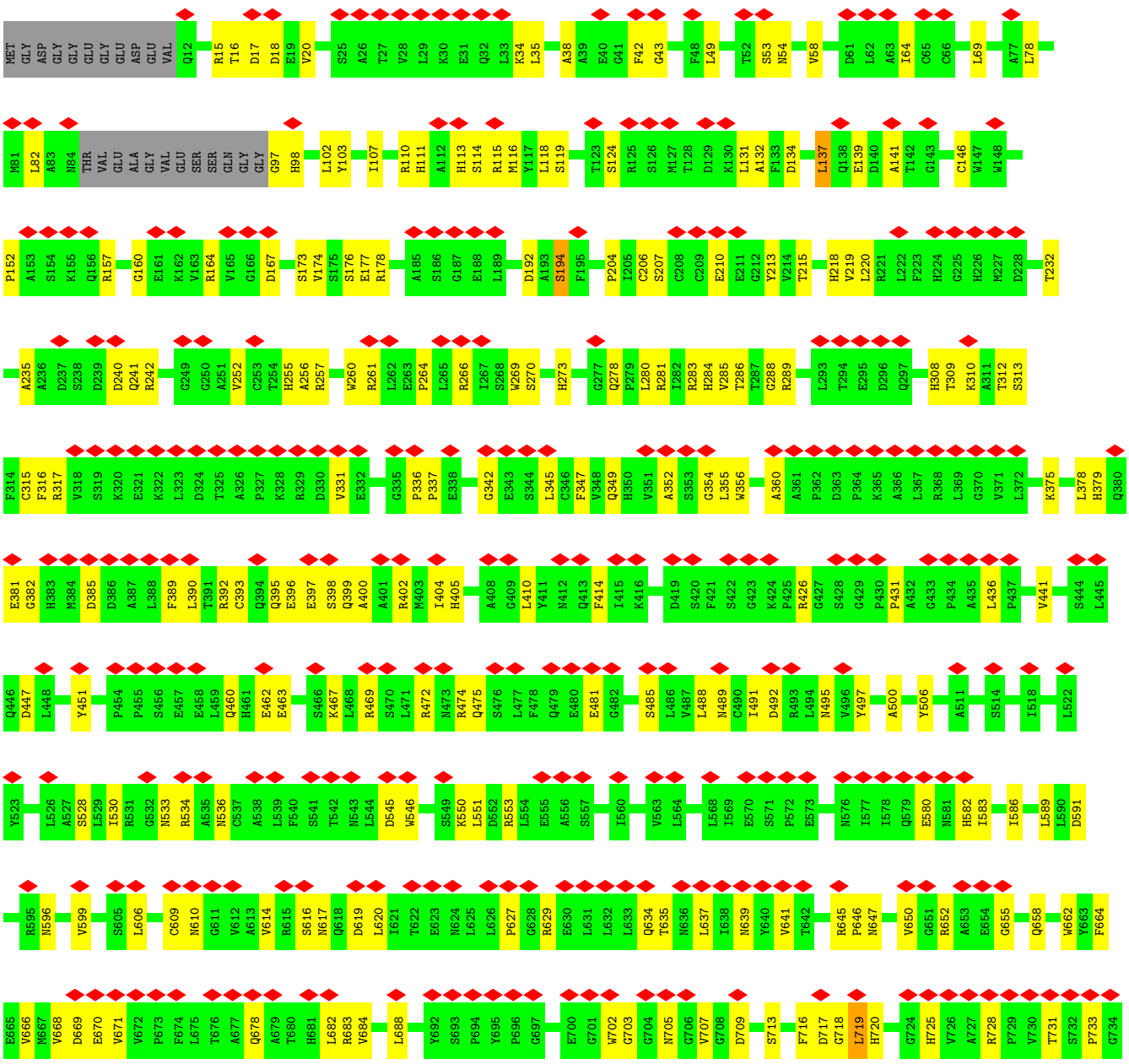
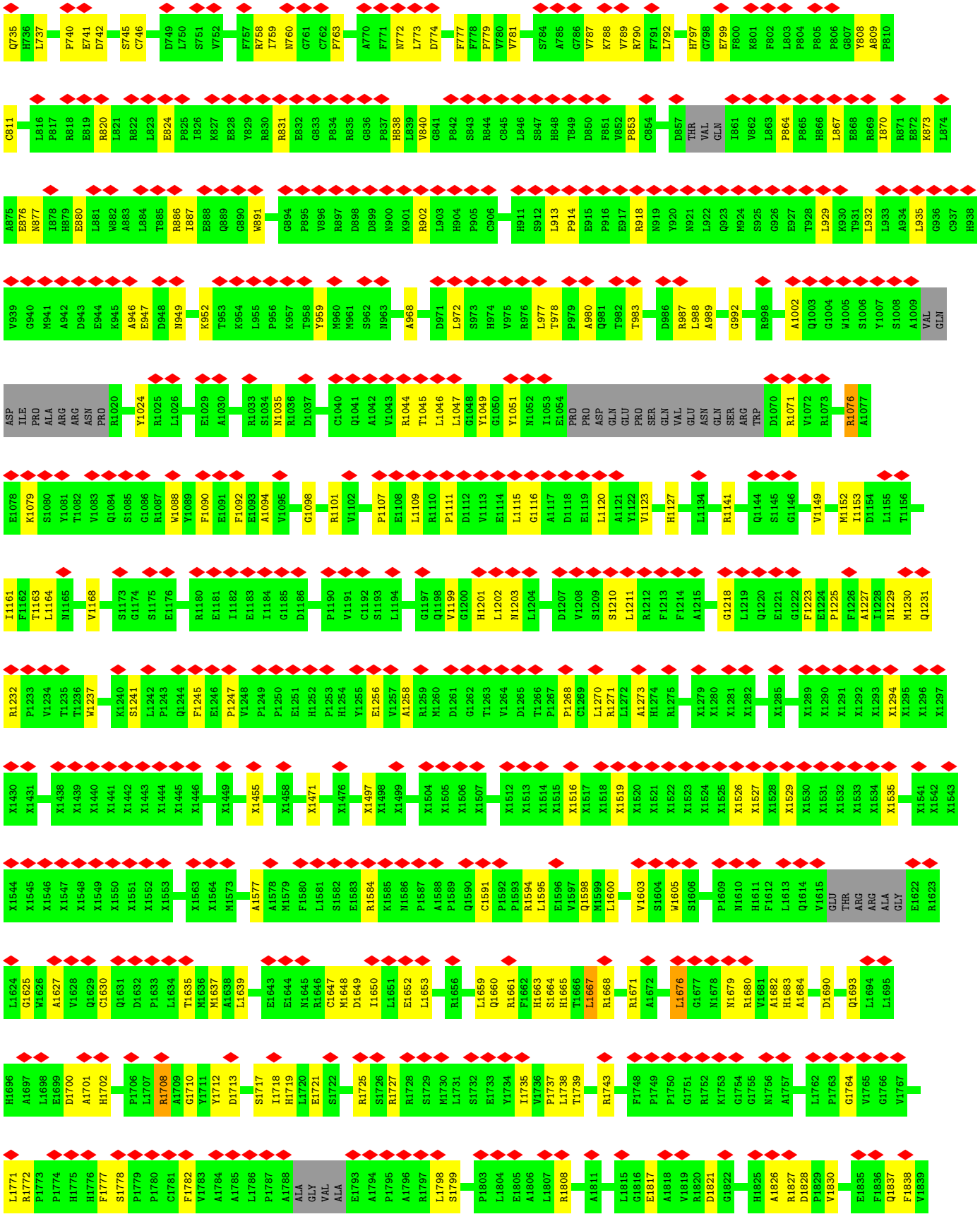




• Molecule 2: ryanodine receptor type 1

Chain I:

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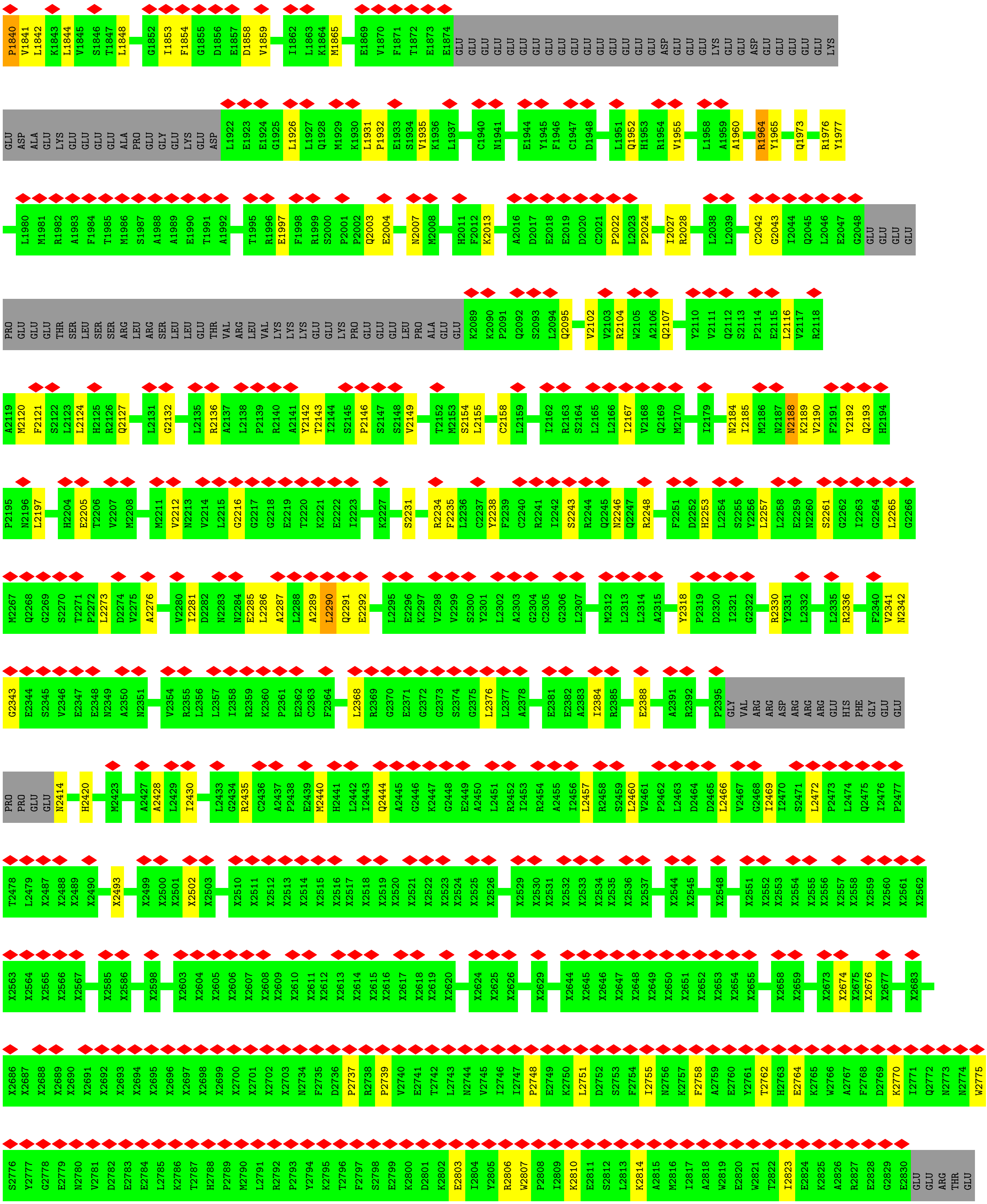
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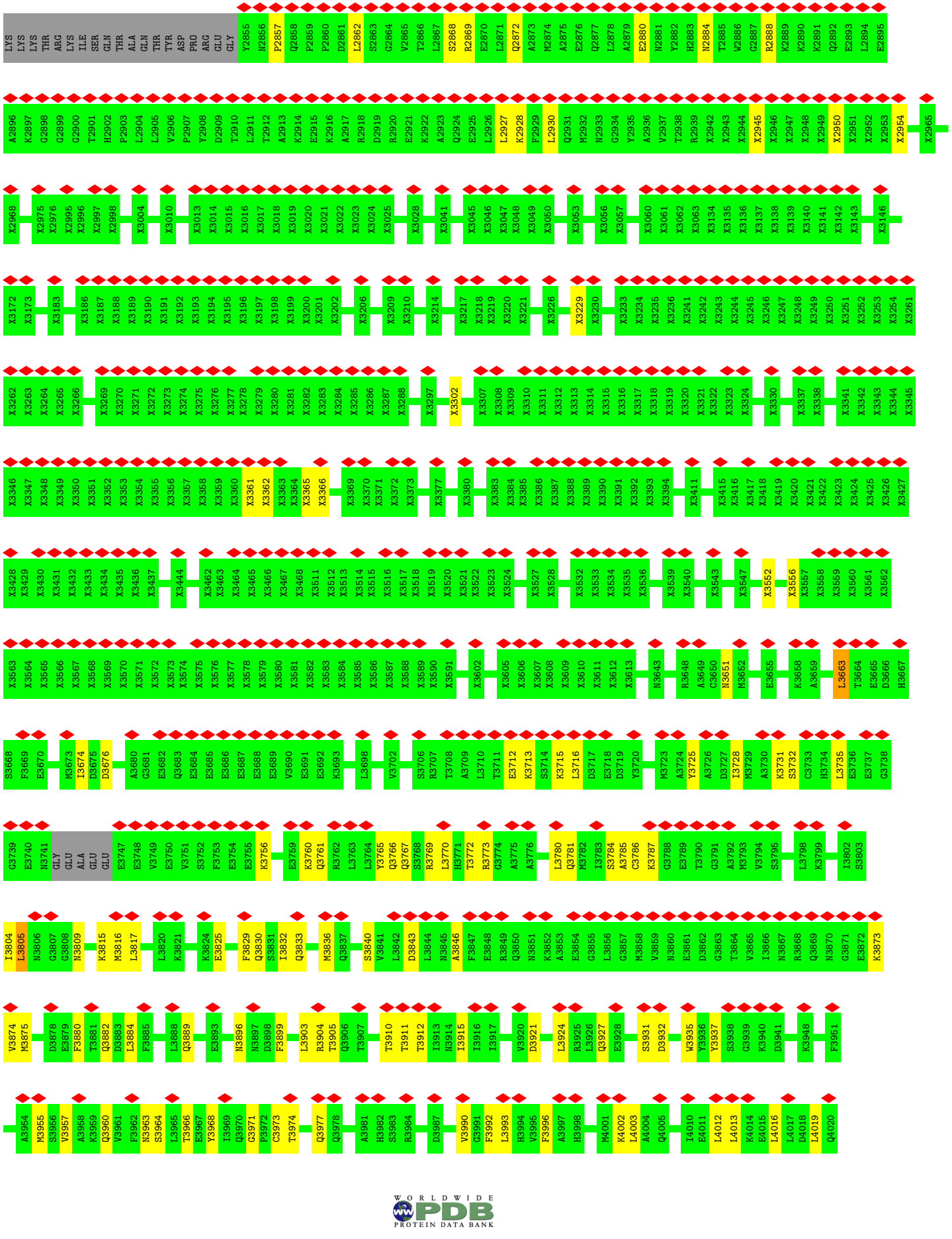
S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818 W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU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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 Y2937 T2938 R2939 X2942 X2943 X2944 X2945 X2946 X2947 X2948 X2949 X2950 X2951 X2952 X2953 X2954 X2965
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X3172 X3173 X3183 X3186 X3187 X3188 X3189 X3190 X3191 X3192 X3193 X3194 X3195 X3196 X3197 X3198 X3199 X3200 X3201 X3202 X3206 X3209 X3210 X3214 X3217 X3218 X3219 X3220 X3221 X3226 X3229 X3230 X3233 X3234 X3235 X3236 X3241 X3242 X3243 X3244 X3245 X3246 X3247 X3248 X3249 X3250 X3251 X3252 X3253 X3254 X3261
X3262 X3263 X3264 X3265 X3266 X3269 X3270 X3271 X3272 X3273 X3274 X3275 X3276 X3277 X3278 X3279 X3280 X3281 X3282 X3283 X3284 X3285 X3286 X3287 X3288 X3297 X3302 X3307 X3308 X3309 X3310 X3311 X3312 X3313 X3314 X3315 X3316 X3317 X3318 X3319 X3320 X3321 X3322 X3323 X3324 X3330 X3337 X3338 X3341 X3342 X3343 X3344 X3345
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S3668 F3669 E3670 M3673 I3674 D3675 D3676 A3680 G3681 E3682 Q3683 E3684 E3685 E3686 E3687 E3688 E3689 V3690 E3691 E3692 K3693 L3698 V3702 S3706 R3707 T3708 A3709 L3710 T3711 E3712 K3713 S3714 K3715 L3716 D3717 E3718 D3719 Y3720 M3723 A3724 Y3725 A3726 D3727 I3728 M3729 A3730 K3731 S3732 C3733 H3734 L3735 E3736 E3737 G3738
G3739 E3740 N3741 GLY GLU ALA GLU GLU E3747 E3748 V3749 E3750 V3751 S3752 F3753 E3754 E3755 K3756 E3759 K3760 Q3761 R3762 L3763 L3764 Y3765 Q3766 Q3767 S3768 R3769 L3770 H3771 T3772 R3773 G3774 A3775 A3776 L3780 Q3781 M3782 I3783 S3784 A3785 C3786 K3787 G3788 E3789 T3790 G3791 A3792 M3793 V3794 S3795 L3798 K3799 I3802 S3803
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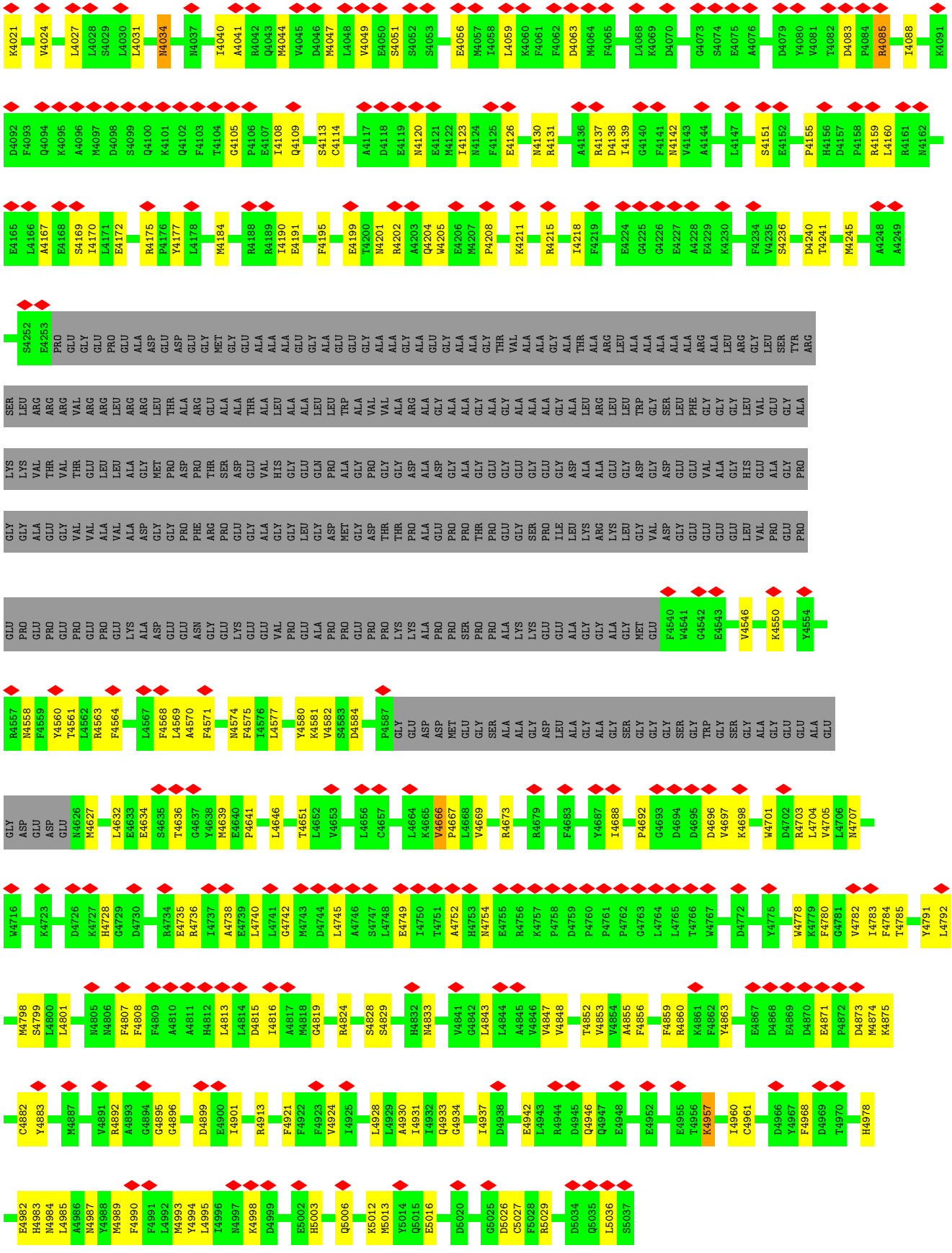
V3874 M3875 D3878 E3879 F3880 T3881 Q3882 D3883 L3884 F3885 L3888 Q3889 E3893 N3896 N3897 D3898 F3899 L3903 R3904 T3905 Q3906 T3907 T3910 T3911 T3912 I3913 N3914 I3915 I3916 I3917 V3920 D3921 L3924 R3925 L3926 Q3927 E3928 S3931 D3932 W3935 Y3936 Y3937 S3938 G3939 K3940 D3941 K3948 F3961
A3954 M3955 S3956 V3957 A3958 K3959 Q3960 V3961 F3962 N3963 S3964 L3965 T3966 E3967 Y3968 I3969 Q3970 G3971 P3972 C3973 T3974 Q3977 Q3978 A3981 H3982 S3983 R3984 D3987 V3990 G3991 F3992 L3993 H3994 Y3995 F3996 A3997 H3998 M4001 K4002 L4003 A4004 Q4005 I4010 E4011 L4012 L4013 K4014 E4015 L4016 L4017 D4018 L4019 Q4020



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	791956	Depositor
Resolution determination method	OTHER	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	0.486	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.16	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, CA

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	0.33	0/834	0.59	0/1123
1	F	0.33	0/834	0.59	0/1123
1	H	0.33	0/834	0.59	0/1123
1	J	0.33	0/834	0.59	0/1123
2	B	0.34	0/25428	0.58	6/34534 (0.0%)
2	E	0.34	0/25428	0.58	6/34534 (0.0%)
2	G	0.34	0/25428	0.58	6/34534 (0.0%)
2	I	0.34	0/25428	0.58	6/34534 (0.0%)
All	All	0.34	0/105048	0.58	24/142628 (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	23
2	E	0	23
2	G	0	23
2	I	0	23
All	All	0	92

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1667	LEU	CA-CB-CG	6.02	129.15	115.30
2	G	1667	LEU	CA-CB-CG	6.02	129.14	115.30
2	B	1667	LEU	CA-CB-CG	5.99	129.08	115.30
2	B	719	LEU	CA-CB-CG	5.98	129.06	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	719	LEU	CA-CB-CG	5.98	129.06	115.30
2	I	1667	LEU	CA-CB-CG	5.98	129.05	115.30
2	I	719	LEU	CA-CB-CG	5.97	129.03	115.30
2	G	719	LEU	CA-CB-CG	5.96	129.01	115.30
2	I	4985	LEU	CA-CB-CG	5.66	128.31	115.30
2	E	4985	LEU	CA-CB-CG	5.66	128.31	115.30
2	G	4985	LEU	CA-CB-CG	5.64	128.28	115.30
2	B	4985	LEU	CA-CB-CG	5.63	128.25	115.30
2	G	977	LEU	CA-CB-CG	5.61	128.19	115.30
2	B	977	LEU	CA-CB-CG	5.60	128.18	115.30
2	E	977	LEU	CA-CB-CG	5.59	128.16	115.30
2	I	977	LEU	CA-CB-CG	5.59	128.15	115.30
2	E	4639	MET	C-N-CA	5.25	134.82	121.70
2	I	4639	MET	C-N-CA	5.25	134.81	121.70
2	B	4639	MET	C-N-CA	5.23	134.77	121.70
2	G	4639	MET	C-N-CA	5.22	134.75	121.70
2	G	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	I	2290	LEU	CA-CB-CG	5.16	127.16	115.30
2	E	2290	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (92) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	LEU	Peptide
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	194	SER	Peptide
2	B	2188	ASN	Peptide
2	B	2291	GLN	Peptide
2	B	2292	GLU	Peptide
2	B	2342	ASN	Peptide
2	B	2343	GLY	Peptide
2	B	240	ASP	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	3786	CYS	Peptide
2	B	3971	GLY	Peptide

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Mol	Chain	Res	Type	Group
2	B	4666	VAL	Peptide
2	B	4696	ASP	Peptide
2	B	4807	PHE	Peptide
2	B	4873	ASP	Peptide
2	B	4901	ILE	Peptide
2	B	808	TYR	Peptide
2	E	137	LEU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	194	SER	Peptide
2	E	2188	ASN	Peptide
2	E	2291	GLN	Peptide
2	E	2292	GLU	Peptide
2	E	2342	ASN	Peptide
2	E	2343	GLY	Peptide
2	E	240	ASP	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	3786	CYS	Peptide
2	E	3971	GLY	Peptide
2	E	4666	VAL	Peptide
2	E	4696	ASP	Peptide
2	E	4807	PHE	Peptide
2	E	4873	ASP	Peptide
2	E	4901	ILE	Peptide
2	E	808	TYR	Peptide
2	G	137	LEU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	194	SER	Peptide
2	G	2188	ASN	Peptide
2	G	2291	GLN	Peptide
2	G	2292	GLU	Peptide
2	G	2342	ASN	Peptide
2	G	2343	GLY	Peptide
2	G	240	ASP	Peptide

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Mol	Chain	Res	Type	Group
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	3786	CYS	Peptide
2	G	3971	GLY	Peptide
2	G	4666	VAL	Peptide
2	G	4696	ASP	Peptide
2	G	4807	PHE	Peptide
2	G	4873	ASP	Peptide
2	G	4901	ILE	Peptide
2	G	808	TYR	Peptide
2	I	137	LEU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	194	SER	Peptide
2	I	2188	ASN	Peptide
2	I	2291	GLN	Peptide
2	I	2292	GLU	Peptide
2	I	2342	ASN	Peptide
2	I	2343	GLY	Peptide
2	I	240	ASP	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	3786	CYS	Peptide
2	I	3971	GLY	Peptide
2	I	4666	VAL	Peptide
2	I	4696	ASP	Peptide
2	I	4807	PHE	Peptide
2	I	4873	ASP	Peptide
2	I	4901	ILE	Peptide
2	I	808	TYR	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	18	0
1	F	818	0	824	20	0
1	H	818	0	824	18	0
1	J	818	0	824	20	0
2	B	29369	0	24713	491	0
2	E	29369	0	24712	503	0
2	G	29369	0	24716	502	0
2	I	29369	0	24713	489	0
3	B	1	0	0	0	0
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	102150	2033	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 9.

All (2033) 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:4859:PHE:HA	2:G:4862:PHE:CD2	1.88	1.08
2:G:4859:PHE:HA	2:G:4862:PHE:HD2	1.28	0.97
2:E:4859:PHE:HA	2:E:4862:PHE:CD2	2.05	0.92
2:E:4859:PHE:HA	2:E:4862:PHE:HD2	1.43	0.83
2:G:4859:PHE:CA	2:G:4862:PHE:HD2	1.99	0.73
2:E:4855:ALA:HA	2:E:4859:PHE:HB2	1.71	0.72
2:I:853:PRO:HB3	2:I:1024:TYR:H	1.56	0.71
2:B:853:PRO:HB3	2:B:1024:TYR:H	1.56	0.71
2:B:2318:TYR:HH	2:B:2414:ASN:N	1.90	0.70
2:I:2318:TYR:HH	2:I:2414:ASN:N	1.90	0.70
2:E:853:PRO:HB3	2:E:1024:TYR:H	1.56	0.69
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.58	0.69
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.58	0.69
2:G:2318:TYR:HH	2:G:2414:ASN:N	1.91	0.69
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.58	0.69
2:G:853:PRO:HB3	2:G:1024:TYR:H	1.56	0.69
2:E:2318:TYR:HH	2:E:2414:ASN:N	1.91	0.69
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.58	0.68
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.26	0.68
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.26	0.68
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.26	0.68
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.26	0.68
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.76	0.68
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.76	0.68
2:G:379:HIS:HD2	2:G:382:GLY:H	1.40	0.68
2:E:379:HIS:HD2	2:E:382:GLY:H	1.40	0.67
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.76	0.67
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.76	0.67
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.76	0.67
2:B:379:HIS:HD2	2:B:382:GLY:H	1.40	0.66
2:I:379:HIS:HD2	2:I:382:GLY:H	1.40	0.66
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.76	0.66
2:B:132:ALA:HA	2:B:194:SER:HB2	1.77	0.66
2:I:2764:GLU:HG3	2:I:2857:PRO:HB2	1.77	0.66
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.78	0.66
2:I:132:ALA:HA	2:I:194:SER:HB2	1.77	0.66
2:E:132:ALA:HA	2:E:194:SER:HB2	1.77	0.66
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.61	0.66
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.78	0.66
2:B:2764:GLU:HG3	2:B:2857:PRO:HB2	1.78	0.65
2:E:4934:GLY:HA3	2:G:4937:ILE:HD12	1.78	0.65
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.30	0.65
2:G:2764:GLU:HG3	2:G:2857:PRO:HB2	1.78	0.65
2:G:4177:TYR:HA	2:G:4202:ARG:HH22	1.61	0.65
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.61	0.65
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.76	0.65
2:G:132:ALA:HA	2:G:194:SER:HB2	1.77	0.65
2:I:4177:TYR:HA	2:I:4202:ARG:HH22	1.61	0.65
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.78	0.65
2:I:1092:PHE:HB3	2:I:1149:VAL:HB	1.79	0.65
2:B:3990:VAL:HG13	2:B:4051:SER:HB2	1.78	0.65
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.78	0.65
2:B:3903:LEU:HG	2:B:3915:ILE:HD12	1.79	0.65
2:E:4177:TYR:HA	2:E:4202:ARG:HH22	1.61	0.65
2:B:1092:PHE:HB3	2:B:1149:VAL:HB	1.79	0.64
2:B:1247:PRO:HA	2:B:1598:GLN:HA	1.79	0.64
2:B:4177:TYR:HA	2:B:4202:ARG:HH22	1.61	0.64
2:E:1667:LEU:HD23	2:E:1671:ARG:HH12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2764:GLU:HG3	2:E:2857:PRO:HB2	1.77	0.64
2:G:1667:LEU:HD23	2:G:1671:ARG:HH12	1.61	0.64
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.61	0.64
2:G:3990:VAL:HG13	2:G:4051:SER:HB2	1.78	0.64
2:E:3903:LEU:HG	2:E:3915:ILE:HD12	1.79	0.64
2:G:3903:LEU:HG	2:G:3915:ILE:HD12	1.79	0.64
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.30	0.64
2:I:1667:LEU:HD23	2:I:1671:ARG:HH12	1.61	0.64
2:G:1232:ARG:HH21	2:G:1701:ALA:HB1	1.63	0.64
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.80	0.64
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.30	0.64
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.30	0.64
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.80	0.64
2:I:3903:LEU:HG	2:I:3915:ILE:HD12	1.79	0.64
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.61	0.64
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.80	0.64
2:B:1667:LEU:HD23	2:B:1671:ARG:HH12	1.61	0.64
2:G:1092:PHE:HB3	2:G:1149:VAL:HB	1.79	0.64
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.80	0.63
2:G:606:LEU:O	2:G:617:ASN:ND2	2.31	0.63
2:E:1232:ARG:HH21	2:E:1701:ALA:HB1	1.63	0.63
2:E:3990:VAL:HG13	2:E:4051:SER:HB2	1.79	0.63
2:B:606:LEU:O	2:B:617:ASN:ND2	2.31	0.63
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.81	0.63
2:I:1232:ARG:HH21	2:I:1701:ALA:HB1	1.63	0.63
2:E:606:LEU:O	2:E:617:ASN:ND2	2.31	0.63
2:E:1092:PHE:HB3	2:E:1149:VAL:HB	1.79	0.63
2:B:111:HIS:HD2	2:B:114:SER:H	1.47	0.63
2:G:1247:PRO:HA	2:G:1598:GLN:HA	1.79	0.63
2:I:3990:VAL:HG13	2:I:4051:SER:HB2	1.78	0.63
2:E:1247:PRO:HA	2:E:1598:GLN:HA	1.79	0.63
2:I:111:HIS:HD2	2:I:114:SER:H	1.47	0.63
2:I:606:LEU:O	2:I:617:ASN:ND2	2.31	0.63
2:I:1247:PRO:HA	2:I:1598:GLN:HA	1.79	0.63
2:B:1232:ARG:HH21	2:B:1701:ALA:HB1	1.63	0.63
2:G:111:HIS:HD2	2:G:114:SER:H	1.47	0.63
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.81	0.63
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.32	0.62
2:G:1700:ASP:OD2	2:G:1708:ARG:NH2	2.32	0.62
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.81	0.62
2:B:3767:GLN:HB3	2:B:3772:THR:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:261:ARG:HB3	2:E:283:ARG:HB3	1.82	0.62
2:G:1101:ARG:HE	2:G:1115:LEU:HB3	1.64	0.62
2:I:1700:ASP:OD2	2:I:1708:ARG:NH2	2.33	0.62
2:I:3767:GLN:HB3	2:I:3772:THR:HG22	1.82	0.62
2:B:1700:ASP:OD2	2:B:1708:ARG:NH2	2.33	0.61
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.82	0.61
2:E:1973:GLN:O	2:E:1977:TYR:N	2.33	0.61
2:E:1101:ARG:HE	2:E:1115:LEU:HB3	1.64	0.61
2:G:261:ARG:HB3	2:G:283:ARG:HB3	1.82	0.61
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.81	0.61
2:E:1700:ASP:OD2	2:E:1708:ARG:NH2	2.32	0.61
2:E:4581:LYS:HB2	2:E:4632:LEU:HB2	1.82	0.61
2:B:1973:GLN:O	2:B:1977:TYR:N	2.33	0.61
2:E:111:HIS:HD2	2:E:114:SER:H	1.47	0.61
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.32	0.61
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.32	0.61
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.32	0.61
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.33	0.61
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.33	0.61
2:G:18:ASP:HB2	2:G:69:LEU:HD12	1.83	0.61
2:G:4581:LYS:HB2	2:G:4632:LEU:HB2	1.82	0.61
2:B:1101:ARG:HE	2:B:1115:LEU:HB3	1.64	0.60
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.60
2:B:261:ARG:HB3	2:B:283:ARG:HB3	1.82	0.60
2:B:1211:LEU:HD11	2:B:1225:PRO:HB3	1.84	0.60
2:E:18:ASP:HB2	2:E:69:LEU:HD12	1.83	0.60
2:G:3882:GLN:HB2	2:G:3957:VAL:HG22	1.82	0.60
2:I:261:ARG:HB3	2:I:283:ARG:HB3	1.82	0.60
2:B:20:VAL:HG12	2:B:204:PRO:HA	1.82	0.60
2:B:4581:LYS:HB2	2:B:4632:LEU:HB2	1.82	0.60
2:G:235:ALA:HA	2:G:257:ARG:HD3	1.83	0.60
2:G:4704:LEU:HD22	2:G:4778:TRP:HB2	1.83	0.60
2:B:4829:SER:O	2:B:4833:ASN:ND2	2.35	0.60
2:E:20:VAL:HG12	2:E:204:PRO:HA	1.82	0.60
2:E:3767:GLN:HB3	2:E:3772:THR:HG22	1.82	0.60
2:G:4961:CYS:SG	2:G:4978:HIS:NE2	2.75	0.60
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.33	0.60
2:I:1101:ARG:HE	2:I:1115:LEU:HB3	1.64	0.60
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.83	0.60
2:I:235:ALA:HA	2:I:257:ARG:HD3	1.84	0.60
2:G:3767:GLN:HB3	2:G:3772:THR:HG22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1973:GLN:O	2:I:1977:TYR:N	2.33	0.60
2:I:4581:LYS:HB2	2:I:4632:LEU:HB2	1.82	0.60
2:I:4961:CYS:SG	2:I:4978:HIS:NE2	2.75	0.60
2:E:742:ASP:HA	2:E:760:ASN:HD21	1.67	0.60
2:E:1649:ASP:HB3	2:E:1652:GLU:HG2	1.84	0.60
2:E:4961:CYS:SG	2:E:4978:HIS:NE2	2.75	0.60
2:B:1649:ASP:HB3	2:B:1652:GLU:HG2	1.84	0.60
2:G:4829:SER:O	2:G:4833:ASN:ND2	2.35	0.60
2:I:742:ASP:HA	2:I:760:ASN:HD21	1.67	0.60
2:E:1211:LEU:HD11	2:E:1225:PRO:HB3	1.84	0.60
2:I:1211:LEU:HD11	2:I:1225:PRO:HB3	1.84	0.60
2:E:4829:SER:O	2:E:4833:ASN:ND2	2.35	0.60
2:I:20:VAL:HG12	2:I:204:PRO:HA	1.82	0.60
2:B:3882:GLN:HB2	2:B:3957:VAL:HG22	1.82	0.59
2:B:4704:LEU:HD22	2:B:4778:TRP:HB2	1.83	0.59
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.83	0.59
2:I:18:ASP:HB2	2:I:69:LEU:HD12	1.83	0.59
2:B:235:ALA:HA	2:B:257:ARG:HD3	1.84	0.59
2:B:742:ASP:HA	2:B:760:ASN:HD21	1.67	0.59
2:E:4704:LEU:HD22	2:E:4778:TRP:HB2	1.83	0.59
2:I:4829:SER:O	2:I:4833:ASN:ND2	2.35	0.59
2:E:3882:GLN:HB2	2:E:3957:VAL:HG22	1.83	0.59
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.83	0.59
2:E:1271:ARG:HA	2:E:1471:UNK:HA	1.85	0.59
2:G:1649:ASP:HB3	2:G:1652:GLU:HG2	1.84	0.59
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.36	0.59
2:I:3882:GLN:HB2	2:I:3957:VAL:HG22	1.82	0.59
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.36	0.59
2:G:20:VAL:HG12	2:G:204:PRO:HA	1.82	0.59
2:G:1211:LEU:HD11	2:G:1225:PRO:HB3	1.83	0.59
2:I:1777:PHE:HA	2:I:1799:SER:HB2	1.85	0.59
2:B:18:ASP:HB2	2:B:69:LEU:HD12	1.83	0.59
2:G:742:ASP:HA	2:G:760:ASN:HD21	1.67	0.59
2:G:1777:PHE:HA	2:G:1799:SER:HB2	1.85	0.59
2:G:2205:GLU:HG2	2:G:2253:HIS:HE1	1.67	0.59
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.36	0.59
2:G:1218:GLY:HA2	2:G:1223:PHE:HB2	1.85	0.59
2:E:4895:GLY:O	2:G:4892:ARG:NH2	2.34	0.59
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.83	0.59
2:I:4704:LEU:HD22	2:I:4778:TRP:HB2	1.83	0.59
2:B:1218:GLY:HA2	2:B:1223:PHE:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:235:ALA:HA	2:E:257:ARG:HD3	1.83	0.59
2:G:1808:ARG:NH1	2:G:1853:ILE:O	2.36	0.59
2:G:1973:GLN:O	2:G:1977:TYR:N	2.33	0.59
2:B:1777:PHE:HA	2:B:1799:SER:HB2	1.85	0.59
2:I:1218:GLY:HA2	2:I:1223:PHE:HB2	1.85	0.59
2:E:2205:GLU:HG2	2:E:2253:HIS:HE1	1.67	0.58
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.85	0.58
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.85	0.58
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.85	0.58
2:I:1649:ASP:HB3	2:I:1652:GLU:HG2	1.83	0.58
2:B:2205:GLU:HG2	2:B:2253:HIS:HE1	1.67	0.58
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.85	0.58
2:E:1777:PHE:HA	2:E:1799:SER:HB2	1.85	0.58
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.85	0.58
2:I:1808:ARG:NH1	2:I:1853:ILE:O	2.36	0.58
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.33	0.58
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.85	0.58
2:I:2205:GLU:HG2	2:I:2253:HIS:HE1	1.67	0.58
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.86	0.58
2:B:4241:THR:HB	2:B:4989:MET:HE1	1.85	0.58
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.85	0.58
1:A:6:THR:HA	1:A:72:ALA:HA	1.85	0.58
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.76	0.58
2:B:3846:ALA:HB1	2:B:3873:LYS:HG2	1.86	0.58
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.36	0.58
2:E:1808:ARG:NH1	2:E:1853:ILE:O	2.36	0.58
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.85	0.58
2:I:627:PRO:HB2	1:J:92:PRO:HD3	1.85	0.58
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.85	0.58
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.85	0.58
1:F:6:THR:HA	1:F:72:ALA:HA	1.85	0.58
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.58
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.85	0.58
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.86	0.58
2:E:3846:ALA:HB1	2:E:3873:LYS:HG2	1.86	0.58
2:E:242:ARG:NH1	2:E:481:GLU:OE1	2.37	0.58
2:G:242:ARG:NH1	2:G:481:GLU:OE1	2.37	0.58
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.86	0.58
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.85	0.58
1:J:27:THR:HB	1:J:100:ASP:HB3	1.86	0.58
2:B:1808:ARG:NH1	2:B:1853:ILE:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.85	0.57
2:E:1218:GLY:HA2	2:E:1223:PHE:HB2	1.85	0.57
1:A:27:THR:HB	1:A:100:ASP:HB3	1.86	0.57
2:B:242:ARG:NH1	2:B:481:GLU:OE1	2.37	0.57
2:E:2440:MET:O	2:E:2444:GLN:N	2.36	0.57
1:H:27:THR:HB	1:H:100:ASP:HB3	1.86	0.57
2:I:242:ARG:NH1	2:I:481:GLU:OE1	2.37	0.57
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.85	0.57
2:B:546:TRP:O	2:B:550:LYS:NZ	2.31	0.57
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.85	0.57
2:B:3780:LEU:HD11	2:B:3816:MET:HG3	1.86	0.57
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.85	0.57
2:E:3780:LEU:HD11	2:E:3816:MET:HG3	1.87	0.57
2:G:1830:VAL:HB	2:G:1837:GLN:HA	1.87	0.57
2:G:3780:LEU:HD11	2:G:3816:MET:HG3	1.87	0.57
1:F:27:THR:HB	1:F:100:ASP:HB3	1.86	0.57
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.86	0.57
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.85	0.57
2:I:210:GLU:HG3	2:I:337:PRO:HG3	1.86	0.57
2:I:2440:MET:O	2:I:2444:GLN:N	2.36	0.57
2:I:3780:LEU:HD11	2:I:3816:MET:HG3	1.86	0.57
1:J:6:THR:HA	1:J:72:ALA:HA	1.85	0.57
2:B:1271:ARG:HA	2:B:1471:UNK:HA	1.86	0.57
2:B:4937:ILE:HD12	2:I:4934:GLY:HA3	1.86	0.57
2:G:210:GLU:HG3	2:G:337:PRO:HG3	1.86	0.57
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.37	0.57
2:I:1271:ARG:HA	2:I:1471:UNK:HA	1.86	0.57
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.86	0.57
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.76	0.57
2:I:3846:ALA:HB1	2:I:3873:LYS:HG2	1.86	0.57
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.86	0.57
2:I:2287:ALA:HA	2:I:2290:LEU:HD13	1.87	0.57
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.85	0.57
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.38	0.57
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.85	0.57
2:G:645:ARG:N	2:G:824:GLU:O	2.38	0.57
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.86	0.57
2:I:1830:VAL:HB	2:I:1837:GLN:HA	1.87	0.57
2:B:210:GLU:HG3	2:B:337:PRO:HG3	1.86	0.57
2:B:4177:TYR:HE1	2:B:4199:GLU:HB2	1.70	0.57
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3846:ALA:HB1	2:G:3873:LYS:HG2	1.86	0.57
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.38	0.57
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.87	0.57
2:B:4151:SER:HA	2:B:4160:LEU:HD21	1.87	0.57
2:E:1830:VAL:HB	2:E:1837:GLN:HA	1.87	0.57
2:E:3843:ASP:H	2:E:3874:VAL:HG13	1.70	0.57
2:E:4201:ASN:O	2:E:4205:TRP:N	2.38	0.57
2:G:683:ARG:NH1	2:G:707:VAL:O	2.37	0.57
2:B:645:ARG:N	2:B:824:GLU:O	2.38	0.56
2:E:4859:PHE:CA	2:E:4862:PHE:HD2	2.18	0.56
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.38	0.56
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.76	0.56
2:B:4126:GLU:O	2:B:4130:ASN:ND2	2.38	0.56
2:E:210:GLU:HG3	2:E:337:PRO:HG3	1.86	0.56
2:G:4151:SER:HA	2:G:4160:LEU:HD21	1.87	0.56
2:G:4177:TYR:HE1	2:G:4199:GLU:HB2	1.70	0.56
2:G:4815:ASP:O	2:G:4819:GLY:N	2.37	0.56
2:I:609:CYS:SG	2:I:610:ASN:N	2.78	0.56
2:I:4151:SER:HA	2:I:4160:LEU:HD21	1.87	0.56
2:E:315:CYS:SG	2:E:316:PHE:N	2.79	0.56
2:E:683:ARG:NH1	2:E:707:VAL:O	2.37	0.56
2:G:451:TYR:O	2:G:474:ARG:NH1	2.38	0.56
2:G:2281:ILE:HG23	2:G:2341:VAL:HG11	1.88	0.56
2:I:645:ARG:N	2:I:824:GLU:O	2.38	0.56
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.85	0.56
2:E:609:CYS:SG	2:E:610:ASN:N	2.78	0.56
2:G:4126:GLU:O	2:G:4130:ASN:ND2	2.38	0.56
1:H:6:THR:HA	1:H:72:ALA:HA	1.85	0.56
2:I:4126:GLU:O	2:I:4130:ASN:ND2	2.38	0.56
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.87	0.56
2:B:1830:VAL:HB	2:B:1837:GLN:HA	1.86	0.56
2:E:4012:LEU:O	2:E:4016:LEU:N	2.39	0.56
2:E:4151:SER:HA	2:E:4160:LEU:HD21	1.87	0.56
2:E:4177:TYR:HE1	2:E:4199:GLU:HB2	1.70	0.56
2:I:683:ARG:NH1	2:I:707:VAL:O	2.37	0.56
2:E:4126:GLU:O	2:E:4130:ASN:ND2	2.38	0.56
2:G:609:CYS:SG	2:G:610:ASN:N	2.78	0.56
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.87	0.56
2:G:315:CYS:SG	2:G:316:PHE:N	2.79	0.56
2:G:682:LEU:HD13	2:G:787:VAL:HG11	1.88	0.56
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:CYS:SG	2:B:316:PHE:N	2.79	0.56
2:E:2287:ALA:HA	2:E:2290:LEU:HD13	1.87	0.56
2:I:4201:ASN:O	2:I:4205:TRP:N	2.38	0.56
2:B:609:CYS:SG	2:B:610:ASN:N	2.78	0.56
2:B:2287:ALA:HA	2:B:2290:LEU:HD13	1.87	0.56
2:E:451:TYR:O	2:E:474:ARG:NH1	2.38	0.56
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.38	0.56
2:G:2287:ALA:HA	2:G:2290:LEU:HD13	1.87	0.56
2:G:3765:TYR:O	2:G:3769:ARG:N	2.36	0.56
2:I:682:LEU:HD13	2:I:787:VAL:HG11	1.88	0.56
2:E:4241:THR:HB	2:E:4989:MET:HE1	1.86	0.55
2:G:17:ASP:HB2	2:G:98:HIS:HE1	1.71	0.55
2:G:4241:THR:HB	2:G:4989:MET:HE1	1.86	0.55
2:I:2281:ILE:HG23	2:I:2341:VAL:HG11	1.88	0.55
2:B:451:TYR:O	2:B:474:ARG:NH1	2.39	0.55
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.76	0.55
2:I:551:LEU:HD11	2:I:589:LEU:HD13	1.87	0.55
2:B:17:ASP:HB2	2:B:98:HIS:HE1	1.71	0.55
2:B:682:LEU:HD13	2:B:787:VAL:HG11	1.88	0.55
2:B:3843:ASP:H	2:B:3874:VAL:HG13	1.71	0.55
2:I:635:THR:O	1:J:34:LYS:NZ	2.34	0.55
2:E:2281:ILE:HG23	2:E:2341:VAL:HG11	1.88	0.55
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.40	0.55
2:I:315:CYS:SG	2:I:316:PHE:N	2.79	0.55
2:I:4815:ASP:O	2:I:4819:GLY:N	2.37	0.55
2:B:4563:ARG:NH1	2:B:4815:ASP:OD2	2.36	0.55
2:E:682:LEU:HD13	2:E:787:VAL:HG11	1.88	0.55
2:E:4924:VAL:O	2:E:4928:LEU:N	2.35	0.55
2:G:157:ARG:NH2	2:G:167:ASP:OD1	2.38	0.55
2:G:3843:ASP:H	2:G:3874:VAL:HG13	1.70	0.55
2:G:4114:CYS:O	2:G:4131:ARG:NH2	2.40	0.55
2:G:4184:MET:HB3	2:G:4190:ILE:HD13	1.89	0.55
2:B:551:LEU:HD11	2:B:589:LEU:HD13	1.87	0.55
2:B:1090:PHE:HD2	2:B:1202:LEU:HD11	1.72	0.55
2:B:2440:MET:O	2:B:2444:GLN:N	2.36	0.55
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.40	0.55
2:I:718:GLY:HA3	2:I:737:LEU:HA	1.88	0.55
2:B:718:GLY:HA3	2:B:737:LEU:HA	1.88	0.55
2:B:4697:VAL:O	2:B:4701:TRP:N	2.39	0.55
2:I:451:TYR:O	2:I:474:ARG:NH1	2.38	0.55
2:B:1667:LEU:O	2:B:1671:ARG:NH1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:LEU:HD11	2:E:589:LEU:HD13	1.88	0.55
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.80	0.55
2:G:4201:ASN:O	2:G:4205:TRP:N	2.38	0.55
2:I:2189:LYS:HA	2:I:2192:TYR:HD2	1.72	0.55
2:I:4114:CYS:O	2:I:4131:ARG:NH2	2.40	0.55
2:I:4563:ARG:NH1	2:I:4815:ASP:OD2	2.36	0.55
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.40	0.55
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.40	0.55
2:B:4815:ASP:O	2:B:4819:GLY:N	2.37	0.55
2:E:331:VAL:HG11	2:E:336:PRO:HD2	1.89	0.55
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.40	0.55
2:G:551:LEU:HD11	2:G:589:LEU:HD13	1.88	0.55
2:G:1667:LEU:O	2:G:1671:ARG:NH1	2.40	0.55
2:I:1090:PHE:HD2	2:I:1202:LEU:HD11	1.72	0.55
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.40	0.55
2:I:4177:TYR:HE1	2:I:4199:GLU:HB2	1.70	0.55
2:B:1679:ASN:HA	2:B:1682:ALA:HB3	1.89	0.55
2:B:2281:ILE:HG23	2:B:2341:VAL:HG11	1.88	0.55
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.55
2:B:4114:CYS:O	2:B:4131:ARG:NH2	2.40	0.55
2:E:4114:CYS:O	2:E:4131:ARG:NH2	2.40	0.55
2:I:17:ASP:HB2	2:I:98:HIS:HE1	1.71	0.55
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.89	0.55
2:I:1258:ALA:HB3	2:I:1271:ARG:HB3	1.89	0.55
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.89	0.54
2:B:2189:LYS:HA	2:B:2192:TYR:HD2	1.72	0.54
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.40	0.54
2:G:331:VAL:HG11	2:G:336:PRO:HD2	1.89	0.54
2:G:635:THR:O	1:H:34:LYS:NZ	2.40	0.54
2:G:1258:ALA:HB3	2:G:1271:ARG:HB3	1.89	0.54
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.80	0.54
2:I:488:LEU:O	2:I:492:ASP:N	2.39	0.54
2:B:683:ARG:NH1	2:B:707:VAL:O	2.37	0.54
2:E:1667:LEU:O	2:E:1671:ARG:NH1	2.40	0.54
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.40	0.54
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.38	0.54
2:I:4184:MET:HB3	2:I:4190:ILE:HD13	1.89	0.54
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.80	0.54
2:E:718:GLY:HA3	2:E:737:LEU:HA	1.88	0.54
2:E:1090:PHE:HD2	2:E:1202:LEU:HD11	1.72	0.54
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.40	0.54
2:I:1679:ASN:HA	2:I:1682:ALA:HB3	1.89	0.54
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.40	0.54
2:E:4184:MET:HB3	2:E:4190:ILE:HD13	1.89	0.54
2:G:718:GLY:HA3	2:G:737:LEU:HA	1.88	0.54
2:I:331:VAL:HG11	2:I:336:PRO:HD2	1.89	0.54
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.40	0.54
2:B:3992:PHE:O	2:B:3996:PHE:N	2.38	0.54
2:E:645:ARG:N	2:E:824:GLU:O	2.38	0.54
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.40	0.54
2:E:2189:LYS:HA	2:E:2192:TYR:HD2	1.72	0.54
2:E:4697:VAL:O	2:E:4701:TRP:N	2.39	0.54
2:G:3830:GLN:HA	2:G:3833:GLN:HG2	1.89	0.54
2:B:1258:ALA:HB3	2:B:1271:ARG:HB3	1.89	0.54
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.40	0.54
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.40	0.54
2:G:731:THR:OG1	2:G:1519:UNK:O	2.25	0.54
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.37	0.54
2:G:2189:LYS:HA	2:G:2192:TYR:HD2	1.72	0.54
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.40	0.54
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.80	0.54
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.89	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:I:1667:LEU:O	2:I:1671:ARG:NH1	2.40	0.54
2:I:3843:ASP:H	2:I:3874:VAL:HG13	1.71	0.54
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.40	0.54
2:B:3830:GLN:HA	2:B:3833:GLN:HG2	1.89	0.54
2:E:1258:ALA:HB3	2:E:1271:ARG:HB3	1.89	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:E:4815:ASP:O	2:E:4819:GLY:N	2.37	0.54
2:I:4012:LEU:O	2:I:4016:LEU:N	2.39	0.54
2:B:647:ASN:ND2	2:B:820:ARG:O	2.41	0.54
2:B:731:THR:OG1	2:B:1519:UNK:O	2.27	0.54
2:B:4012:LEU:O	2:B:4016:LEU:N	2.39	0.54
2:E:3830:GLN:HA	2:E:3833:GLN:HG2	1.89	0.54
2:I:157:ARG:NH2	2:I:167:ASP:OD1	2.38	0.54
2:I:1713:ASP:O	2:I:1717:SER:N	2.41	0.54
2:I:4848:VAL:HG23	2:I:4883:TYR:HE1	1.73	0.54
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.90	0.54
2:E:17:ASP:HB2	2:E:98:HIS:HE1	1.71	0.53
2:G:1090:PHE:HD2	2:G:1202:LEU:HD11	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1271:ARG:HA	2:G:1471:UNK:HA	1.89	0.53
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	1.90	0.53
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.41	0.53
2:G:4012:LEU:O	2:G:4016:LEU:N	2.39	0.53
2:B:157:ARG:NH2	2:B:167:ASP:OD1	2.38	0.53
2:B:331:VAL:HG11	2:B:336:PRO:HD2	1.89	0.53
2:B:3932:ASP:HA	2:B:3935:TRP:HD1	1.73	0.53
2:B:4184:MET:HB3	2:B:4190:ILE:HD13	1.89	0.53
2:E:4848:VAL:HG23	2:E:4883:TYR:HE1	1.73	0.53
2:G:2336:ARG:HD3	2:G:2435:ARG:HD2	1.89	0.53
2:G:4848:VAL:HG23	2:G:4883:TYR:HE1	1.73	0.53
2:I:4024:VAL:HG23	2:I:4027:LEU:HD12	1.90	0.53
2:B:111:HIS:N	2:B:116:MET:O	2.36	0.53
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	1.91	0.53
2:E:4824:ARG:O	2:E:4828:SER:N	2.38	0.53
2:I:281:ARG:NH2	2:I:309:THR:OG1	2.41	0.53
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.53
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.40	0.53
2:B:891:TRP:HA	2:B:902:ARG:HB3	1.90	0.53
2:E:3992:PHE:O	2:E:3996:PHE:N	2.38	0.53
2:G:281:ARG:NH2	2:G:309:THR:OG1	2.41	0.53
2:G:2440:MET:O	2:G:2444:GLN:N	2.36	0.53
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	1.91	0.53
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.42	0.53
2:B:1721:GLU:HG2	2:B:1725:ARG:HH12	1.73	0.53
2:B:4924:VAL:O	2:B:4928:LEU:N	2.35	0.53
2:E:1231:GLN:NE2	2:E:1821:ASP:O	2.42	0.53
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.38	0.53
2:I:3932:ASP:HA	2:I:3935:TRP:HD1	1.73	0.53
2:I:4088:ILE:HG23	2:I:4123:ILE:HB	1.90	0.53
2:B:2336:ARG:HD3	2:B:2435:ARG:HD2	1.89	0.53
2:E:256:ALA:HB1	2:E:286:THR:HG21	1.91	0.53
2:E:1679:ASN:HA	2:E:1682:ALA:HB3	1.89	0.53
1:F:62:GLY:HA3	1:F:74:LEU:HD21	1.90	0.53
2:G:4088:ILE:HG23	2:G:4123:ILE:HB	1.90	0.53
2:I:1231:GLN:NE2	2:I:1821:ASP:O	2.42	0.53
2:I:3830:GLN:HA	2:I:3833:GLN:HG2	1.89	0.53
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.90	0.53
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	1.90	0.53
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.42	0.53
2:G:3781:GLN:HA	2:G:3784:SER:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.42	0.53
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.42	0.53
2:E:731:THR:OG1	2:E:1519:UNK:O	2.27	0.53
2:E:891:TRP:HA	2:E:902:ARG:HB3	1.90	0.53
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.39	0.53
2:E:2336:ARG:HD3	2:E:2435:ARG:HD2	1.89	0.53
2:G:1679:ASN:HA	2:G:1682:ALA:HB3	1.89	0.53
2:G:2257:LEU:HD11	2:G:2276:ALA:HB2	1.91	0.53
2:I:647:ASN:ND2	2:I:820:ARG:O	2.41	0.53
2:I:2336:ARG:HD3	2:I:2435:ARG:HD2	1.89	0.53
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.38	0.53
2:B:4978:HIS:HA	2:B:4982:GLU:HB2	1.90	0.53
2:E:488:LEU:O	2:E:492:ASP:N	2.39	0.53
2:E:4978:HIS:HA	2:E:4982:GLU:HB2	1.90	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.42	0.53
2:E:157:ARG:NH2	2:E:167:ASP:OD1	2.38	0.53
2:E:1721:GLU:HG2	2:E:1725:ARG:HH12	1.73	0.53
2:G:15:ARG:HD3	2:G:98:HIS:HB3	1.91	0.53
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.40	0.53
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.42	0.53
2:G:891:TRP:HA	2:G:902:ARG:HB3	1.90	0.53
2:G:3932:ASP:HA	2:G:3935:TRP:HD1	1.73	0.53
2:G:4024:VAL:HG23	2:G:4027:LEU:HD12	1.90	0.53
2:I:15:ARG:HD3	2:I:98:HIS:HB3	1.91	0.53
2:I:891:TRP:HA	2:I:902:ARG:HB3	1.90	0.53
2:I:3781:GLN:HA	2:I:3784:SER:HB3	1.91	0.53
2:I:4697:VAL:O	2:I:4701:TRP:N	2.39	0.53
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.91	0.52
2:B:877:ASN:HD22	2:B:1045:THR:HG23	1.74	0.52
2:B:1838:PHE:HB3	2:B:1842:LEU:HD11	1.91	0.52
2:B:4201:ASN:O	2:B:4205:TRP:N	2.38	0.52
2:B:4892:ARG:NH2	2:I:4899:ASP:OD1	2.40	0.52
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.91	0.52
2:G:488:LEU:O	2:G:492:ASP:N	2.39	0.52
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.42	0.52
2:B:281:ARG:NH2	2:B:309:THR:OG1	2.41	0.52
2:B:4780:PHE:O	2:B:4784:PHE:N	2.42	0.52
2:E:877:ASN:HD22	2:E:1045:THR:HG23	1.74	0.52
2:E:2257:LEU:HD11	2:E:2276:ALA:HB2	1.91	0.52
2:G:395:GLN:HG3	2:G:397:GLU:H	1.75	0.52
2:G:1231:GLN:NE2	2:G:1821:ASP:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4782:VAL:O	2:G:4785:THR:OG1	2.26	0.52
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.91	0.52
2:I:1838:PHE:HB3	2:I:1842:LEU:HD11	1.92	0.52
2:E:206:CYS:SG	2:E:207:SER:N	2.83	0.52
2:I:1865:MET:N	2:I:1865:MET:SD	2.83	0.52
2:B:1865:MET:N	2:B:1865:MET:SD	2.83	0.52
2:B:4024:VAL:HG23	2:B:4027:LEU:HD12	1.90	0.52
2:B:4782:VAL:O	2:B:4785:THR:OG1	2.26	0.52
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.91	0.52
2:E:281:ARG:NH2	2:E:309:THR:OG1	2.41	0.52
2:E:2265:LEU:HB3	2:E:2330:ARG:HG2	1.92	0.52
1:H:62:GLY:HA3	1:H:74:LEU:HD21	1.90	0.52
2:I:4978:HIS:HA	2:I:4982:GLU:HB2	1.90	0.52
1:A:57:LYS:HB2	1:A:80:VAL:HB	1.92	0.52
2:B:206:CYS:SG	2:B:207:SER:N	2.83	0.52
2:B:256:ALA:HB1	2:B:286:THR:HG21	1.91	0.52
2:B:1713:ASP:O	2:B:1717:SER:N	2.41	0.52
2:B:4892:ARG:NH2	2:I:4895:GLY:O	2.43	0.52
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.42	0.52
2:E:3932:ASP:HA	2:E:3935:TRP:HD1	1.73	0.52
2:G:256:ALA:HB1	2:G:286:THR:HG21	1.91	0.52
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.43	0.52
2:B:1231:GLN:NE2	2:B:1821:ASP:O	2.42	0.52
2:B:4848:VAL:HG23	2:B:4883:TYR:HE1	1.73	0.52
2:E:647:ASN:ND2	2:E:820:ARG:O	2.41	0.52
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.43	0.52
2:E:4024:VAL:HG23	2:E:4027:LEU:HD12	1.90	0.52
1:F:57:LYS:HB2	1:F:80:VAL:HB	1.92	0.52
2:G:1721:GLU:HG2	2:G:1725:ARG:HH12	1.74	0.52
2:G:4697:VAL:O	2:G:4701:TRP:N	2.39	0.52
2:B:395:GLN:HG3	2:B:397:GLU:H	1.74	0.52
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.43	0.52
2:E:4782:VAL:O	2:E:4785:THR:OG1	2.26	0.52
2:G:206:CYS:SG	2:G:207:SER:N	2.83	0.52
2:G:2265:LEU:HB3	2:G:2330:ARG:HG2	1.92	0.52
2:G:4824:ARG:O	2:G:4828:SER:N	2.38	0.52
2:G:4924:VAL:O	2:G:4928:LEU:N	2.35	0.52
2:I:317:ARG:HB2	2:I:347:PHE:HB2	1.92	0.52
2:I:4782:VAL:O	2:I:4785:THR:OG1	2.26	0.52
2:B:4040:ILE:O	2:B:4044:MET:N	2.41	0.52
2:E:395:GLN:HG3	2:E:397:GLU:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1653:LEU:HB3	2:E:1660:GLN:HB2	1.92	0.52
2:E:4088:ILE:HG23	2:E:4123:ILE:HB	1.90	0.52
2:E:4563:ARG:NH1	2:E:4815:ASP:OD2	2.36	0.52
2:G:317:ARG:HB2	2:G:347:PHE:HB2	1.92	0.52
2:G:647:ASN:ND2	2:G:820:ARG:O	2.41	0.52
2:I:877:ASN:HD22	2:I:1045:THR:HG23	1.74	0.52
2:I:880:GLU:OE1	2:I:968:ALA:N	2.43	0.52
2:I:1653:LEU:HB3	2:I:1660:GLN:HB2	1.92	0.52
2:I:2457:LEU:HD23	2:I:2460:LEU:HD12	1.92	0.52
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.52
2:E:15:ARG:HD3	2:E:98:HIS:HB3	1.91	0.52
2:E:3781:GLN:HA	2:E:3784:SER:HB3	1.91	0.52
2:G:877:ASN:HD22	2:G:1045:THR:HG23	1.74	0.52
2:G:1653:LEU:HB3	2:G:1660:GLN:HB2	1.92	0.52
2:G:1838:PHE:HB3	2:G:1842:LEU:HD11	1.92	0.52
2:G:1865:MET:N	2:G:1865:MET:SD	2.83	0.52
2:G:3992:PHE:O	2:G:3996:PHE:N	2.38	0.52
2:I:1721:GLU:HG2	2:I:1725:ARG:HH12	1.73	0.52
2:B:3781:GLN:HA	2:B:3784:SER:HB3	1.91	0.52
2:E:728:ARG:NH2	2:E:1527:UNK:O	2.43	0.52
2:E:2368:LEU:HD13	2:E:2376:LEU:HB2	1.91	0.52
2:G:111:HIS:CD2	2:G:114:SER:H	2.28	0.52
2:G:2457:LEU:HD23	2:G:2460:LEU:HD12	1.92	0.52
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.42	0.52
1:J:25:HIS:HB3	1:J:40:ARG:HD3	1.92	0.52
2:B:1653:LEU:HB3	2:B:1660:GLN:HB2	1.92	0.51
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.42	0.51
2:B:2257:LEU:HD11	2:B:2276:ALA:HB2	1.91	0.51
2:B:2368:LEU:HD13	2:B:2376:LEU:HB2	1.91	0.51
2:B:4088:ILE:HG23	2:B:4123:ILE:HB	1.90	0.51
2:E:1838:PHE:HB3	2:E:1842:LEU:HD11	1.92	0.51
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.91	0.51
2:G:792:LEU:HD22	2:G:799:GLU:H	1.75	0.51
2:G:2368:LEU:HD13	2:G:2376:LEU:HB2	1.91	0.51
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.40	0.51
2:I:1684:ALA:HA	2:I:1782:PHE:HZ	1.75	0.51
2:I:4780:PHE:O	2:I:4784:PHE:N	2.42	0.51
2:I:4855:ALA:HA	2:I:4859:PHE:HB2	1.92	0.51
2:B:15:ARG:HD3	2:B:98:HIS:HB3	1.91	0.51
2:B:2457:LEU:HD23	2:B:2460:LEU:HD12	1.92	0.51
2:E:1865:MET:N	2:E:1865:MET:SD	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.43	0.51
2:G:4978:HIS:HA	2:G:4982:GLU:HB2	1.90	0.51
2:I:103:TYR:HB3	2:I:152:PRO:HD3	1.92	0.51
2:I:206:CYS:SG	2:I:207:SER:N	2.83	0.51
2:I:256:ALA:HB1	2:I:286:THR:HG21	1.91	0.51
2:I:1727:ARG:HH12	2:I:1772:ARG:HB3	1.76	0.51
2:I:4571:PHE:O	2:I:4575:PHE:N	2.43	0.51
2:B:43:GLY:N	2:B:447:ASP:OD2	2.43	0.51
2:B:1659:LEU:O	2:B:1663:HIS:N	2.41	0.51
2:E:111:HIS:CD2	2:E:114:SER:H	2.28	0.51
2:G:1684:ALA:HA	2:G:1782:PHE:HZ	1.76	0.51
2:G:1713:ASP:O	2:G:1717:SER:N	2.41	0.51
2:I:111:HIS:N	2:I:116:MET:O	2.36	0.51
2:I:4824:ARG:O	2:I:4828:SER:N	2.38	0.51
2:B:111:HIS:CD2	2:B:114:SER:H	2.28	0.51
1:F:87:HIS:N	1:F:91:ILE:O	2.44	0.51
2:G:103:TYR:HB3	2:G:152:PRO:HD3	1.91	0.51
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	1.93	0.51
2:G:4040:ILE:O	2:G:4044:MET:N	2.41	0.51
1:H:57:LYS:HB2	1:H:80:VAL:HB	1.92	0.51
1:H:87:HIS:N	1:H:91:ILE:O	2.44	0.51
2:I:2257:LEU:HD11	2:I:2276:ALA:HB2	1.91	0.51
2:I:4040:ILE:O	2:I:4044:MET:N	2.41	0.51
1:A:87:HIS:N	1:A:91:ILE:O	2.44	0.51
2:B:317:ARG:HB2	2:B:347:PHE:HB2	1.92	0.51
2:B:1727:ARG:HH12	2:B:1772:ARG:HB3	1.76	0.51
2:E:2190:VAL:HA	2:E:2193:GLN:HB2	1.93	0.51
2:E:4780:PHE:O	2:E:4784:PHE:N	2.42	0.51
2:E:4998:LYS:HB3	2:E:5003:HIS:HE1	1.76	0.51
2:I:792:LEU:HD22	2:I:799:GLU:H	1.76	0.51
2:I:2368:LEU:HD13	2:I:2376:LEU:HB2	1.91	0.51
1:J:57:LYS:HB2	1:J:80:VAL:HB	1.92	0.51
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.93	0.51
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	1.93	0.51
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.42	0.51
2:E:3552:UNK:O	2:E:3556:UNK:N	2.43	0.51
2:G:728:ARG:NH2	2:G:1527:UNK:O	2.44	0.51
2:I:111:HIS:CD2	2:I:114:SER:H	2.28	0.51
2:B:792:LEU:HD22	2:B:799:GLU:H	1.76	0.51
2:B:2758:PHE:O	2:B:2762:THR:N	2.43	0.51
2:E:43:GLY:N	2:E:447:ASP:OD2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:HIS:N	2:E:116:MET:O	2.36	0.51
2:E:792:LEU:HD22	2:E:799:GLU:H	1.76	0.51
2:E:4899:ASP:OD1	2:G:4892:ARG:NH2	2.37	0.51
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.93	0.51
2:G:3552:UNK:O	2:G:3556:UNK:N	2.44	0.51
2:G:4918:ILE:HD13	2:I:4892:ARG:HD3	1.92	0.51
2:I:3756:LYS:O	2:I:3760:LYS:NZ	2.37	0.51
2:B:103:TYR:HB3	2:B:152:PRO:HD3	1.92	0.51
2:B:2265:LEU:HB3	2:B:2330:ARG:HG2	1.92	0.51
2:B:3552:UNK:O	2:B:3556:UNK:N	2.44	0.51
2:B:4934:GLY:HA3	2:E:4937:ILE:HD12	1.92	0.51
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.93	0.51
2:G:639:ASN:H	2:G:678:GLN:HE22	1.59	0.51
2:G:1727:ARG:HH12	2:G:1772:ARG:HB3	1.76	0.51
2:G:2235:PHE:HA	2:G:2238:TYR:HD2	1.76	0.51
2:G:4859:PHE:CA	2:G:4862:PHE:CD2	2.75	0.51
2:I:2235:PHE:HA	2:I:2238:TYR:HD2	1.76	0.51
2:I:2265:LEU:HB3	2:I:2330:ARG:HG2	1.92	0.51
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	1.93	0.51
1:J:29:MET:HB3	1:J:98:ILE:HB	1.93	0.51
2:B:4855:ALA:HA	2:B:4859:PHE:HB2	1.92	0.51
2:E:103:TYR:HB3	2:E:152:PRO:HD3	1.92	0.51
2:E:880:GLU:OE1	2:E:968:ALA:N	2.43	0.51
2:E:1713:ASP:O	2:E:1717:SER:N	2.41	0.51
2:E:2248:ARG:NH2	2:E:2285:GLU:OE1	2.44	0.51
2:E:4843:LEU:HD22	2:E:4928:LEU:HD11	1.93	0.51
2:G:1778:SER:N	2:G:1799:SER:O	2.44	0.51
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.42	0.51
2:B:709:ASP:O	2:B:725:HIS:ND1	2.44	0.51
2:B:1071:ARG:HD3	2:B:1241:SER:HB3	1.93	0.51
2:B:2248:ARG:NH2	2:B:2285:GLU:OE1	2.44	0.51
2:B:3904:ARG:NH2	2:B:3973:CYS:SG	2.84	0.51
2:E:317:ARG:HB2	2:E:347:PHE:HB2	1.92	0.51
2:E:2013:LYS:HA	2:E:2028:ARG:HB2	1.93	0.51
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.93	0.51
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	1.93	0.51
2:E:4745:LEU:O	2:E:4749:GLU:N	2.43	0.51
2:I:43:GLY:N	2:I:447:ASP:OD2	2.43	0.51
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.93	0.51
2:I:731:THR:OG1	2:I:1519:UNK:O	2.29	0.51
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2190:VAL:HA	2:I:2193:GLN:HB2	1.93	0.51
2:I:4570:ALA:O	2:I:4574:ASN:ND2	2.44	0.51
2:B:639:ASN:H	2:B:678:GLN:HE22	1.59	0.50
2:B:1684:ALA:HA	2:B:1782:PHE:HZ	1.75	0.50
2:E:639:ASN:H	2:E:678:GLN:HE22	1.59	0.50
2:I:2248:ARG:NH2	2:I:2285:GLU:OE1	2.44	0.50
2:I:4998:LYS:HB3	2:I:5003:HIS:HE1	1.76	0.50
2:B:134:ASP:HA	2:B:192:ASP:HA	1.94	0.50
2:B:1865:MET:HB3	2:B:1926:LEU:HB2	1.94	0.50
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.94	0.50
2:E:1865:MET:HB3	2:E:1926:LEU:HB2	1.94	0.50
2:E:4570:ALA:O	2:E:4574:ASN:ND2	2.44	0.50
1:F:25:HIS:HB3	1:F:40:ARG:HD3	1.92	0.50
2:G:1071:ARG:HD3	2:G:1241:SER:HB3	1.92	0.50
2:G:4843:LEU:HD22	2:G:4928:LEU:HD11	1.93	0.50
2:I:396:GLU:O	2:I:400:ALA:N	2.40	0.50
2:I:1659:LEU:O	2:I:1663:HIS:N	2.41	0.50
2:B:932:LEU:HD23	2:B:935:LEU:HD12	1.94	0.50
2:B:4998:LYS:HB3	2:B:5003:HIS:HE1	1.76	0.50
2:E:54:ASN:O	2:E:58:VAL:N	2.43	0.50
2:E:1241:SER:HA	2:E:1603:VAL:HA	1.92	0.50
2:E:3889:GLN:OE1	2:E:3960:GLN:NE2	2.45	0.50
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.92	0.50
2:G:709:ASP:O	2:G:725:HIS:ND1	2.44	0.50
2:I:395:GLN:HG3	2:I:397:GLU:H	1.74	0.50
2:I:932:LEU:HD23	2:I:935:LEU:HD12	1.94	0.50
2:B:2235:PHE:HA	2:B:2238:TYR:HD2	1.76	0.50
2:B:4570:ALA:O	2:B:4574:ASN:ND2	2.44	0.50
2:E:69:LEU:HD22	2:E:107:ILE:HD11	1.93	0.50
2:E:134:ASP:HA	2:E:192:ASP:HA	1.94	0.50
2:E:232:THR:HB	2:E:252:VAL:HG11	1.93	0.50
2:E:1727:ARG:HH12	2:E:1772:ARG:HB3	1.76	0.50
2:E:2235:PHE:HA	2:E:2238:TYR:HD2	1.76	0.50
2:G:2248:ARG:NH2	2:G:2285:GLU:OE1	2.44	0.50
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.93	0.50
2:I:3772:THR:OG1	2:I:3815:LYS:NZ	2.44	0.50
2:I:4109:GLN:O	2:I:4113:SER:N	2.43	0.50
2:I:4843:LEU:HD22	2:I:4928:LEU:HD11	1.93	0.50
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	1.93	0.50
2:E:1684:ALA:HA	2:E:1782:PHE:HZ	1.76	0.50
2:E:1778:SER:N	2:E:1799:SER:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2457:LEU:HD23	2:E:2460:LEU:HD12	1.92	0.50
2:G:880:GLU:OE1	2:G:968:ALA:N	2.43	0.50
2:G:2190:VAL:HA	2:G:2193:GLN:HB2	1.93	0.50
2:G:4855:ALA:HA	2:G:4859:PHE:HB2	1.92	0.50
1:H:29:MET:HB3	1:H:98:ILE:HB	1.93	0.50
2:I:2013:LYS:HA	2:I:2028:ARG:HB2	1.93	0.50
2:B:1241:SER:HA	2:B:1603:VAL:HA	1.92	0.50
2:B:3765:TYR:O	2:B:3769:ARG:N	2.36	0.50
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.94	0.50
2:G:932:LEU:HD23	2:G:935:LEU:HD12	1.94	0.50
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	1.93	0.50
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	1.94	0.50
2:G:2257:LEU:O	2:G:2261:SER:N	2.45	0.50
2:G:2466:LEU:HA	2:G:2469:ILE:HD12	1.94	0.50
2:G:3904:ARG:NH2	2:G:3973:CYS:SG	2.84	0.50
2:I:2758:PHE:O	2:I:2762:THR:N	2.43	0.50
2:B:1721:GLU:O	2:B:1725:ARG:NH2	2.45	0.50
2:B:1778:SER:N	2:B:1799:SER:O	2.44	0.50
2:B:3910:THR:HG23	2:B:3911:THR:HG23	1.93	0.50
2:B:4634:GLU:HG3	2:B:4636:THR:H	1.77	0.50
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.93	0.50
2:E:1071:ARG:HD3	2:E:1241:SER:HB3	1.92	0.50
2:E:2466:LEU:HA	2:E:2469:ILE:HD12	1.94	0.50
2:G:69:LEU:HD22	2:G:107:ILE:HD11	1.93	0.50
2:G:1721:GLU:O	2:G:1725:ARG:NH2	2.45	0.50
2:G:2013:LYS:HA	2:G:2028:ARG:HB2	1.93	0.50
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.94	0.50
2:G:4998:LYS:HB3	2:G:5003:HIS:HE1	1.76	0.50
2:I:639:ASN:H	2:I:678:GLN:HE22	1.59	0.50
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.94	0.50
2:I:3552:UNK:O	2:I:3556:UNK:N	2.44	0.50
2:I:4634:GLU:HG3	2:I:4636:THR:H	1.77	0.50
2:B:488:LEU:O	2:B:492:ASP:N	2.39	0.50
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.93	0.50
2:B:2013:LYS:HA	2:B:2028:ARG:HB2	1.93	0.50
2:B:4843:LEU:HD22	2:B:4928:LEU:HD11	1.93	0.50
2:E:932:LEU:HD23	2:E:935:LEU:HD12	1.94	0.50
2:E:1163:THR:HA	2:E:1168:VAL:HA	1.94	0.50
2:G:1865:MET:HB3	2:G:1926:LEU:HB2	1.94	0.50
2:G:4634:GLU:HG3	2:G:4636:THR:H	1.77	0.50
1:H:25:HIS:HB3	1:H:40:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:134:ASP:HA	2:I:192:ASP:HA	1.94	0.50
2:I:709:ASP:O	2:I:725:HIS:ND1	2.44	0.50
2:I:1721:GLU:O	2:I:1725:ARG:NH2	2.45	0.50
2:I:3910:THR:HG23	2:I:3911:THR:HG23	1.93	0.50
2:B:3889:GLN:OE1	2:B:3960:GLN:NE2	2.45	0.50
2:E:124:SER:HA	2:E:132:ALA:HB3	1.93	0.50
2:E:1721:GLU:O	2:E:1725:ARG:NH2	2.45	0.50
2:E:4634:GLU:HG3	2:E:4636:THR:H	1.77	0.50
2:G:670:GLU:H	2:G:740:PRO:HB3	1.77	0.50
2:G:1241:SER:HA	2:G:1603:VAL:HA	1.92	0.50
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.33	0.50
2:G:3889:GLN:OE1	2:G:3960:GLN:NE2	2.45	0.50
2:I:379:HIS:CD2	2:I:382:GLY:H	2.27	0.50
2:I:1778:SER:N	2:I:1799:SER:O	2.44	0.50
2:B:4571:PHE:O	2:B:4575:PHE:N	2.43	0.49
2:E:684:VAL:HG23	2:E:781:VAL:HB	1.94	0.49
2:E:709:ASP:O	2:E:725:HIS:ND1	2.44	0.49
2:E:3904:ARG:NH2	2:E:3973:CYS:SG	2.84	0.49
2:E:4571:PHE:O	2:E:4575:PHE:N	2.43	0.49
2:G:134:ASP:HA	2:G:192:ASP:HA	1.94	0.49
2:G:3761:GLN:HB3	2:G:4754:ASN:HA	1.93	0.49
2:G:3772:THR:OG1	2:G:3815:LYS:NZ	2.44	0.49
2:G:4560:TYR:O	2:G:4564:PHE:N	2.45	0.49
2:G:5012:LYS:O	2:G:5016:GLU:N	2.44	0.49
2:I:1865:MET:HB3	2:I:1926:LEU:HB2	1.94	0.49
2:I:2257:LEU:O	2:I:2261:SER:N	2.45	0.49
2:I:4924:VAL:O	2:I:4928:LEU:N	2.35	0.49
1:J:87:HIS:N	1:J:91:ILE:O	2.44	0.49
2:B:2132:GLY:O	2:B:2136:ARG:N	2.46	0.49
2:B:3756:LYS:O	2:B:3760:LYS:NZ	2.37	0.49
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.94	0.49
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	1.94	0.49
2:G:546:TRP:O	2:G:550:LYS:NZ	2.31	0.49
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.92	0.49
2:I:1241:SER:HA	2:I:1603:VAL:HA	1.92	0.49
2:I:3904:ARG:NH2	2:I:3973:CYS:SG	2.84	0.49
1:A:25:HIS:HB3	1:A:40:ARG:HD3	1.92	0.49
2:B:124:SER:HA	2:B:132:ALA:HB3	1.94	0.49
2:B:670:GLU:H	2:B:740:PRO:HB3	1.77	0.49
2:E:670:GLU:H	2:E:740:PRO:HB3	1.77	0.49
2:E:2257:LEU:O	2:E:2261:SER:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2758:PHE:O	2:E:2762:THR:N	2.44	0.49
2:E:3910:THR:HG23	2:E:3911:THR:HG23	1.93	0.49
2:E:4875:LYS:HB3	2:E:4882:CYS:HA	1.95	0.49
2:G:124:SER:HA	2:G:132:ALA:HB3	1.94	0.49
2:G:1111:PRO:HD3	2:G:1605:TRP:HE1	1.78	0.49
2:G:4875:LYS:HB3	2:G:4882:CYS:HA	1.95	0.49
2:I:670:GLU:H	2:I:740:PRO:HB3	1.77	0.49
2:I:2466:LEU:HA	2:I:2469:ILE:HD12	1.94	0.49
2:B:684:VAL:HG23	2:B:781:VAL:HB	1.94	0.49
2:B:2190:VAL:HA	2:B:2193:GLN:HB2	1.93	0.49
2:B:3761:GLN:HB3	2:B:4754:ASN:HA	1.93	0.49
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	1.93	0.49
2:E:4040:ILE:O	2:E:4044:MET:N	2.41	0.49
2:E:4546:VAL:O	2:E:4550:LYS:N	2.42	0.49
2:G:232:THR:HB	2:G:252:VAL:HG11	1.93	0.49
2:G:4570:ALA:O	2:G:4574:ASN:ND2	2.44	0.49
2:I:124:SER:HA	2:I:132:ALA:HB3	1.94	0.49
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	1.94	0.49
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.94	0.49
2:B:5012:LYS:O	2:B:5016:GLU:N	2.44	0.49
2:G:1163:THR:HA	2:G:1168:VAL:HA	1.94	0.49
2:G:2132:GLY:O	2:G:2136:ARG:N	2.46	0.49
2:G:3910:THR:HG23	2:G:3911:THR:HG23	1.93	0.49
2:I:164:ARG:N	2:I:167:ASP:OD2	2.46	0.49
2:I:1071:ARG:HD3	2:I:1241:SER:HB3	1.93	0.49
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	1.94	0.49
2:I:2132:GLY:O	2:I:2136:ARG:N	2.46	0.49
2:I:3889:GLN:OE1	2:I:3960:GLN:NE2	2.45	0.49
2:I:5012:LYS:O	2:I:5016:GLU:N	2.44	0.49
2:B:3772:THR:OG1	2:B:3815:LYS:NZ	2.44	0.49
2:B:4863:TYR:HB2	2:B:4874:MET:HE2	1.95	0.49
1:F:29:MET:HB3	1:F:98:ILE:HB	1.93	0.49
2:G:43:GLY:N	2:G:447:ASP:OD2	2.43	0.49
2:I:252:VAL:HA	2:I:255:HIS:HB2	1.94	0.49
2:I:988:LEU:O	2:I:992:GLY:N	2.44	0.49
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.94	0.49
2:I:4875:LYS:HB3	2:I:4882:CYS:HA	1.95	0.49
2:B:988:LEU:O	2:B:992:GLY:N	2.45	0.49
2:E:3761:GLN:HB3	2:E:4754:ASN:HA	1.93	0.49
2:E:3765:TYR:O	2:E:3769:ARG:N	2.36	0.49
2:G:78:LEU:O	2:G:82:LEU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.49
2:I:1841:VAL:HA	2:I:1844:LEU:HB3	1.95	0.49
2:I:3761:GLN:HB3	2:I:4754:ASN:HA	1.93	0.49
2:B:1841:VAL:HA	2:B:1844:LEU:HB3	1.95	0.49
2:B:3840:SER:OG	2:B:3875:MET:O	2.25	0.49
2:E:495:ASN:HD21	2:E:550:LYS:HD2	1.77	0.49
2:E:1841:VAL:HA	2:E:1844:LEU:HB3	1.95	0.49
2:I:69:LEU:HD22	2:I:107:ILE:HD11	1.93	0.49
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.49
2:I:1163:THR:HA	2:I:1168:VAL:HA	1.94	0.49
2:I:3905:THR:HA	2:I:3912:THR:HG23	1.95	0.49
2:I:4241:THR:HB	2:I:4989:MET:HE1	1.93	0.49
2:I:4560:TYR:O	2:I:4564:PHE:N	2.45	0.49
2:B:396:GLU:O	2:B:400:ALA:N	2.40	0.49
2:B:867:LEU:HD22	2:B:929:LEU:HD22	1.95	0.49
2:B:2466:LEU:HA	2:B:2469:ILE:HD12	1.94	0.49
2:B:4875:LYS:HB3	2:B:4882:CYS:HA	1.95	0.49
2:E:1111:PRO:HD3	2:E:1605:TRP:HE1	1.78	0.49
2:E:1229:ASN:O	2:E:1827:ARG:N	2.42	0.49
2:E:1737:PRO:HG2	2:E:1739:THR:HG23	1.95	0.49
2:E:3756:LYS:O	2:E:3760:LYS:NZ	2.37	0.49
2:G:1841:VAL:HA	2:G:1844:LEU:HB3	1.95	0.49
2:I:2336:ARG:NH2	2:I:2428:ALA:O	2.46	0.49
2:B:379:HIS:CD2	2:B:382:GLY:H	2.27	0.49
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.38	0.49
2:B:2257:LEU:O	2:B:2261:SER:N	2.45	0.49
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.49
1:H:7:ILE:HG22	1:H:9:PRO:HD2	1.94	0.49
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.78	0.49
2:I:1663:HIS:O	2:I:1667:LEU:N	2.46	0.49
2:I:3840:SER:OG	2:I:3875:MET:O	2.25	0.49
2:B:232:THR:HB	2:B:252:VAL:HG11	1.93	0.48
2:B:252:VAL:HA	2:B:255:HIS:HB2	1.95	0.48
2:B:797:HIS:HB3	2:B:1625:GLY:H	1.78	0.48
2:B:1163:THR:HA	2:B:1168:VAL:HA	1.94	0.48
2:G:54:ASN:O	2:G:58:VAL:N	2.43	0.48
2:G:867:LEU:HD22	2:G:929:LEU:HD22	1.95	0.48
2:G:988:LEU:O	2:G:992:GLY:N	2.45	0.48
2:I:867:LEU:HD22	2:I:929:LEU:HD22	1.95	0.48
2:I:1952:GLN:HA	2:I:1955:VAL:HG12	1.95	0.48
2:I:2104:ARG:HA	2:I:2107:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2868:SER:O	2:I:2872:GLN:N	2.46	0.48
1:A:7:ILE:HG22	1:A:9:PRO:HD2	1.94	0.48
2:B:164:ARG:N	2:B:167:ASP:OD2	2.46	0.48
2:B:629:ARG:HB3	2:B:634:GLN:NE2	2.29	0.48
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.78	0.48
2:E:2868:SER:O	2:E:2872:GLN:N	2.46	0.48
2:G:1229:ASN:O	2:G:1827:ARG:N	2.42	0.48
2:G:4863:TYR:HB2	2:G:4874:MET:HE2	1.94	0.48
2:I:2318:TYR:OH	2:I:2414:ASN:N	2.45	0.48
1:A:29:MET:HB3	1:A:98:ILE:HB	1.93	0.48
2:B:54:ASN:O	2:B:58:VAL:N	2.43	0.48
2:B:69:LEU:HD22	2:B:107:ILE:HD11	1.93	0.48
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.48
2:B:1952:GLN:HA	2:B:1955:VAL:HG12	1.95	0.48
2:E:1659:LEU:O	2:E:1663:HIS:N	2.40	0.48
2:G:2868:SER:O	2:G:2872:GLN:N	2.46	0.48
2:I:266:ARG:NH2	2:I:269:TRP:O	2.46	0.48
2:I:1294:UNK:HA	2:I:1455:UNK:HA	1.96	0.48
2:E:913:LEU:HD13	2:E:918:ARG:HA	1.96	0.48
2:E:3772:THR:OG1	2:E:3815:LYS:NZ	2.44	0.48
1:F:7:ILE:HG22	1:F:9:PRO:HD2	1.94	0.48
2:G:266:ARG:NH2	2:G:269:TRP:O	2.46	0.48
2:G:629:ARG:HB3	2:G:634:GLN:NE2	2.28	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.46	0.48
2:I:495:ASN:HD21	2:I:550:LYS:HD2	1.77	0.48
2:I:4863:TYR:HB2	2:I:4874:MET:HE2	1.95	0.48
2:B:1227:ALA:HB1	2:B:1230:MET:HG3	1.95	0.48
2:E:988:LEU:O	2:E:992:GLY:N	2.45	0.48
2:E:2318:TYR:OH	2:E:2414:ASN:N	2.45	0.48
2:E:4705:VAL:HB	2:E:4778:TRP:CG	2.48	0.48
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.48	0.48
2:G:2104:ARG:HA	2:G:2107:GLN:HB3	1.95	0.48
2:G:4928:LEU:HA	2:G:4931:ILE:HD12	1.95	0.48
2:I:913:LEU:HD13	2:I:918:ARG:HA	1.96	0.48
2:I:4705:VAL:HB	2:I:4778:TRP:CG	2.49	0.48
2:B:2104:ARG:HA	2:B:2107:GLN:HB3	1.95	0.48
2:B:2318:TYR:OH	2:B:2414:ASN:N	2.45	0.48
2:B:2868:SER:O	2:B:2872:GLN:N	2.46	0.48
2:E:266:ARG:NH2	2:E:269:TRP:O	2.47	0.48
2:E:629:ARG:HB3	2:E:634:GLN:NE2	2.29	0.48
2:E:867:LEU:HD22	2:E:929:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3993:LEU:HA	2:E:3996:PHE:HB2	1.96	0.48
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.96	0.48
2:I:232:THR:HB	2:I:252:VAL:HG11	1.93	0.48
2:I:1668:ARG:HA	2:I:1671:ARG:HH11	1.79	0.48
2:I:3992:PHE:O	2:I:3996:PHE:N	2.38	0.48
2:I:4745:LEU:O	2:I:4749:GLU:N	2.43	0.48
2:B:266:ARG:NH2	2:B:269:TRP:O	2.46	0.48
2:B:4705:VAL:HB	2:B:4778:TRP:CG	2.49	0.48
2:E:164:ARG:N	2:E:167:ASP:OD2	2.46	0.48
2:E:1668:ARG:HA	2:E:1671:ARG:HH11	1.79	0.48
2:G:164:ARG:N	2:G:167:ASP:OD2	2.46	0.48
2:G:252:VAL:HA	2:G:255:HIS:HB2	1.95	0.48
2:G:396:GLU:O	2:G:400:ALA:N	2.41	0.48
2:G:495:ASN:HD21	2:G:550:LYS:HD2	1.77	0.48
2:G:684:VAL:HG23	2:G:781:VAL:HB	1.94	0.48
2:G:1203:ASN:ND2	2:G:1210:SER:O	2.47	0.48
2:G:1952:GLN:HA	2:G:1955:VAL:HG12	1.95	0.48
2:G:4705:VAL:HB	2:G:4778:TRP:CG	2.48	0.48
2:I:668:VAL:HG22	2:I:789:VAL:HG23	1.96	0.48
2:I:1227:ALA:HB1	2:I:1230:MET:HG3	1.95	0.48
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.49	0.48
1:J:7:ILE:HG22	1:J:9:PRO:HD2	1.94	0.48
2:B:4138:ASP:OD1	2:B:4138:ASP:N	2.46	0.48
2:B:4745:LEU:O	2:B:4749:GLU:N	2.43	0.48
2:E:220:LEU:HD11	2:E:390:LEU:HD22	1.95	0.48
2:E:2336:ARG:NH2	2:E:2428:ALA:O	2.46	0.48
2:G:220:LEU:HD11	2:G:390:LEU:HD22	1.95	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.46	0.48
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.96	0.48
2:B:469:ARG:HH21	2:B:3712:GLU:HB3	1.79	0.48
2:B:495:ASN:HD21	2:B:550:LYS:HD2	1.77	0.48
2:B:1203:ASN:ND2	2:B:1210:SER:O	2.47	0.48
2:B:1764:GLY:HA3	2:B:1859:VAL:HG11	1.96	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.96	0.48
2:E:914:PRO:O	2:E:918:ARG:N	2.46	0.48
2:E:1854:PHE:HD1	2:E:1858:ASP:HB3	1.79	0.48
2:E:3829:PHE:HA	2:E:3832:ILE:HD12	1.95	0.48
2:G:637:LEU:HG	2:G:1693:GLN:HB3	1.96	0.48
2:G:797:HIS:HB3	2:G:1625:GLY:H	1.78	0.48
2:G:1659:LEU:O	2:G:1663:HIS:N	2.41	0.48
2:G:1976:ARG:NH1	2:G:1997:GLU:OE2	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:78:LEU:O	2:I:82:LEU:N	2.44	0.48
2:I:684:VAL:HG23	2:I:781:VAL:HB	1.94	0.48
2:I:1764:GLY:HA3	2:I:1859:VAL:HG11	1.96	0.48
2:B:497:TYR:HB3	2:B:500:ALA:HB2	1.96	0.48
2:B:1668:ARG:HA	2:B:1671:ARG:HH11	1.79	0.48
2:E:252:VAL:HA	2:E:255:HIS:HB2	1.95	0.48
2:E:1764:GLY:HA3	2:E:1859:VAL:HG11	1.96	0.48
2:E:1952:GLN:HA	2:E:1955:VAL:HG12	1.95	0.48
2:E:3905:THR:HA	2:E:3912:THR:HG23	1.95	0.48
2:G:288:GLY:HA3	2:G:405:HIS:CE1	2.49	0.48
2:G:379:HIS:CD2	2:G:382:GLY:H	2.27	0.48
2:G:1668:ARG:HA	2:G:1671:ARG:HH11	1.79	0.48
2:I:54:ASN:O	2:I:58:VAL:N	2.43	0.48
2:I:637:LEU:HG	2:I:1693:GLN:HB3	1.96	0.48
2:I:709:ASP:HB3	2:I:725:HIS:CE1	2.49	0.48
2:I:797:HIS:HB3	2:I:1625:GLY:H	1.78	0.48
2:I:4942:GLU:O	2:I:4946:GLN:N	2.43	0.48
2:B:2336:ARG:NH2	2:B:2428:ALA:O	2.46	0.47
2:E:469:ARG:HH21	2:E:3712:GLU:HB3	1.79	0.47
2:E:497:TYR:HB3	2:E:500:ALA:HB2	1.96	0.47
2:E:546:TRP:O	2:E:550:LYS:NZ	2.31	0.47
2:E:637:LEU:HG	2:E:1693:GLN:HB3	1.96	0.47
2:E:668:VAL:HG22	2:E:789:VAL:HG23	1.96	0.47
2:E:1203:ASN:ND2	2:E:1210:SER:O	2.47	0.47
2:E:1848:LEU:HB3	2:E:1853:ILE:HB	1.95	0.47
2:I:497:TYR:HB3	2:I:500:ALA:HB2	1.96	0.47
2:I:1203:ASN:ND2	2:I:1210:SER:O	2.47	0.47
2:I:3829:PHE:HA	2:I:3832:ILE:HD12	1.95	0.47
2:I:4928:LEU:HA	2:I:4931:ILE:HD12	1.96	0.47
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.49	0.47
2:B:4560:TYR:O	2:B:4564:PHE:N	2.45	0.47
2:G:1227:ALA:HB1	2:G:1230:MET:HG3	1.95	0.47
2:G:3905:THR:HA	2:G:3912:THR:HG23	1.95	0.47
2:G:4571:PHE:O	2:G:4575:PHE:N	2.43	0.47
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.96	0.47
2:I:1737:PRO:HG2	2:I:1739:THR:HG23	1.95	0.47
2:B:913:LEU:HD13	2:B:918:ARG:HA	1.95	0.47
2:B:1229:ASN:O	2:B:1827:ARG:N	2.42	0.47
2:B:1737:PRO:HG2	2:B:1739:THR:HG23	1.95	0.47
2:E:809:ALA:O	2:E:811:CYS:N	2.47	0.47
2:E:1227:ALA:HB1	2:E:1230:MET:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:139:GLU:O	2:G:141:ALA:N	2.47	0.47
2:G:4780:PHE:O	2:G:4784:PHE:N	2.42	0.47
2:I:629:ARG:HB3	2:I:634:GLN:NE2	2.29	0.47
2:I:4584:ASP:HA	2:I:4627:MET:HA	1.97	0.47
2:B:288:GLY:HA3	2:B:405:HIS:CE1	2.49	0.47
2:B:668:VAL:HG22	2:B:789:VAL:HG23	1.96	0.47
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.96	0.47
2:B:1817:GLU:O	2:B:1821:ASP:N	2.45	0.47
2:B:4584:ASP:HA	2:B:4627:MET:HA	1.97	0.47
2:E:1663:HIS:O	2:E:1667:LEU:N	2.46	0.47
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.48	0.47
2:E:4056:GLU:HA	2:E:4059:LEU:HB2	1.97	0.47
2:G:173:SER:OG	2:G:174:VAL:N	2.48	0.47
2:G:410:LEU:HD21	2:G:441:VAL:HA	1.96	0.47
2:G:497:TYR:HB3	2:G:500:ALA:HB2	1.96	0.47
2:G:709:ASP:HB3	2:G:725:HIS:CE1	2.50	0.47
2:G:913:LEU:HD13	2:G:918:ARG:HA	1.96	0.47
2:G:1044:ARG:HA	2:G:1047:LEU:HD12	1.97	0.47
2:G:1764:GLY:HA3	2:G:1859:VAL:HG11	1.96	0.47
2:G:3829:PHE:HA	2:G:3832:ILE:HD12	1.95	0.47
2:I:652:ARG:HB3	2:I:773:LEU:HD13	1.97	0.47
2:B:173:SER:OG	2:B:174:VAL:N	2.47	0.47
2:B:4928:LEU:HA	2:B:4931:ILE:HD12	1.96	0.47
2:E:288:GLY:HA3	2:E:405:HIS:CE1	2.49	0.47
2:E:797:HIS:HB3	2:E:1625:GLY:H	1.78	0.47
2:E:952:LYS:HB3	2:E:968:ALA:HB1	1.96	0.47
2:E:3927:GLN:O	2:E:3931:SER:N	2.43	0.47
2:G:1737:PRO:HG2	2:G:1739:THR:HG23	1.95	0.47
2:G:2318:TYR:OH	2:G:2414:ASN:N	2.45	0.47
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.48	0.47
2:I:4896:GLY:HA2	2:I:4921:PHE:HB2	1.97	0.47
2:B:220:LEU:HD11	2:B:390:LEU:HD22	1.95	0.47
2:B:637:LEU:HG	2:B:1693:GLN:HB3	1.96	0.47
2:B:2154:SER:O	2:B:2184:ASN:ND2	2.47	0.47
2:B:3674:ILE:HG13	2:B:3732:SER:HB3	1.96	0.47
2:B:3993:LEU:HA	2:B:3996:PHE:HB2	1.96	0.47
2:B:4546:VAL:O	2:B:4550:LYS:N	2.42	0.47
2:E:4059:LEU:O	2:E:4063:ASP:N	2.47	0.47
2:E:4858:PHE:O	2:E:4862:PHE:HE2	1.98	0.47
2:G:1848:LEU:HB3	2:G:1853:ILE:HB	1.95	0.47
2:G:4172:GLU:HA	2:G:4175:ARG:HE	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:952:LYS:HB3	2:I:968:ALA:HB1	1.96	0.47
2:I:1044:ARG:HA	2:I:1047:LEU:HD12	1.97	0.47
2:B:118:LEU:HD12	2:B:137:LEU:HB3	1.97	0.47
2:B:410:LEU:HD21	2:B:441:VAL:HA	1.96	0.47
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.96	0.47
2:B:709:ASP:HB3	2:B:725:HIS:CE1	2.49	0.47
2:B:1848:LEU:HD22	2:B:1853:ILE:HG13	1.97	0.47
2:B:1848:LEU:HB3	2:B:1853:ILE:HB	1.95	0.47
2:B:4021:LYS:HA	2:B:4024:VAL:HG12	1.97	0.47
2:B:4109:GLN:O	2:B:4113:SER:N	2.43	0.47
2:B:4688:ILE:HG21	2:B:4728:HIS:HB3	1.96	0.47
2:B:4710:SER:OG	2:B:4772:ASP:OD2	2.28	0.47
2:B:4896:GLY:HA2	2:B:4921:PHE:HB2	1.97	0.47
2:E:652:ARG:HB3	2:E:773:LEU:HD13	1.97	0.47
2:E:709:ASP:HB3	2:E:725:HIS:CE1	2.49	0.47
2:E:1046:LEU:HB3	2:E:1051:TYR:HB2	1.97	0.47
2:E:2095:GLN:NE2	2:E:2127:GLN:O	2.48	0.47
2:E:2104:ARG:HA	2:E:2107:GLN:HB3	1.95	0.47
2:E:2132:GLY:O	2:E:2136:ARG:N	2.45	0.47
2:E:2154:SER:O	2:E:2184:ASN:ND2	2.47	0.47
2:E:4021:LYS:HA	2:E:4024:VAL:HG12	1.97	0.47
2:G:118:LEU:HD12	2:G:137:LEU:HB3	1.97	0.47
2:G:652:ARG:HB3	2:G:773:LEU:HD13	1.97	0.47
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.96	0.47
2:G:1516:UNK:N	2:G:1529:UNK:O	2.47	0.47
2:G:4056:GLU:HA	2:G:4059:LEU:HB2	1.97	0.47
2:G:4138:ASP:OD1	2:G:4138:ASP:N	2.46	0.47
2:G:4688:ILE:HG21	2:G:4728:HIS:HB3	1.96	0.47
2:I:220:LEU:HD11	2:I:390:LEU:HD22	1.95	0.47
2:I:1848:LEU:HB3	2:I:1853:ILE:HB	1.95	0.47
2:I:4172:GLU:HA	2:I:4175:ARG:HE	1.79	0.47
2:B:139:GLU:O	2:B:141:ALA:N	2.47	0.47
2:B:914:PRO:O	2:B:918:ARG:N	2.46	0.47
2:B:3905:THR:HA	2:B:3912:THR:HG23	1.95	0.47
2:E:139:GLU:O	2:E:141:ALA:N	2.47	0.47
2:E:485:SER:O	2:E:489:ASN:N	2.46	0.47
2:E:2430:ILE:HG21	2:E:2502:UNK:HA	1.97	0.47
2:E:4928:LEU:HA	2:E:4931:ILE:HD12	1.96	0.47
2:G:668:VAL:HG22	2:G:789:VAL:HG23	1.96	0.47
2:G:809:ALA:O	2:G:811:CYS:N	2.47	0.47
2:G:1046:LEU:HB3	2:G:1051:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1854:PHE:HD1	2:G:1858:ASP:HB3	1.79	0.47
2:G:4201:ASN:ND2	2:G:4993:MET:SD	2.88	0.47
2:I:118:LEU:HD12	2:I:137:LEU:HB3	1.97	0.47
2:I:218:HIS:HB3	2:I:392:ARG:HD3	1.97	0.47
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	1.97	0.47
2:I:1848:LEU:HD22	2:I:1853:ILE:HG13	1.97	0.47
2:B:475:GLN:NE2	2:B:528:SER:O	2.48	0.47
2:B:1046:LEU:HB3	2:B:1051:TYR:HB2	1.97	0.47
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	1.97	0.47
2:B:1854:PHE:HD1	2:B:1858:ASP:HB3	1.79	0.47
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.97	0.47
2:E:4083:ASP:HA	2:E:4085:ARG:HH11	1.80	0.47
2:E:4201:ASN:ND2	2:E:4993:MET:SD	2.88	0.47
2:E:4860:ARG:HD2	2:G:4582:VAL:HG11	1.97	0.47
2:E:4863:TYR:HB2	2:E:4874:MET:HE2	1.95	0.47
2:G:4584:ASP:HA	2:G:4627:MET:HA	1.96	0.47
2:I:546:TRP:O	2:I:550:LYS:NZ	2.31	0.47
2:I:3765:TYR:O	2:I:3769:ARG:N	2.36	0.47
1:A:23:VAL:HB	1:A:105:ASN:HA	1.97	0.47
2:B:176:SER:HB2	2:B:178:ARG:HD3	1.97	0.47
2:B:652:ARG:HB3	2:B:773:LEU:HD13	1.97	0.47
2:B:1044:ARG:HA	2:B:1047:LEU:HD12	1.97	0.47
2:E:173:SER:OG	2:E:174:VAL:N	2.48	0.47
2:E:410:LEU:HD21	2:E:441:VAL:HA	1.96	0.47
2:E:702:TRP:O	2:E:705:ASN:ND2	2.46	0.47
2:E:4138:ASP:N	2:E:4138:ASP:OD1	2.46	0.47
2:G:176:SER:HB2	2:G:178:ARG:HD3	1.97	0.47
2:G:241:GLN:O	2:G:289:ARG:NH1	2.42	0.47
2:G:952:LYS:HB3	2:G:968:ALA:HB1	1.96	0.47
2:G:2154:SER:O	2:G:2184:ASN:ND2	2.47	0.47
2:G:4896:GLY:HA2	2:G:4921:PHE:HB2	1.97	0.47
2:I:469:ARG:HH21	2:I:3712:GLU:HB3	1.80	0.47
2:I:4138:ASP:OD1	2:I:4138:ASP:N	2.46	0.47
2:B:460:GLN:HG2	2:B:462:GLU:H	1.80	0.46
2:E:379:HIS:CD2	2:E:382:GLY:H	2.27	0.46
2:E:4584:ASP:HA	2:E:4627:MET:HA	1.96	0.46
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.97	0.46
1:F:23:VAL:HB	1:F:105:ASN:HA	1.97	0.46
2:G:469:ARG:HH21	2:G:3712:GLU:HB3	1.80	0.46
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.48	0.46
2:G:3674:ILE:HG13	2:G:3732:SER:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:3927:GLN:O	2:G:3931:SER:N	2.43	0.46
2:G:4083:ASP:HA	2:G:4085:ARG:HH11	1.80	0.46
2:G:4858:PHE:O	2:G:4862:PHE:HE2	1.98	0.46
2:I:139:GLU:O	2:I:141:ALA:N	2.48	0.46
2:I:173:SER:OG	2:I:174:VAL:N	2.47	0.46
2:I:410:LEU:HD21	2:I:441:VAL:HA	1.96	0.46
2:I:1046:LEU:HB3	2:I:1051:TYR:HB2	1.97	0.46
2:I:1149:VAL:HG22	2:I:1164:LEU:HD13	1.97	0.46
2:I:1976:ARG:NH1	2:I:1997:GLU:OE2	2.35	0.46
2:I:3993:LEU:HA	2:I:3996:PHE:HB2	1.96	0.46
2:B:34:LYS:N	2:B:53:SER:OG	2.43	0.46
2:B:1149:VAL:HG22	2:B:1164:LEU:HD13	1.97	0.46
2:B:2880:GLU:O	2:B:2884:ASN:N	2.45	0.46
2:B:3829:PHE:HA	2:B:3832:ILE:HD12	1.95	0.46
2:B:4083:ASP:HA	2:B:4085:ARG:HH11	1.80	0.46
2:E:118:LEU:HD12	2:E:137:LEU:HB3	1.97	0.46
2:E:218:HIS:HB3	2:E:392:ARG:HD3	1.97	0.46
2:E:1098:GLY:HA2	2:E:1127:HIS:CD2	2.51	0.46
2:E:4688:ILE:HG21	2:E:4728:HIS:HB3	1.96	0.46
2:G:111:HIS:N	2:G:116:MET:O	2.36	0.46
2:G:385:ASP:OD1	2:G:385:ASP:N	2.48	0.46
2:G:1098:GLY:HA2	2:G:1127:HIS:CD2	2.51	0.46
2:G:4563:ARG:NH1	2:G:4815:ASP:OD2	2.36	0.46
2:I:460:GLN:HG2	2:I:462:GLU:H	1.80	0.46
2:B:4172:GLU:HA	2:B:4175:ARG:HE	1.79	0.46
2:E:396:GLU:O	2:E:400:ALA:N	2.40	0.46
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.96	0.46
2:E:3674:ILE:HG13	2:E:3732:SER:HB3	1.97	0.46
2:E:4172:GLU:HA	2:E:4175:ARG:HE	1.80	0.46
2:G:2336:ARG:NH2	2:G:2428:ALA:O	2.46	0.46
2:I:475:GLN:NE2	2:I:528:SER:O	2.48	0.46
2:I:3674:ILE:HG13	2:I:3732:SER:HB3	1.97	0.46
2:I:4056:GLU:HA	2:I:4059:LEU:HB2	1.97	0.46
2:E:176:SER:HB2	2:E:178:ARG:HD3	1.97	0.46
2:E:2212:VAL:O	2:E:2216:GLY:N	2.46	0.46
2:E:4896:GLY:HA2	2:E:4921:PHE:HB2	1.97	0.46
2:G:426:ARG:HG2	2:G:431:PRO:HA	1.98	0.46
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	1.97	0.46
2:G:2758:PHE:O	2:G:2762:THR:N	2.44	0.46
2:I:1854:PHE:HD1	2:I:1858:ASP:HB3	1.79	0.46
2:I:4688:ILE:HG21	2:I:4728:HIS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:HG2	2:B:431:PRO:HA	1.98	0.46
2:B:702:TRP:O	2:B:705:ASN:ND2	2.46	0.46
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.48	0.46
2:B:2430:ILE:HG21	2:B:2502:UNK:HA	1.98	0.46
2:B:4824:ARG:O	2:B:4828:SER:N	2.38	0.46
2:G:742:ASP:OD1	2:G:760:ASN:ND2	2.49	0.46
2:G:1848:LEU:HD22	2:G:1853:ILE:HG13	1.97	0.46
2:G:4021:LYS:HA	2:G:4024:VAL:HG12	1.97	0.46
2:I:176:SER:HB2	2:I:178:ARG:HD3	1.97	0.46
2:I:288:GLY:HA3	2:I:405:HIS:CE1	2.49	0.46
2:I:4546:VAL:O	2:I:4550:LYS:N	2.42	0.46
2:B:485:SER:O	2:B:489:ASN:N	2.46	0.46
2:B:952:LYS:HB3	2:B:968:ALA:HB1	1.96	0.46
2:B:1663:HIS:O	2:B:1667:LEU:N	2.46	0.46
2:E:1848:LEU:HD22	2:E:1853:ILE:HG13	1.97	0.46
2:G:264:PRO:HA	2:G:280:LEU:HA	1.97	0.46
2:G:355:LEU:HB3	2:G:378:LEU:HB3	1.97	0.46
2:G:1149:VAL:HG22	2:G:1164:LEU:HD13	1.97	0.46
2:G:3993:LEU:HA	2:G:3996:PHE:HB2	1.96	0.46
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.98	0.46
2:I:2154:SER:O	2:I:2184:ASN:ND2	2.47	0.46
2:I:4021:LYS:HA	2:I:4024:VAL:HG12	1.97	0.46
2:I:4853:VAL:HA	2:I:4856:PHE:HB3	1.98	0.46
2:B:583:ILE:HA	2:B:586:ILE:HD12	1.98	0.46
2:E:426:ARG:HG2	2:E:431:PRO:HA	1.98	0.46
2:E:475:GLN:NE2	2:E:528:SER:O	2.48	0.46
2:E:1149:VAL:HG22	2:E:1164:LEU:HD13	1.97	0.46
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	1.98	0.46
2:G:218:HIS:HB3	2:G:392:ARG:HD3	1.97	0.46
1:H:14:THR:N	1:H:67:SER:OG	2.49	0.46
2:I:34:LYS:N	2:I:53:SER:OG	2.43	0.46
2:I:385:ASP:N	2:I:385:ASP:OD1	2.48	0.46
2:I:426:ARG:HG2	2:I:431:PRO:HA	1.98	0.46
2:I:2143:THR:O	2:I:3651:ASN:ND2	2.38	0.46
2:B:2231:SER:HA	2:B:2234:ARG:HG2	1.98	0.46
2:E:1044:ARG:HA	2:E:1047:LEU:HD12	1.97	0.46
2:E:2158:CYS:HB2	2:E:2184:ASN:HD22	1.81	0.46
2:E:4105:GLY:HA2	2:E:4108:ILE:HD12	1.98	0.46
2:G:1647:CYS:SG	2:G:1648:MET:N	2.89	0.46
2:G:4934:GLY:HA3	2:I:4937:ILE:HD12	1.97	0.46
2:I:1098:GLY:HA2	2:I:1127:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4083:ASP:HA	2:I:4085:ARG:HH11	1.80	0.46
2:B:218:HIS:HB3	2:B:392:ARG:HD3	1.97	0.46
2:B:650:VAL:HB	2:B:777:PHE:HB2	1.98	0.46
2:B:2158:CYS:HB2	2:B:2184:ASN:HD22	1.81	0.46
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.49	0.46
2:E:583:ILE:HA	2:E:586:ILE:HD12	1.98	0.46
2:E:2231:SER:HA	2:E:2234:ARG:HG2	1.98	0.46
2:G:34:LYS:N	2:G:53:SER:OG	2.43	0.46
2:I:742:ASP:OD1	2:I:760:ASN:ND2	2.49	0.46
2:I:1661:ARG:O	2:I:1664:SER:OG	2.32	0.46
2:I:1817:GLU:O	2:I:1821:ASP:N	2.45	0.46
2:I:2231:SER:HA	2:I:2234:ARG:HG2	1.98	0.46
2:I:4201:ASN:ND2	2:I:4993:MET:SD	2.88	0.46
2:B:278:GLN:N	2:B:315:CYS:SG	2.89	0.46
2:B:4056:GLU:HA	2:B:4059:LEU:HB2	1.97	0.46
2:B:4201:ASN:ND2	2:B:4993:MET:SD	2.88	0.46
2:B:4942:GLU:O	2:B:4946:GLN:N	2.43	0.46
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.98	0.46
2:G:475:GLN:NE2	2:G:528:SER:O	2.48	0.46
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.81	0.46
2:G:4059:LEU:O	2:G:4063:ASP:N	2.49	0.46
2:I:264:PRO:HA	2:I:280:LEU:HA	1.97	0.46
2:I:355:LEU:HB3	2:I:378:LEU:HB3	1.97	0.46
2:I:1647:CYS:SG	2:I:1648:MET:N	2.89	0.46
2:I:2243:SER:HB3	2:I:2246:ASN:H	1.81	0.46
2:I:2430:ILE:HG21	2:I:2502:UNK:HA	1.98	0.46
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.97	0.46
2:B:666:VAL:HG21	2:B:684:VAL:HG21	1.98	0.45
2:B:1647:CYS:SG	2:B:1648:MET:N	2.89	0.45
2:B:3805:LEU:H	2:B:3805:LEU:HG	1.61	0.45
2:E:1965:TYR:HE1	2:E:2027:ILE:HB	1.82	0.45
2:E:4577:LEU:HG	2:E:4580:TYR:HE2	1.81	0.45
2:E:4813:LEU:HA	2:E:4816:ILE:HG12	1.99	0.45
1:F:14:THR:N	1:F:67:SER:OG	2.49	0.45
2:G:583:ILE:HA	2:G:586:ILE:HD12	1.98	0.45
2:G:650:VAL:HB	2:G:777:PHE:HB2	1.98	0.45
2:G:1694:LEU:O	2:G:1712:TYR:OH	2.24	0.45
2:G:4853:VAL:HA	2:G:4856:PHE:HB3	1.98	0.45
2:I:110:ARG:HH21	2:I:115:ARG:HB3	1.81	0.45
2:I:668:VAL:O	2:I:741:GLU:N	2.49	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:4577:LEU:HG	2:I:4580:TYR:HE2	1.81	0.45
2:B:742:ASP:OD1	2:B:760:ASN:ND2	2.49	0.45
2:B:2869:ARG:HH12	2:B:2945:UNK:C	2.29	0.45
2:B:4895:GLY:O	2:E:4892:ARG:NH2	2.48	0.45
2:E:355:LEU:HB3	2:E:378:LEU:HB3	1.97	0.45
2:E:5012:LYS:O	2:E:5016:GLU:N	2.44	0.45
2:G:110:ARG:HH21	2:G:115:ARG:HB3	1.81	0.45
2:G:2243:SER:HB3	2:G:2246:ASN:H	1.81	0.45
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.98	0.45
2:G:4105:GLY:HA2	2:G:4108:ILE:HD12	1.98	0.45
2:G:4109:GLN:O	2:G:4113:SER:N	2.43	0.45
2:I:3927:GLN:O	2:I:3931:SER:N	2.43	0.45
2:I:4961:CYS:HB3	2:I:4983:HIS:CE1	2.51	0.45
1:J:14:THR:N	1:J:67:SER:OG	2.49	0.45
2:B:264:PRO:HA	2:B:280:LEU:HA	1.97	0.45
2:B:668:VAL:O	2:B:741:GLU:N	2.49	0.45
2:B:2243:SER:HB3	2:B:2246:ASN:H	1.81	0.45
2:B:4041:ALA:HA	2:B:4044:MET:HB2	1.99	0.45
2:B:4813:LEU:HA	2:B:4816:ILE:HG12	1.98	0.45
2:E:264:PRO:HA	2:E:280:LEU:HA	1.97	0.45
2:E:460:GLN:HG2	2:E:462:GLU:H	1.80	0.45
2:E:742:ASP:OD1	2:E:760:ASN:ND2	2.49	0.45
2:E:1516:UNK:N	2:E:1529:UNK:O	2.50	0.45
2:G:702:TRP:O	2:G:705:ASN:ND2	2.46	0.45
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.38	0.45
2:G:4041:ALA:HA	2:G:4044:MET:HB2	1.99	0.45
2:G:4546:VAL:O	2:G:4550:LYS:N	2.42	0.45
2:I:278:GLN:N	2:I:315:CYS:SG	2.89	0.45
2:I:583:ILE:HA	2:I:586:ILE:HD12	1.98	0.45
2:I:2869:ARG:HH12	2:I:2945:UNK:C	2.29	0.45
2:I:3676:ASP:N	2:I:3676:ASP:OD1	2.49	0.45
2:I:4813:LEU:HA	2:I:4816:ILE:HG12	1.98	0.45
2:B:983:THR:O	2:B:987:ARG:N	2.48	0.45
2:B:1098:GLY:HA2	2:B:1127:HIS:CD2	2.51	0.45
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.98	0.45
2:B:4780:PHE:HA	2:B:4783:ILE:HD12	1.99	0.45
2:E:983:THR:O	2:E:987:ARG:N	2.48	0.45
2:E:4041:ALA:HA	2:E:4044:MET:HB2	1.99	0.45
2:E:4780:PHE:HA	2:E:4783:ILE:HD12	1.99	0.45
2:G:870:ILE:HD11	2:G:1049:TYR:CG	2.52	0.45
2:G:2231:SER:HA	2:G:2234:ARG:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4780:PHE:HA	2:G:4783:ILE:HD12	1.99	0.45
1:H:23:VAL:HB	1:H:105:ASN:HA	1.97	0.45
2:I:838:HIS:CE1	2:I:1201:HIS:HD2	2.35	0.45
2:I:2212:VAL:O	2:I:2216:GLY:N	2.46	0.45
2:I:2869:ARG:HA	2:I:2872:GLN:HB3	1.98	0.45
2:I:2880:GLU:O	2:I:2884:ASN:N	2.45	0.45
2:I:4044:MET:HA	2:I:4047:MET:HG2	1.98	0.45
2:B:838:HIS:CE1	2:B:1201:HIS:HD2	2.35	0.45
2:B:1245:PHE:HE1	2:B:1600:LEU:HD23	1.82	0.45
2:B:2908:TYR:OH	2:B:2920:ARG:NE	2.44	0.45
2:B:3805:LEU:HA	2:B:3809:ASN:HD22	1.82	0.45
2:B:4105:GLY:HA2	2:B:4108:ILE:HD12	1.98	0.45
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.81	0.45
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.38	0.45
2:E:2869:ARG:HH12	2:E:2945:UNK:C	2.29	0.45
2:G:278:GLN:N	2:G:315:CYS:SG	2.89	0.45
2:G:1663:HIS:O	2:G:1667:LEU:N	2.46	0.45
2:G:1817:GLU:O	2:G:1821:ASP:N	2.45	0.45
2:G:2158:CYS:HB2	2:G:2184:ASN:HD22	1.81	0.45
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.49	0.45
1:J:23:VAL:HB	1:J:105:ASN:HA	1.97	0.45
1:A:14:THR:N	1:A:67:SER:OG	2.49	0.45
2:B:78:LEU:O	2:B:82:LEU:N	2.44	0.45
2:B:684:VAL:HA	2:B:781:VAL:HA	1.99	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.81	0.45
2:B:4044:MET:HA	2:B:4047:MET:HG2	1.98	0.45
2:E:838:HIS:CE1	2:E:1201:HIS:HD2	2.35	0.45
2:E:1647:CYS:SG	2:E:1648:MET:N	2.89	0.45
2:E:1694:LEU:O	2:E:1712:TYR:OH	2.24	0.45
2:G:684:VAL:HA	2:G:781:VAL:HA	1.99	0.45
2:G:4044:MET:HA	2:G:4047:MET:HG2	1.98	0.45
2:I:1245:PHE:HE1	2:I:1600:LEU:HD23	1.82	0.45
2:I:4780:PHE:HA	2:I:4783:ILE:HD12	1.99	0.45
2:B:1092:PHE:N	2:B:1149:VAL:O	2.37	0.45
2:E:110:ARG:HH21	2:E:115:ARG:HB3	1.82	0.45
2:E:278:GLN:N	2:E:315:CYS:SG	2.89	0.45
2:E:666:VAL:HG21	2:E:684:VAL:HG21	1.98	0.45
2:E:4853:VAL:HA	2:E:4856:PHE:HB3	1.98	0.45
2:G:3649:ALA:O	2:G:3653:PHE:N	2.47	0.45
2:G:3805:LEU:HA	2:G:3809:ASN:HD22	1.82	0.45
2:G:4031:LEU:HB3	2:G:4034:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2158:CYS:HB2	2:I:2184:ASN:HD22	1.81	0.45
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.98	0.45
2:B:809:ALA:O	2:B:811:CYS:N	2.47	0.45
2:B:1679:ASN:O	2:B:1683:HIS:ND1	2.36	0.45
2:B:3927:GLN:O	2:B:3931:SER:N	2.43	0.45
2:B:4031:LEU:HB3	2:B:4034:ASN:HB2	1.99	0.45
2:E:684:VAL:HA	2:E:781:VAL:HA	1.99	0.45
2:E:840:VAL:HB	2:E:1199:VAL:HG12	1.99	0.45
2:E:2869:ARG:HA	2:E:2872:GLN:HB3	1.98	0.45
2:E:2950:UNK:O	2:E:2954:UNK:N	2.50	0.45
2:G:666:VAL:HG21	2:G:684:VAL:HG21	1.98	0.45
2:G:840:VAL:HB	2:G:1199:VAL:HG12	1.99	0.45
2:G:4942:GLU:O	2:G:4946:GLN:N	2.43	0.45
2:I:4105:GLY:HA2	2:I:4108:ILE:HD12	1.98	0.45
2:B:349:GLN:HA	2:B:356:TRP:HA	1.99	0.45
2:B:355:LEU:HB3	2:B:378:LEU:HB3	1.97	0.45
2:B:870:ILE:HD11	2:B:1049:TYR:CG	2.52	0.45
2:B:4853:VAL:HA	2:B:4856:PHE:HB3	1.98	0.45
2:B:4961:CYS:HB3	2:B:4983:HIS:CE1	2.51	0.45
2:E:1817:GLU:O	2:E:1821:ASP:N	2.45	0.45
2:E:4031:LEU:HB3	2:E:4034:ASN:HB2	1.99	0.45
2:E:4169:SER:HA	2:E:4172:GLU:HB3	1.99	0.45
2:G:4813:LEU:HA	2:G:4816:ILE:HG12	1.99	0.45
2:G:4961:CYS:HB3	2:G:4983:HIS:CE1	2.51	0.45
2:I:666:VAL:HG21	2:I:684:VAL:HG21	1.98	0.45
2:I:3805:LEU:HA	2:I:3809:ASN:HD22	1.82	0.45
2:I:3963:ASN:O	2:I:3966:THR:OG1	2.28	0.45
2:I:4735:GLU:HA	2:I:4738:ALA:HB3	1.99	0.45
2:B:1735:ILE:HG23	2:B:1771:LEU:HD23	1.99	0.45
2:B:2950:UNK:O	2:B:2954:UNK:N	2.50	0.45
2:B:4577:LEU:HG	2:B:4580:TYR:HE2	1.81	0.45
2:G:349:GLN:HA	2:G:356:TRP:HA	1.99	0.45
2:G:1735:ILE:HG23	2:G:1771:LEU:HD23	1.99	0.45
2:G:2950:UNK:O	2:G:2954:UNK:N	2.50	0.45
2:G:4735:GLU:HA	2:G:4738:ALA:HB3	1.99	0.45
2:G:4859:PHE:C	2:G:4862:PHE:HD2	2.20	0.45
2:I:4031:LEU:HB3	2:I:4034:ASN:HB2	1.99	0.45
2:I:4968:PHE:HE1	2:I:5029:ARG:HD3	1.82	0.45
2:B:317:ARG:N	2:B:347:PHE:O	2.50	0.44
2:B:385:ASP:OD1	2:B:385:ASP:N	2.48	0.44
2:B:2869:ARG:HA	2:B:2872:GLN:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1679:ASN:O	2:E:1683:HIS:ND1	2.36	0.44
2:E:2116:LEU:O	2:E:2120:MET:N	2.46	0.44
2:E:4109:GLN:O	2:E:4113:SER:N	2.43	0.44
2:E:4735:GLU:HA	2:E:4738:ALA:HB3	1.99	0.44
2:E:4961:CYS:HB3	2:E:4983:HIS:CE1	2.51	0.44
2:E:4968:PHE:HE1	2:E:5029:ARG:HD3	1.82	0.44
2:G:1965:TYR:HE1	2:G:2027:ILE:HB	1.82	0.44
2:G:3963:ASN:O	2:G:3966:THR:OG1	2.29	0.44
2:I:870:ILE:HD11	2:I:1049:TYR:CG	2.52	0.44
2:E:317:ARG:N	2:E:347:PHE:O	2.50	0.44
2:E:650:VAL:HB	2:E:777:PHE:HB2	1.98	0.44
2:E:1245:PHE:HE1	2:E:1600:LEU:HD23	1.82	0.44
2:E:2243:SER:HB3	2:E:2246:ASN:H	1.81	0.44
2:E:2908:TYR:OH	2:E:2920:ARG:NE	2.44	0.44
2:E:3974:THR:HA	2:E:3977:GLN:HB2	1.99	0.44
2:G:281:ARG:HA	2:G:312:THR:HG21	2.00	0.44
2:G:460:GLN:HG2	2:G:462:GLU:H	1.80	0.44
2:G:983:THR:O	2:G:987:ARG:N	2.48	0.44
2:G:1245:PHE:HE1	2:G:1600:LEU:HD23	1.82	0.44
2:G:1497:UNK:HA	2:G:1535:UNK:HA	1.99	0.44
2:G:2116:LEU:O	2:G:2120:MET:N	2.46	0.44
2:G:4169:SER:HA	2:G:4172:GLU:HB3	1.99	0.44
2:G:4558:ASN:HB2	2:G:4561:THR:HB	2.00	0.44
2:I:392:ARG:HH12	2:I:398:SER:HB2	1.83	0.44
2:I:580:GLU:HG3	2:I:620:LEU:HD22	1.99	0.44
2:I:2950:UNK:O	2:I:2954:UNK:N	2.50	0.44
2:B:264:PRO:HG2	2:B:270:SER:HB2	2.00	0.44
2:B:4735:GLU:HA	2:B:4738:ALA:HB3	1.99	0.44
2:E:349:GLN:HA	2:E:356:TRP:HA	1.99	0.44
2:E:870:ILE:HD11	2:E:1049:TYR:CG	2.52	0.44
2:E:4560:TYR:O	2:E:4564:PHE:N	2.45	0.44
2:G:317:ARG:N	2:G:347:PHE:O	2.50	0.44
2:G:580:GLU:HG3	2:G:620:LEU:HD22	1.99	0.44
2:G:4577:LEU:HG	2:G:4580:TYR:HE2	1.81	0.44
2:I:349:GLN:HA	2:I:356:TRP:HA	1.99	0.44
2:I:4041:ALA:HA	2:I:4044:MET:HB2	1.99	0.44
2:B:1965:TYR:HE1	2:B:2027:ILE:HB	1.82	0.44
2:B:2452:ARG:HH12	2:I:177:GLU:HG3	1.83	0.44
2:E:1735:ILE:HG23	2:E:1771:LEU:HD23	2.00	0.44
2:E:1965:TYR:OH	2:E:2027:ILE:O	2.26	0.44
2:G:392:ARG:HH12	2:G:398:SER:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4568:PHE:HA	2:G:4571:PHE:HD2	1.83	0.44
2:G:4968:PHE:HE1	2:G:5029:ARG:HD3	1.83	0.44
2:I:684:VAL:HA	2:I:781:VAL:HA	1.99	0.44
2:I:1735:ILE:HG23	2:I:1771:LEU:HD23	1.99	0.44
2:I:4568:PHE:HA	2:I:4571:PHE:HD2	1.82	0.44
2:B:110:ARG:HH21	2:B:115:ARG:HB3	1.81	0.44
2:B:392:ARG:HH12	2:B:398:SER:HB2	1.83	0.44
2:B:772:ASN:ND2	2:B:774:ASP:OD2	2.50	0.44
2:B:1931:LEU:HD22	2:B:1935:VAL:HG11	2.00	0.44
2:B:2212:VAL:O	2:B:2216:GLY:N	2.46	0.44
2:E:772:ASN:ND2	2:E:774:ASP:OD2	2.50	0.44
2:E:3361:UNK:O	2:E:3365:UNK:N	2.51	0.44
2:E:4139:ILE:HA	2:E:4142:ASN:HD22	1.82	0.44
2:G:360:ALA:N	2:G:375:LYS:O	2.50	0.44
2:I:650:VAL:HB	2:I:777:PHE:HB2	1.98	0.44
2:I:1931:LEU:HD22	2:I:1935:VAL:HG11	2.00	0.44
2:I:4558:ASN:HB2	2:I:4561:THR:HB	2.00	0.44
2:B:4139:ILE:HA	2:B:4142:ASN:HD22	1.82	0.44
2:B:4990:PHE:O	2:B:4994:TYR:N	2.48	0.44
2:E:16:THR:OG1	2:E:97:GLY:O	2.35	0.44
2:E:392:ARG:HH12	2:E:398:SER:HB2	1.83	0.44
2:E:1976:ARG:NH1	2:E:1997:GLU:OE2	2.35	0.44
2:E:2142:TYR:CG	2:E:2197:LEU:HD13	2.53	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.83	0.44
2:G:3974:THR:HA	2:G:3977:GLN:HB2	1.99	0.44
2:I:264:PRO:HG2	2:I:270:SER:HB2	2.00	0.44
2:I:283:ARG:HH21	2:I:402:ARG:HH12	1.65	0.44
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.35	0.44
2:B:4059:LEU:O	2:B:4063:ASP:N	2.50	0.44
2:E:876:GLU:O	2:E:880:GLU:N	2.48	0.44
2:E:3805:LEU:HA	2:E:3809:ASN:HD22	1.82	0.44
2:G:668:VAL:O	2:G:741:GLU:N	2.49	0.44
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.83	0.44
2:G:4745:LEU:O	2:G:4749:GLU:N	2.43	0.44
2:I:840:VAL:HB	2:I:1199:VAL:HG12	1.99	0.44
2:I:1965:TYR:HE1	2:I:2027:ILE:HB	1.82	0.44
2:B:580:GLU:HG3	2:B:620:LEU:HD22	1.99	0.44
2:B:1497:UNK:HA	2:B:1535:UNK:HA	2.00	0.44
2:B:3361:UNK:O	2:B:3365:UNK:N	2.50	0.44
2:E:38:ALA:HB1	2:E:64:ILE:HG13	1.99	0.44
2:E:668:VAL:O	2:E:741:GLU:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4044:MET:HA	2:E:4047:MET:HG2	1.98	0.44
2:G:533:ASN:HB3	2:G:536:ASN:HB2	2.00	0.44
2:G:838:HIS:CE1	2:G:1201:HIS:HD2	2.35	0.44
2:G:3361:UNK:O	2:G:3365:UNK:N	2.51	0.44
2:I:983:THR:O	2:I:987:ARG:N	2.48	0.44
2:I:1232:ARG:HD3	2:I:1702:HIS:HB3	2.00	0.44
2:B:283:ARG:HH21	2:B:402:ARG:HH12	1.65	0.44
2:B:840:VAL:HB	2:B:1199:VAL:HG12	1.99	0.44
2:B:1661:ARG:O	2:B:1664:SER:OG	2.32	0.44
2:B:3713:LYS:HG2	2:B:3715:LYS:H	1.83	0.44
2:B:4169:SER:HA	2:B:4172:GLU:HB3	1.99	0.44
2:B:4968:PHE:HE1	2:B:5029:ARG:HD3	1.83	0.44
2:E:385:ASP:OD1	2:E:385:ASP:N	2.48	0.44
2:E:1676:LEU:HD22	2:E:2167:ILE:HG13	2.00	0.44
2:E:1779:PRO:HG2	1:F:44:LYS:HE3	2.00	0.44
2:G:2869:ARG:HA	2:G:2872:GLN:HB3	1.98	0.44
2:I:281:ARG:HA	2:I:312:THR:HG21	2.00	0.44
2:I:463:GLU:OE2	2:I:467:LYS:NZ	2.51	0.44
2:I:596:ASN:HB3	2:I:599:VAL:HG22	2.00	0.44
2:I:1676:LEU:HD22	2:I:2167:ILE:HG13	2.00	0.44
2:I:2142:TYR:CG	2:I:2197:LEU:HD13	2.53	0.44
2:B:635:THR:HB	2:B:1639:LEU:HD23	2.00	0.43
2:B:2142:TYR:CG	2:B:2197:LEU:HD13	2.53	0.43
2:E:177:GLU:HG3	2:G:2452:ARG:HH12	1.83	0.43
2:E:1577:ALA:HB1	2:E:1584:ARG:HA	2.00	0.43
2:E:4215:ARG:HA	2:E:4218:ILE:HD12	2.00	0.43
2:E:4942:GLU:O	2:E:4946:GLN:N	2.43	0.43
2:G:1232:ARG:HD3	2:G:1702:HIS:HB3	1.99	0.43
2:G:1286:UNK:HA	2:G:1461:UNK:HA	1.99	0.43
2:I:702:TRP:O	2:I:705:ASN:ND2	2.46	0.43
2:I:4139:ILE:HA	2:I:4142:ASN:HD22	1.82	0.43
2:B:213:TYR:CG	2:B:337:PRO:HB2	2.53	0.43
2:B:1294:UNK:HA	2:B:1455:UNK:HA	1.98	0.43
2:E:4568:PHE:HA	2:E:4571:PHE:HD2	1.83	0.43
2:G:113:HIS:CE1	2:G:399:GLN:HA	2.53	0.43
2:G:1577:ALA:HB1	2:G:1584:ARG:HA	2.01	0.43
2:I:655:GLY:HA2	2:I:1002:ALA:HB2	2.01	0.43
2:I:4989:MET:HE2	2:I:4989:MET:HB3	1.91	0.43
2:B:1738:LEU:H	2:B:2146:PRO:HD3	1.83	0.43
2:B:4918:ILE:HD13	2:E:4892:ARG:HD3	2.01	0.43
2:E:463:GLU:OE2	2:E:467:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ALA:HB1	2:G:64:ILE:HG13	1.99	0.43
2:G:530:ILE:HA	2:G:536:ASN:HB3	2.00	0.43
2:G:914:PRO:O	2:G:918:ARG:N	2.46	0.43
2:G:3731:LYS:O	2:G:3735:LEU:N	2.50	0.43
2:I:113:HIS:CE1	2:I:399:GLN:HA	2.53	0.43
2:I:261:ARG:N	2:I:283:ARG:O	2.44	0.43
2:I:360:ALA:N	2:I:375:LYS:O	2.50	0.43
2:I:4059:LEU:O	2:I:4063:ASP:N	2.51	0.43
1:J:2:VAL:HG21	1:J:61:GLU:HB2	2.00	0.43
2:B:655:GLY:HA2	2:B:1002:ALA:HB2	2.01	0.43
2:B:831:ARG:HH21	2:B:840:VAL:HG11	1.84	0.43
2:B:3953:LYS:O	2:B:3956:SER:OG	2.29	0.43
2:B:4558:ASN:HB2	2:B:4561:THR:HB	1.99	0.43
2:B:4568:PHE:HA	2:B:4571:PHE:HD2	1.83	0.43
2:E:113:HIS:CE1	2:E:399:GLN:HA	2.53	0.43
2:E:3731:LYS:O	2:E:3735:LEU:N	2.50	0.43
2:E:4651:THR:HA	2:E:4799:SER:HB3	2.00	0.43
2:G:215:THR:HG22	2:G:273:HIS:HA	2.00	0.43
2:G:2142:TYR:CG	2:G:2197:LEU:HD13	2.53	0.43
2:G:4139:ILE:HA	2:G:4142:ASN:HD22	1.82	0.43
2:I:213:TYR:CG	2:I:337:PRO:HB2	2.53	0.43
2:I:658:GLN:O	2:I:662:TRP:NE1	2.51	0.43
2:I:1738:LEU:H	2:I:2146:PRO:HD3	1.83	0.43
2:B:596:ASN:HB3	2:B:599:VAL:HG22	2.00	0.43
2:B:733:PRO:HD2	2:B:763:PRO:HD2	2.00	0.43
2:B:1516:UNK:N	2:B:1529:UNK:O	2.51	0.43
2:B:3674:ILE:HD11	2:B:3728:ILE:HG22	2.01	0.43
2:E:281:ARG:HA	2:E:312:THR:HG21	2.00	0.43
2:E:978:THR:HB	2:E:980:ALA:H	1.83	0.43
2:E:1232:ARG:HD3	2:E:1702:HIS:HB3	1.99	0.43
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.83	0.43
2:G:264:PRO:HG2	2:G:270:SER:HB2	1.99	0.43
2:G:1738:LEU:H	2:G:2146:PRO:HD3	1.83	0.43
2:G:2869:ARG:HH12	2:G:2945:UNK:C	2.32	0.43
2:G:2880:GLU:O	2:G:2884:ASN:N	2.45	0.43
2:I:215:THR:HG22	2:I:273:HIS:HA	2.01	0.43
2:I:317:ARG:N	2:I:347:PHE:O	2.50	0.43
2:B:1232:ARG:HD3	2:B:1702:HIS:HB3	1.99	0.43
2:B:1577:ALA:HB1	2:B:1584:ARG:HA	2.01	0.43
2:B:4215:ARG:HA	2:B:4218:ILE:HD12	2.00	0.43
2:E:264:PRO:HG2	2:E:270:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:635:THR:O	1:F:34:LYS:NZ	2.49	0.43
2:E:2286:LEU:HA	2:E:2289:ALA:HB3	2.01	0.43
2:E:4918:ILE:HD11	2:G:4888:TYR:HA	2.01	0.43
2:G:379:HIS:CD2	2:G:381:GLU:H	2.37	0.43
2:G:596:ASN:HB3	2:G:599:VAL:HG22	2.00	0.43
2:G:2155:LEU:HD23	2:G:2185:ILE:HG22	2.01	0.43
2:G:2286:LEU:HA	2:G:2289:ALA:HB3	2.01	0.43
2:G:3674:ILE:HD11	2:G:3728:ILE:HG22	2.01	0.43
2:I:545:ASP:HA	2:I:582:HIS:CE1	2.54	0.43
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.01	0.43
2:I:3713:LYS:HG2	2:I:3715:LYS:H	1.83	0.43
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.83	0.43
2:I:4169:SER:HA	2:I:4172:GLU:HB3	1.99	0.43
1:J:7:ILE:N	1:J:71:ARG:O	2.47	0.43
2:B:342:GLY:HA2	2:B:389:PHE:HD2	1.83	0.43
2:B:463:GLU:OE2	2:B:467:LYS:NZ	2.51	0.43
2:B:614:VAL:HG22	2:B:616:SER:H	1.84	0.43
2:B:1229:ASN:HB3	2:B:1826:ALA:HA	2.01	0.43
2:E:215:THR:HG22	2:E:273:HIS:HA	2.01	0.43
2:E:360:ALA:N	2:E:375:LYS:O	2.50	0.43
2:E:2155:LEU:HD23	2:E:2185:ILE:HG22	2.01	0.43
2:E:3676:ASP:OD1	2:E:3676:ASP:N	2.49	0.43
2:G:213:TYR:CG	2:G:337:PRO:HB2	2.53	0.43
2:G:313:SER:HB3	2:G:352:ALA:H	1.84	0.43
2:G:2185:ILE:HA	2:G:2188:ASN:HD21	1.84	0.43
2:G:3953:LYS:O	2:G:3956:SER:OG	2.29	0.43
2:G:4791:TYR:HD2	2:G:4792:LEU:HD22	1.84	0.43
2:G:4895:GLY:O	2:I:4892:ARG:NH2	2.50	0.43
2:I:38:ALA:HB1	2:I:64:ILE:HG13	1.99	0.43
2:I:831:ARG:HH21	2:I:840:VAL:HG11	1.84	0.43
2:I:3674:ILE:HD11	2:I:3728:ILE:HG22	2.01	0.43
2:B:2286:LEU:HA	2:B:2289:ALA:HB3	2.01	0.43
2:E:283:ARG:HH21	2:E:402:ARG:HH12	1.66	0.43
2:E:655:GLY:HA2	2:E:1002:ALA:HB2	2.01	0.43
2:G:772:ASN:ND2	2:G:774:ASP:OD2	2.50	0.43
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.00	0.43
2:G:5026:ASP:OD1	2:G:5027:CYS:N	2.52	0.43
2:I:530:ILE:HA	2:I:536:ASN:HB3	2.00	0.43
2:I:809:ALA:O	2:I:811:CYS:N	2.47	0.43
2:I:1229:ASN:HB3	2:I:1826:ALA:HA	2.01	0.43
2:I:1649:ASP:OD1	2:I:1650:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3974:THR:HA	2:I:3977:GLN:HB2	1.99	0.43
2:B:38:ALA:HB1	2:B:64:ILE:HG13	1.99	0.43
2:B:313:SER:HB3	2:B:352:ALA:H	1.84	0.43
2:B:530:ILE:HA	2:B:536:ASN:HB3	2.00	0.43
2:B:5026:ASP:OD1	2:B:5027:CYS:N	2.52	0.43
2:E:213:TYR:CG	2:E:337:PRO:HB2	2.53	0.43
2:E:313:SER:HB3	2:E:352:ALA:H	1.84	0.43
2:E:342:GLY:HA2	2:E:389:PHE:HD2	1.83	0.43
2:E:703:GLY:H	2:E:1647:CYS:HB3	1.84	0.43
2:E:3674:ILE:HD11	2:E:3728:ILE:HG22	2.01	0.43
2:E:4558:ASN:HB2	2:E:4561:THR:HB	2.00	0.43
2:G:342:GLY:HA2	2:G:389:PHE:HD2	1.83	0.43
2:G:635:THR:HB	2:G:1639:LEU:HD23	2.00	0.43
2:G:831:ARG:HH21	2:G:840:VAL:HG11	1.84	0.43
2:G:3713:LYS:HG2	2:G:3715:LYS:H	1.83	0.43
1:H:16:PRO:HD2	1:H:64:ALA:HA	2.01	0.43
2:I:1152:MET:HB2	2:I:1161:ILE:HB	2.01	0.43
2:I:1229:ASN:O	2:I:1827:ARG:N	2.42	0.43
2:I:1577:ALA:HB1	2:I:1584:ARG:HA	2.01	0.43
2:I:2286:LEU:HA	2:I:2289:ALA:HB3	2.01	0.43
1:J:16:PRO:HD2	1:J:64:ALA:HA	2.00	0.43
2:B:113:HIS:CE1	2:B:399:GLN:HA	2.53	0.43
2:B:281:ARG:HA	2:B:312:THR:HG21	2.00	0.43
2:B:978:THR:HB	2:B:980:ALA:H	1.83	0.43
2:B:2185:ILE:HA	2:B:2188:ASN:HD21	1.84	0.43
2:B:3974:THR:HA	2:B:3977:GLN:HB2	1.99	0.43
2:E:530:ILE:HA	2:E:536:ASN:HB3	1.99	0.43
2:E:580:GLU:HG3	2:E:620:LEU:HD22	1.99	0.43
2:E:635:THR:HB	2:E:1639:LEU:HD23	2.01	0.43
2:E:1738:LEU:H	2:E:2146:PRO:HD3	1.83	0.43
2:E:1931:LEU:HD22	2:E:1935:VAL:HG11	2.00	0.43
2:E:2880:GLU:O	2:E:2884:ASN:N	2.45	0.43
2:E:3805:LEU:H	2:E:3805:LEU:HG	1.61	0.43
2:E:4990:PHE:O	2:E:4994:TYR:N	2.48	0.43
2:E:4995:LEU:HA	2:E:4995:LEU:HD22	1.81	0.43
2:G:1676:LEU:HD22	2:G:2167:ILE:HG13	2.00	0.43
2:G:2006:ILE:O	2:G:2010:LEU:N	2.45	0.43
2:G:4651:THR:HA	2:G:4799:SER:HB3	2.00	0.43
2:G:4670:ILE:O	2:G:4674:GLU:N	2.44	0.43
1:H:2:VAL:HG21	1:H:61:GLU:HB2	2.00	0.43
2:I:313:SER:HB3	2:I:352:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1516:UNK:N	2:I:1529:UNK:O	2.52	0.43
2:I:3731:LYS:O	2:I:3735:LEU:N	2.50	0.43
2:I:3825:GLU:OE1	2:I:3825:GLU:N	2.52	0.43
2:I:4990:PHE:O	2:I:4994:TYR:N	2.48	0.43
1:J:26:TYR:OH	1:J:42:ARG:NH2	2.39	0.43
2:B:404:ILE:HG21	2:B:481:GLU:HG3	2.01	0.42
2:E:545:ASP:HA	2:E:582:HIS:CE1	2.54	0.42
2:E:614:VAL:HG22	2:E:616:SER:H	1.84	0.42
2:E:831:ARG:HH21	2:E:840:VAL:HG11	1.84	0.42
2:E:1649:ASP:OD1	2:E:1650:ILE:N	2.52	0.42
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.01	0.42
2:E:3649:ALA:O	2:E:3653:PHE:N	2.48	0.42
1:F:83:GLY:O	1:F:94:ASN:N	2.52	0.42
2:G:283:ARG:HH21	2:G:402:ARG:HH12	1.65	0.42
2:G:545:ASP:HA	2:G:582:HIS:CE1	2.54	0.42
2:G:4215:ARG:HA	2:G:4218:ILE:HD12	2.00	0.42
2:I:342:GLY:HA2	2:I:389:PHE:HD2	1.83	0.42
2:I:703:GLY:H	2:I:1647:CYS:HB3	1.84	0.42
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.01	0.42
2:E:345:LEU:HD23	2:E:389:PHE:HB3	2.01	0.42
2:G:463:GLU:OE2	2:G:467:LYS:NZ	2.51	0.42
2:G:655:GLY:HA2	2:G:1002:ALA:HB2	2.01	0.42
2:G:733:PRO:HD2	2:G:763:PRO:HD2	2.00	0.42
2:I:379:HIS:CD2	2:I:381:GLU:H	2.37	0.42
2:I:404:ILE:HG21	2:I:481:GLU:HG3	2.01	0.42
2:I:947:GLU:HG3	2:I:1049:TYR:HD1	1.84	0.42
2:I:3361:UNK:O	2:I:3365:UNK:N	2.52	0.42
2:I:5026:ASP:OD1	2:I:5027:CYS:N	2.52	0.42
2:B:215:THR:HG22	2:B:273:HIS:HA	2.01	0.42
2:B:545:ASP:HA	2:B:582:HIS:CE1	2.54	0.42
2:E:596:ASN:HB3	2:E:599:VAL:HG22	2.00	0.42
2:G:404:ILE:HG21	2:G:481:GLU:HG3	2.01	0.42
2:G:1931:LEU:HD22	2:G:1935:VAL:HG11	1.99	0.42
2:G:3880:PHE:O	2:G:3884:LEU:N	2.52	0.42
2:I:614:VAL:HG22	2:I:616:SER:H	1.84	0.42
2:I:772:ASN:ND2	2:I:774:ASP:OD2	2.50	0.42
2:I:2185:ILE:HA	2:I:2188:ASN:HD21	1.84	0.42
2:I:3229:UNK:HA	2:I:3302:UNK:HA	2.02	0.42
2:B:260:TRP:CE2	2:B:284:HIS:HD2	2.38	0.42
2:B:533:ASN:HB3	2:B:536:ASN:HB2	2.00	0.42
2:B:703:GLY:H	2:B:1647:CYS:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:947:GLU:HG3	2:B:1049:TYR:HD1	1.85	0.42
2:B:1152:MET:HB2	2:B:1161:ILE:HB	2.01	0.42
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.83	0.42
2:B:3825:GLU:OE1	2:B:3825:GLU:N	2.52	0.42
2:E:404:ILE:HG21	2:E:481:GLU:HG3	2.01	0.42
2:E:733:PRO:HD2	2:E:763:PRO:HD2	2.00	0.42
2:E:3880:PHE:O	2:E:3884:LEU:N	2.52	0.42
2:E:4670:ILE:O	2:E:4674:GLU:N	2.44	0.42
2:E:4791:TYR:HD2	2:E:4792:LEU:HD22	1.84	0.42
2:G:703:GLY:H	2:G:1647:CYS:HB3	1.84	0.42
2:G:1649:ASP:OD1	2:G:1650:ILE:N	2.52	0.42
2:G:2212:VAL:O	2:G:2216:GLY:N	2.46	0.42
2:I:16:THR:OG1	2:I:97:GLY:O	2.35	0.42
2:I:533:ASN:HB3	2:I:536:ASN:HB2	2.00	0.42
2:I:733:PRO:HD2	2:I:763:PRO:HD2	2.00	0.42
2:I:870:ILE:HD12	2:I:870:ILE:HA	1.87	0.42
2:I:4651:THR:HA	2:I:4799:SER:HB3	2.00	0.42
2:I:4791:TYR:HD2	2:I:4792:LEU:HD22	1.84	0.42
1:A:2:VAL:HG21	1:A:61:GLU:HB2	2.00	0.42
2:B:1649:ASP:OD1	2:B:1650:ILE:N	2.52	0.42
2:B:2144:ILE:H	2:B:2144:ILE:HG13	1.72	0.42
2:B:2155:LEU:HD23	2:B:2185:ILE:HG22	2.01	0.42
2:B:3880:PHE:O	2:B:3884:LEU:N	2.52	0.42
2:E:119:SER:HA	2:E:146:CYS:HA	2.01	0.42
2:E:379:HIS:CD2	2:E:381:GLU:H	2.37	0.42
2:E:3825:GLU:OE1	2:E:3825:GLU:N	2.52	0.42
1:F:2:VAL:HG21	1:F:61:GLU:HB2	2.00	0.42
1:F:55:VAL:HG23	1:F:60:GLU:HB2	2.02	0.42
2:G:614:VAL:HG22	2:G:616:SER:H	1.84	0.42
2:G:1771:LEU:HD11	2:G:2149:VAL:HB	2.01	0.42
2:I:260:TRP:CE2	2:I:284:HIS:HD2	2.38	0.42
2:I:873:LYS:HB3	2:I:1049:TYR:CZ	2.55	0.42
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.02	0.42
2:I:2155:LEU:HD23	2:I:2185:ILE:HG22	2.01	0.42
1:A:16:PRO:HD2	1:A:64:ALA:HA	2.00	0.42
2:B:1676:LEU:HD22	2:B:2167:ILE:HG13	2.00	0.42
2:B:4651:THR:HA	2:B:4799:SER:HB3	2.00	0.42
2:E:273:HIS:CE1	2:E:337:PRO:HB3	2.55	0.42
1:F:16:PRO:HD2	1:F:64:ALA:HA	2.00	0.42
2:G:3663:LEU:H	2:G:3663:LEU:HG	1.64	0.42
2:I:345:LEU:HD23	2:I:389:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1771:LEU:HD11	2:I:2149:VAL:HB	2.01	0.42
2:I:4960:ILE:HD12	2:I:4983:HIS:HB3	2.02	0.42
2:B:119:SER:HA	2:B:146:CYS:HA	2.01	0.42
2:B:345:LEU:HD23	2:B:389:PHE:HB3	2.01	0.42
2:B:3770:LEU:HD22	2:B:3804:ILE:HD11	2.01	0.42
2:B:4960:ILE:HD12	2:B:4983:HIS:HB3	2.02	0.42
2:E:790:ARG:HG2	2:E:1627:ALA:HA	2.02	0.42
2:E:1229:ASN:HB3	2:E:1826:ALA:HA	2.01	0.42
2:E:2185:ILE:HA	2:E:2188:ASN:HD21	1.84	0.42
2:E:3713:LYS:HG2	2:E:3715:LYS:H	1.83	0.42
2:G:345:LEU:HD23	2:G:389:PHE:HB3	2.01	0.42
2:G:1152:MET:HB2	2:G:1161:ILE:HB	2.01	0.42
1:H:7:ILE:N	1:H:71:ARG:O	2.47	0.42
1:H:83:GLY:O	1:H:94:ASN:N	2.52	0.42
2:I:4215:ARG:HA	2:I:4218:ILE:HD12	2.00	0.42
1:A:55:VAL:HG23	1:A:60:GLU:HB2	2.02	0.42
2:B:273:HIS:CE1	2:B:337:PRO:HB3	2.55	0.42
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.87	0.42
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.02	0.42
2:E:260:TRP:CE2	2:E:284:HIS:HD2	2.38	0.42
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.02	0.42
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.02	0.42
2:G:1229:ASN:HB3	2:G:1826:ALA:HA	2.01	0.42
2:G:3770:LEU:HD22	2:G:3804:ILE:HD11	2.01	0.42
2:G:3825:GLU:OE1	2:G:3825:GLU:N	2.52	0.42
2:G:4692:PRO:HG2	2:G:4703:ARG:HH21	1.84	0.42
2:G:4852:THR:HG21	2:G:4883:TYR:HB2	2.02	0.42
2:I:102:LEU:HB3	2:I:160:GLY:HA2	2.02	0.42
2:I:241:GLN:O	2:I:289:ARG:NH1	2.42	0.42
2:B:379:HIS:CD2	2:B:381:GLU:H	2.37	0.42
2:B:1771:LEU:HD11	2:B:2149:VAL:HB	2.02	0.42
2:B:1976:ARG:NH1	2:B:1997:GLU:OE2	2.35	0.42
2:B:3963:ASN:O	2:B:3966:THR:OG1	2.29	0.42
2:E:533:ASN:HB3	2:E:536:ASN:HB2	2.00	0.42
2:E:1152:MET:HB2	2:E:1161:ILE:HB	2.01	0.42
2:E:1936:LYS:O	2:E:1940:CYS:N	2.48	0.42
2:E:4736:ARG:O	2:E:4740:LEU:N	2.53	0.42
2:E:4960:ILE:HD12	2:E:4983:HIS:HB3	2.02	0.42
2:E:5026:ASP:OD1	2:E:5027:CYS:N	2.52	0.42
2:G:349:GLN:HE21	2:G:354:GLY:HA2	1.85	0.42
2:G:873:LYS:HB3	2:G:1049:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1936:LYS:O	2:G:1940:CYS:N	2.48	0.42
2:G:4736:ARG:O	2:G:4740:LEU:N	2.53	0.42
2:B:3716:LEU:HD22	2:B:3785:ALA:HB1	2.02	0.42
2:B:3927:GLN:NE2	2:B:3988:ALA:O	2.46	0.42
2:B:4791:TYR:HD2	2:B:4792:LEU:HD22	1.84	0.42
2:E:488:LEU:HA	2:E:491:ILE:HB	2.02	0.42
2:E:947:GLU:HG3	2:E:1049:TYR:HD1	1.84	0.42
2:G:35:LEU:HD13	2:G:49:LEU:HD13	2.02	0.42
2:G:131:LEU:HD22	2:G:178:ARG:NH1	2.35	0.42
2:G:4859:PHE:HA	2:G:4862:PHE:CE2	2.47	0.42
2:G:4956:THR:O	2:G:4965:SER:N	2.52	0.42
2:I:273:HIS:CE1	2:I:337:PRO:HB3	2.55	0.42
2:I:349:GLN:HE21	2:I:354:GLY:HA2	1.84	0.42
1:A:83:GLY:O	1:A:94:ASN:N	2.52	0.41
2:B:35:LEU:HD13	2:B:49:LEU:HD13	2.02	0.41
2:B:102:LEU:HB3	2:B:160:GLY:HA2	2.02	0.41
2:B:110:ARG:NH2	2:B:115:ARG:HB3	2.35	0.41
2:B:873:LYS:HB3	2:B:1049:TYR:CZ	2.55	0.41
2:B:946:ALA:HA	2:B:949:ASN:HB2	2.02	0.41
2:B:1256:GLU:HG2	2:B:1273:ALA:HB3	2.02	0.41
2:B:3766:GLN:O	2:B:3770:LEU:N	2.50	0.41
2:B:3773:ARG:HG2	2:B:3815:LYS:HD3	2.03	0.41
2:B:4167:ALA:HA	2:B:4170:ILE:HD12	2.02	0.41
2:E:261:ARG:N	2:E:283:ARG:O	2.44	0.41
2:E:658:GLN:O	2:E:662:TRP:NE1	2.51	0.41
2:E:3716:LEU:HD22	2:E:3785:ALA:HB1	2.02	0.41
2:E:3770:LEU:HD22	2:E:3804:ILE:HD11	2.01	0.41
2:E:4167:ALA:HA	2:E:4170:ILE:HD12	2.02	0.41
2:E:4208:PRO:HA	2:E:4211:LYS:HB3	2.02	0.41
2:G:260:TRP:CE2	2:G:284:HIS:HD2	2.38	0.41
2:G:273:HIS:CE1	2:G:337:PRO:HB3	2.55	0.41
2:G:488:LEU:HA	2:G:491:ILE:HB	2.02	0.41
2:G:947:GLU:HG3	2:G:1049:TYR:HD1	1.84	0.41
2:G:1661:ARG:O	2:G:1664:SER:OG	2.32	0.41
2:G:2430:ILE:HG21	2:G:2502:UNK:HA	2.02	0.41
2:G:4960:ILE:HD12	2:G:4983:HIS:HB3	2.02	0.41
2:I:110:ARG:NH2	2:I:115:ARG:HB3	2.35	0.41
2:I:978:THR:HB	2:I:980:ALA:H	1.83	0.41
2:I:3880:PHE:O	2:I:3884:LEU:N	2.52	0.41
1:J:83:GLY:O	1:J:94:ASN:N	2.52	0.41
1:A:34:LYS:NZ	2:B:634:GLN:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.89	0.41
2:B:1268:PRO:HB2	2:B:1591:CYS:HB2	2.03	0.41
2:E:639:ASN:HD22	2:E:1635:THR:HA	1.85	0.41
2:E:873:LYS:HB3	2:E:1049:TYR:CZ	2.55	0.41
2:E:1771:LEU:HD11	2:E:2149:VAL:HB	2.02	0.41
2:E:3901:ASN:OD1	2:E:3904:ARG:NH1	2.49	0.41
2:I:488:LEU:HA	2:I:491:ILE:HB	2.02	0.41
2:I:639:ASN:HD22	2:I:1635:THR:HA	1.85	0.41
2:I:1679:ASN:O	2:I:1683:HIS:ND1	2.36	0.41
2:I:3770:LEU:HD22	2:I:3804:ILE:HD11	2.01	0.41
2:I:4692:PRO:HG2	2:I:4703:ARG:HH21	1.84	0.41
2:I:4852:THR:HG21	2:I:4883:TYR:HB2	2.02	0.41
2:B:1041:GLN:O	2:B:1045:THR:OG1	2.30	0.41
2:E:131:LEU:HB3	2:G:2459:SER:HB2	2.01	0.41
2:E:3963:ASN:O	2:E:3966:THR:OG1	2.29	0.41
2:G:639:ASN:HD22	2:G:1635:THR:HA	1.85	0.41
2:G:658:GLN:O	2:G:662:TRP:NE1	2.51	0.41
2:G:3646:THR:O	2:G:3650:CYS:N	2.51	0.41
2:G:3716:LEU:HD22	2:G:3785:ALA:HB1	2.02	0.41
2:G:3756:LYS:O	2:G:3760:LYS:NZ	2.37	0.41
2:G:4208:PRO:HA	2:G:4211:LYS:HB3	2.02	0.41
2:I:635:THR:HB	2:I:1639:LEU:HD23	2.00	0.41
2:I:1076:ARG:HD3	2:I:1237:TRP:HB2	2.02	0.41
2:I:1268:PRO:HB2	2:I:1591:CYS:HB2	2.03	0.41
2:I:2862:LEU:HB3	2:I:2928:LYS:HB3	2.02	0.41
2:I:3964:SER:HG	2:I:3968:TYR:HH	1.67	0.41
1:J:55:VAL:HG23	1:J:60:GLU:HB2	2.02	0.41
1:A:26:TYR:OH	1:A:42:ARG:NH2	2.39	0.41
2:B:728:ARG:NH2	2:B:1527:UNK:O	2.53	0.41
2:B:3915:ILE:H	2:B:3915:ILE:HG13	1.63	0.41
2:B:4692:PRO:HG2	2:B:4703:ARG:HH21	1.84	0.41
2:B:4736:ARG:O	2:B:4740:LEU:N	2.53	0.41
2:B:4801:LEU:HB3	2:B:4808:PHE:CG	2.56	0.41
2:E:78:LEU:O	2:E:82:LEU:N	2.44	0.41
2:E:241:GLN:O	2:E:289:ARG:NH1	2.42	0.41
2:G:790:ARG:HG2	2:G:1627:ALA:HA	2.02	0.41
2:G:2265:LEU:HD21	2:G:2273:LEU:HD13	2.02	0.41
2:G:3927:GLN:NE2	2:G:3988:ALA:O	2.46	0.41
2:I:1256:GLU:HG2	2:I:1273:ALA:HB3	2.02	0.41
2:B:131:LEU:HD22	2:B:178:ARG:NH1	2.35	0.41
2:B:639:ASN:HD22	2:B:1635:THR:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:790:ARG:HG2	2:B:1627:ALA:HA	2.02	0.41
2:B:4195:PHE:HZ	2:B:4987:ASN:HB3	1.86	0.41
2:E:35:LEU:HD13	2:E:49:LEU:HD13	2.02	0.41
2:E:1076:ARG:HD3	2:E:1237:TRP:HB2	2.02	0.41
2:E:3645:PRO:O	2:E:3649:ALA:N	2.53	0.41
2:E:4692:PRO:HG2	2:E:4703:ARG:HH21	1.84	0.41
2:E:4801:LEU:HB3	2:E:4808:PHE:CG	2.56	0.41
2:G:119:SER:HA	2:G:146:CYS:HA	2.01	0.41
2:G:3229:UNK:HA	2:G:3302:UNK:HA	2.02	0.41
1:H:55:VAL:HG23	1:H:60:GLU:HB2	2.02	0.41
2:I:914:PRO:O	2:I:918:ARG:N	2.46	0.41
2:I:3773:ARG:HG2	2:I:3815:LYS:HD3	2.02	0.41
2:B:349:GLN:HE21	2:B:354:GLY:HA2	1.85	0.41
2:B:4707:ASN:OD1	2:B:4742:GLY:N	2.49	0.41
2:B:4822:THR:O	2:B:4825:THR:OG1	2.30	0.41
2:B:4957:LYS:HE3	2:B:4957:LYS:HB3	1.83	0.41
2:E:131:LEU:HD22	2:E:178:ARG:NH1	2.35	0.41
2:E:1497:UNK:HA	2:E:1535:UNK:HA	2.02	0.41
2:G:110:ARG:NH2	2:G:115:ARG:HB3	2.35	0.41
2:G:1256:GLU:HG2	2:G:1273:ALA:HB3	2.02	0.41
2:G:2862:LEU:HB3	2:G:2928:LYS:HB3	2.02	0.41
2:G:2908:TYR:OH	2:G:2920:ARG:NE	2.44	0.41
2:I:876:GLU:O	2:I:880:GLU:N	2.48	0.41
2:B:1088:TRP:HB2	2:B:1153:ILE:HG22	2.03	0.41
2:B:3649:ALA:O	2:B:3653:PHE:N	2.48	0.41
2:E:110:ARG:NH2	2:E:115:ARG:HB3	2.35	0.41
2:E:1116:GLY:HA3	2:E:1123:VAL:HG12	2.02	0.41
2:E:1270:LEU:HD11	2:E:1595:LEU:HB3	2.03	0.41
2:G:16:THR:OG1	2:G:97:GLY:O	2.35	0.41
2:G:946:ALA:HA	2:G:949:ASN:HB2	2.02	0.41
2:G:4990:PHE:O	2:G:4994:TYR:N	2.48	0.41
2:B:805:PRO:HA	2:B:806:PRO:HD3	1.95	0.41
2:B:1808:ARG:HD3	2:B:1853:ILE:HG22	2.03	0.41
2:E:34:LYS:N	2:E:53:SER:OG	2.43	0.41
2:E:308:HIS:CE1	2:E:310:LYS:HB2	2.56	0.41
2:E:349:GLN:HE21	2:E:354:GLY:HA2	1.85	0.41
2:E:2144:ILE:H	2:E:2144:ILE:HG13	1.72	0.41
2:E:3773:ARG:HG2	2:E:3815:LYS:HD3	2.03	0.41
2:E:4195:PHE:HZ	2:E:4987:ASN:HB3	1.86	0.41
2:E:4847:VAL:HG11	2:E:4924:VAL:HG11	2.03	0.41
2:G:102:LEU:HB3	2:G:160:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:805:PRO:HA	2:G:806:PRO:HD3	1.94	0.41
2:G:1088:TRP:HB2	2:G:1153:ILE:HG22	2.03	0.41
2:G:1808:ARG:HD3	2:G:1853:ILE:HG22	2.03	0.41
2:G:3921:ASP:HA	2:G:3924:LEU:HB3	2.03	0.41
2:G:4847:VAL:HG11	2:G:4924:VAL:HG11	2.03	0.41
2:I:119:SER:HA	2:I:146:CYS:HA	2.01	0.41
2:I:3915:ILE:H	2:I:3915:ILE:HG13	1.63	0.41
2:I:4049:VAL:HG21	2:I:4159:ARG:HD2	2.03	0.41
2:B:17:ASP:HB2	2:B:98:HIS:CE1	2.55	0.41
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.02	0.41
2:B:1116:GLY:HA3	2:B:1123:VAL:HG12	2.02	0.41
2:B:2121:PHE:O	2:B:3725:TYR:OH	2.39	0.41
2:B:2265:LEU:HD21	2:B:2273:LEU:HD13	2.02	0.41
2:B:2342:ASN:OD1	2:B:2342:ASN:N	2.54	0.41
2:B:3153:UNK:O	2:B:3157:UNK:N	2.54	0.41
2:B:3921:ASP:HA	2:B:3924:LEU:HB3	2.03	0.41
2:B:4852:THR:HG21	2:B:4883:TYR:HB2	2.02	0.41
2:E:259:LEU:HA	2:E:259:LEU:HD23	1.87	0.41
2:E:913:LEU:O	2:E:918:ARG:NH2	2.54	0.41
2:E:1088:TRP:HB2	2:E:1153:ILE:HG22	2.03	0.41
2:E:2265:LEU:HD22	2:E:2330:ARG:HB3	2.03	0.41
2:E:3229:UNK:HA	2:E:3302:UNK:HA	2.02	0.41
2:E:3663:LEU:H	2:E:3663:LEU:HG	1.64	0.41
2:E:4958:CYS:SG	2:E:4959:PHE:N	2.94	0.41
2:G:259:LEU:HD23	2:G:259:LEU:HA	1.87	0.41
2:G:1076:ARG:HD3	2:G:1237:TRP:HB2	2.02	0.41
2:G:1116:GLY:HA3	2:G:1123:VAL:HG12	2.02	0.41
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	2.02	0.41
2:G:3773:ARG:HG2	2:G:3815:LYS:HD3	2.03	0.41
2:G:4049:VAL:HG21	2:G:4159:ARG:HD2	2.03	0.41
2:G:4957:LYS:HE3	2:G:4957:LYS:HB3	1.83	0.41
2:I:591:ASP:O	2:I:1594:ARG:NH2	2.54	0.41
2:I:728:ARG:NH2	2:I:1527:UNK:O	2.54	0.41
2:I:946:ALA:HA	2:I:949:ASN:HB2	2.02	0.41
2:I:1088:TRP:HB2	2:I:1153:ILE:HG22	2.03	0.41
2:I:1116:GLY:HA3	2:I:1123:VAL:HG12	2.02	0.41
2:I:1497:UNK:HA	2:I:1535:UNK:HA	2.02	0.41
2:I:2116:LEU:O	2:I:2120:MET:N	2.46	0.41
2:I:2121:PHE:O	2:I:3725:TYR:OH	2.39	0.41
2:I:2265:LEU:HD21	2:I:2273:LEU:HD13	2.02	0.41
2:I:2384:ILE:O	2:I:2388:GLU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3663:LEU:H	2:I:3663:LEU:HG	1.64	0.41
2:I:3716:LEU:HD22	2:I:3785:ALA:HB1	2.02	0.41
2:I:4167:ALA:HA	2:I:4170:ILE:HD12	2.02	0.41
2:I:4195:PHE:HZ	2:I:4987:ASN:HB3	1.86	0.41
2:I:4707:ASN:OD1	2:I:4742:GLY:N	2.49	0.41
2:I:4736:ARG:O	2:I:4740:LEU:N	2.53	0.41
2:I:4847:VAL:HG11	2:I:4924:VAL:HG11	2.03	0.41
2:I:4957:LYS:HB3	2:I:4957:LYS:HE3	1.83	0.41
2:I:5013:MET:HA	2:I:5016:GLU:HB3	2.03	0.41
2:B:308:HIS:CE1	2:B:310:LYS:HB2	2.56	0.41
2:B:1092:PHE:HE2	2:B:1094:ALA:HB2	1.85	0.41
2:B:1936:LYS:O	2:B:1940:CYS:N	2.48	0.41
2:B:2116:LEU:O	2:B:2120:MET:N	2.46	0.41
2:B:2517:UNK:O	2:B:2521:UNK:N	2.54	0.41
2:B:4191:GLU:OE1	2:B:5006:GLN:NE2	2.54	0.41
2:B:4208:PRO:HA	2:B:4211:LYS:HB3	2.03	0.41
2:B:4958:CYS:SG	2:B:4959:PHE:N	2.94	0.41
2:B:5013:MET:HA	2:B:5016:GLU:HB3	2.03	0.41
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.02	0.41
2:E:1256:GLU:HG2	2:E:1273:ALA:HB3	2.02	0.41
2:E:1808:ARG:HD3	2:E:1853:ILE:HG22	2.03	0.41
2:E:4191:GLU:OE1	2:E:5006:GLN:NE2	2.54	0.41
1:F:7:ILE:N	1:F:71:ARG:O	2.47	0.41
2:G:1270:LEU:HD11	2:G:1595:LEU:HB3	2.03	0.41
2:G:2342:ASN:OD1	2:G:2342:ASN:N	2.54	0.41
2:G:4191:GLU:OE1	2:G:5006:GLN:NE2	2.54	0.41
2:I:42:PHE:HD1	2:I:447:ASP:HB3	1.86	0.41
2:I:131:LEU:HD22	2:I:178:ARG:NH1	2.35	0.41
2:I:308:HIS:CE1	2:I:310:LYS:HB2	2.56	0.41
2:I:1808:ARG:HD3	2:I:1853:ILE:HG22	2.03	0.41
2:I:3362:UNK:O	2:I:3366:UNK:N	2.54	0.41
2:I:4191:GLU:OE1	2:I:5006:GLN:NE2	2.54	0.41
2:I:4204:GLN:NE2	2:I:4245:MET:SD	2.94	0.41
2:I:4569:LEU:HD11	2:I:4646:LEU:HD22	2.03	0.41
2:I:4801:LEU:HB3	2:I:4808:PHE:CG	2.56	0.41
2:B:488:LEU:HA	2:B:491:ILE:HB	2.02	0.40
2:B:4091:LYS:HD3	2:B:4091:LYS:HA	1.90	0.40
2:B:4581:LYS:HD2	2:B:4632:LEU:HD13	2.04	0.40
2:E:17:ASP:HB2	2:E:98:HIS:CE1	2.55	0.40
2:E:591:ASP:O	2:E:1594:ARG:NH2	2.54	0.40
2:E:3645:PRO:HB2	2:E:3648:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.56	0.40
2:E:3921:ASP:HA	2:E:3924:LEU:HB3	2.03	0.40
2:E:3953:LYS:O	2:E:3956:SER:OG	2.29	0.40
2:E:4138:ASP:O	2:E:4142:ASN:ND2	2.54	0.40
2:E:4852:THR:HG21	2:E:4883:TYR:HB2	2.02	0.40
2:G:414:PHE:HE1	2:G:436:LEU:HB3	1.86	0.40
2:G:4569:LEU:HD11	2:G:4646:LEU:HD22	2.03	0.40
2:I:35:LEU:HD13	2:I:49:LEU:HD13	2.02	0.40
2:I:4930:ALA:HA	2:I:4933:GLN:HB3	2.03	0.40
2:B:42:PHE:HD1	2:B:447:ASP:HB3	1.86	0.40
2:B:2006:ILE:O	2:B:2010:LEU:N	2.45	0.40
2:B:2196:ASN:OD1	2:B:2199:ARG:NH1	2.54	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:B:3645:PRO:HB2	2:B:3648:ARG:HB3	2.03	0.40
2:E:320:LYS:HG2	2:E:356:TRP:CD1	2.57	0.40
2:E:627:PRO:HB2	1:F:92:PRO:HD3	2.04	0.40
2:E:836:GLY:HA3	2:E:1201:HIS:ND1	2.37	0.40
2:E:1693:GLN:HA	2:E:1696:HIS:HB3	2.04	0.40
2:E:2255:SER:HA	2:E:2258:LEU:HB3	2.04	0.40
2:E:4837:LEU:HD11	2:E:4936:ILE:HD11	2.03	0.40
2:G:1092:PHE:HE2	2:G:1094:ALA:HB2	1.85	0.40
2:G:2121:PHE:O	2:G:3725:TYR:OH	2.39	0.40
2:G:3771:HIS:O	2:G:3774:GLY:N	2.52	0.40
2:I:790:ARG:HG2	2:I:1627:ALA:HA	2.02	0.40
2:I:2810:LYS:O	2:I:2814:LYS:N	2.52	0.40
2:B:414:PHE:HE1	2:B:436:LEU:HB3	1.86	0.40
2:B:591:ASP:O	2:B:1594:ARG:NH2	2.54	0.40
2:B:688:LEU:HB3	2:B:777:PHE:CE1	2.57	0.40
2:B:1270:LEU:HD11	2:B:1595:LEU:HB3	2.03	0.40
2:B:2265:LEU:HD22	2:B:2330:ARG:HB3	2.03	0.40
2:B:4847:VAL:HG11	2:B:4924:VAL:HG11	2.03	0.40
2:B:4875:LYS:HA	2:B:4881:THR:HG22	2.03	0.40
2:E:946:ALA:HA	2:E:949:ASN:HB2	2.02	0.40
2:E:1092:PHE:HE2	2:E:1094:ALA:HB2	1.85	0.40
2:E:2121:PHE:O	2:E:3725:TYR:OH	2.39	0.40
2:E:2318:TYR:HA	2:E:2319:PRO:HD3	1.88	0.40
2:E:3921:ASP:O	2:E:3925:ARG:N	2.51	0.40
2:E:4114:CYS:HB3	2:E:4131:ARG:HH22	1.86	0.40
2:G:149:THR:N	2:G:172:VAL:O	2.55	0.40
2:G:591:ASP:O	2:G:1594:ARG:NH2	2.54	0.40
2:G:913:LEU:O	2:G:918:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:2023:LEU:O	2:G:2025:GLU:N	2.54	0.40
2:G:2384:ILE:O	2:G:2388:GLU:N	2.54	0.40
2:G:2674:UNK:O	2:G:2676:UNK:N	2.55	0.40
2:G:4138:ASP:O	2:G:4142:ASN:ND2	2.55	0.40
2:G:4801:LEU:HB3	2:G:4808:PHE:CG	2.56	0.40
2:G:5013:MET:HA	2:G:5016:GLU:HB3	2.03	0.40
2:I:414:PHE:HE1	2:I:436:LEU:HB3	1.86	0.40
2:I:716:PHE:HE2	2:I:759:ILE:HD11	1.86	0.40
2:I:1092:PHE:HE2	2:I:1094:ALA:HB2	1.85	0.40
2:I:1270:LEU:HD11	2:I:1595:LEU:HB3	2.03	0.40
2:I:2265:LEU:HD22	2:I:2330:ARG:HB3	2.04	0.40
2:I:3766:GLN:O	2:I:3770:LEU:N	2.50	0.40
2:I:3832:ILE:O	2:I:3836:MET:N	2.45	0.40
2:I:3921:ASP:HA	2:I:3924:LEU:HB3	2.03	0.40
2:B:221:ARG:NH2	2:B:255:HIS:O	2.55	0.40
2:B:360:ALA:N	2:B:375:LYS:O	2.50	0.40
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	2.02	0.40
2:B:4850:LEU:HD22	2:E:4814:LEU:HD21	2.03	0.40
2:E:102:LEU:HB3	2:E:160:GLY:HA2	2.02	0.40
2:E:688:LEU:HB3	2:E:777:PHE:CE1	2.57	0.40
2:E:776:LEU:HG	2:E:848:HIS:HA	2.04	0.40
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.54	0.40
2:E:3363:UNK:O	2:E:3367:UNK:N	2.55	0.40
2:E:3915:ILE:H	2:E:3915:ILE:HG13	1.63	0.40
2:E:4956:THR:O	2:E:4965:SER:N	2.52	0.40
2:G:308:HIS:CE1	2:G:310:LYS:HB2	2.56	0.40
2:G:716:PHE:HE2	2:G:759:ILE:HD11	1.86	0.40
2:G:836:GLY:HA3	2:G:1201:HIS:ND1	2.37	0.40
2:G:1268:PRO:HB2	2:G:1591:CYS:HB2	2.03	0.40
2:G:1294:UNK:HA	2:G:1455:UNK:HA	2.03	0.40
2:G:4195:PHE:HZ	2:G:4987:ASN:HB3	1.86	0.40
2:G:4204:GLN:NE2	2:G:4245:MET:SD	2.94	0.40
2:I:913:LEU:O	2:I:918:ARG:NH2	2.54	0.40
2:I:2674:UNK:O	2:I:2676:UNK:N	2.55	0.40
2:I:4138:ASP:O	2:I:4142:ASN:ND2	2.55	0.40
2:I:4208:PRO:HA	2:I:4211:LYS:HB3	2.02	0.40
2:B:716:PHE:HE2	2:B:759:ILE:HD11	1.86	0.40
2:E:1268:PRO:HB2	2:E:1591:CYS:HB2	2.03	0.40
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	2.03	0.40
2:E:2265:LEU:HD21	2:E:2273:LEU:HD13	2.02	0.40
2:G:151:HIS:HB2	2:G:170:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:663:TYR:HB2	2:G:808:TYR:HB3	2.04	0.40
2:G:2196:ASN:OD1	2:G:2199:ARG:NH1	2.54	0.40
2:G:2255:SER:HA	2:G:2258:LEU:HB3	2.04	0.40
2:G:4167:ALA:HA	2:G:4170:ILE:HD12	2.02	0.40
2:I:4236:SER:O	2:I:4240:ASP:N	2.45	0.40
2:I:4978:HIS:O	2:I:4983:HIS:N	2.47	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	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	F	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	H	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
1	J	105/107 (98%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	47	81
2	E	3235/4687 (69%)	2849 (88%)	381 (12%)	5 (0%)	47	81
2	G	3235/4687 (69%)	2848 (88%)	382 (12%)	5 (0%)	47	81
2	I	3235/4687 (69%)	2850 (88%)	380 (12%)	5 (0%)	47	81
All	All	13360/19176 (70%)	11775 (88%)	1565 (12%)	20 (0%)	54	85

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	E	1708	ARG
2	G	1708	ARG
2	I	1708	ARG

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Mol	Chain	Res	Type
2	B	1932	PRO
2	E	1932	PRO
2	G	1932	PRO
2	I	1932	PRO
2	B	4667	PRO
2	E	4667	PRO
2	G	4667	PRO
2	I	4667	PRO
2	B	1840	PRO
2	E	1840	PRO
2	G	1840	PRO
2	I	1840	PRO
2	B	4641	PRO
2	E	4641	PRO
2	G	4641	PRO
2	I	4641	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	88/88 (100%)	88 (100%)	0	100 100
1	F	88/88 (100%)	88 (100%)	0	100 100
1	H	88/88 (100%)	88 (100%)	0	100 100
1	J	88/88 (100%)	88 (100%)	0	100 100
2	B	2493/3209 (78%)	2473 (99%)	20 (1%)	81 89
2	E	2493/3209 (78%)	2473 (99%)	20 (1%)	81 89
2	G	2493/3209 (78%)	2472 (99%)	21 (1%)	81 89
2	I	2493/3209 (78%)	2473 (99%)	20 (1%)	81 89
All	All	10324/13188 (78%)	10243 (99%)	81 (1%)	82 89

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	534	ARG
2	B	553	ARG
2	B	688	LEU
2	B	1076	ARG
2	B	1141	ARG
2	B	1964	ARG
2	B	3663	LEU
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	B	4137	ARG
2	B	4798	MET
2	B	4871	GLU
2	B	4913	ARG
2	B	4957	LYS
2	B	4984	ASN
2	B	4995	LEU
2	E	534	ARG
2	E	553	ARG
2	E	688	LEU
2	E	1076	ARG
2	E	1141	ARG
2	E	1964	ARG
2	E	3663	LEU
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	E	4137	ARG
2	E	4798	MET
2	E	4871	GLU
2	E	4913	ARG
2	E	4957	LYS
2	E	4984	ASN
2	E	4995	LEU
2	G	534	ARG
2	G	553	ARG
2	G	688	LEU

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Mol	Chain	Res	Type
2	G	978	THR
2	G	1076	ARG
2	G	1141	ARG
2	G	1964	ARG
2	G	3663	LEU
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4137	ARG
2	G	4798	MET
2	G	4871	GLU
2	G	4913	ARG
2	G	4957	LYS
2	G	4984	ASN
2	G	4995	LEU
2	I	534	ARG
2	I	553	ARG
2	I	688	LEU
2	I	1076	ARG
2	I	1141	ARG
2	I	1964	ARG
2	I	3663	LEU
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	I	4137	ARG
2	I	4798	MET
2	I	4871	GLU
2	I	4913	ARG
2	I	4957	LYS
2	I	4984	ASN
2	I	4995	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (164) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
2	B	57	ASN
2	B	111	HIS
2	B	151	HIS
2	B	218	HIS
2	B	224	HIS
2	B	273	HIS
2	B	308	HIS
2	B	379	HIS
2	B	383	HIS
2	B	395	GLN
2	B	405	HIS
2	B	479	GLN
2	B	495	ASN
2	B	838	HIS
2	B	1035	ASN
2	B	1158	ASN
2	B	1231	GLN
2	B	1598	GLN
2	B	1679	ASN
2	B	1691	GLN
2	B	1719	HIS
2	B	1775	HIS
2	B	1941	ASN
2	B	1973	GLN
2	B	2005	GLN
2	B	2127	GLN
2	B	3809	ASN
2	B	3889	GLN
2	B	3896	ASN
2	B	3946	GLN
2	B	3950	ASN
2	B	3960	GLN
2	B	3963	ASN
2	B	4120	ASN
2	B	4130	ASN
2	B	4142	ASN
2	B	4728	HIS
2	B	4886	HIS
2	B	4984	ASN
2	B	4987	ASN
2	B	5003	HIS
2	E	57	ASN

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Mol	Chain	Res	Type
2	E	111	HIS
2	E	151	HIS
2	E	218	HIS
2	E	224	HIS
2	E	273	HIS
2	E	308	HIS
2	E	379	HIS
2	E	383	HIS
2	E	395	GLN
2	E	405	HIS
2	E	479	GLN
2	E	495	ASN
2	E	838	HIS
2	E	1035	ASN
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	1941	ASN
2	E	1973	GLN
2	E	2005	GLN
2	E	2127	GLN
2	E	3809	ASN
2	E	3889	GLN
2	E	3896	ASN
2	E	3946	GLN
2	E	3950	ASN
2	E	3960	GLN
2	E	3963	ASN
2	E	4120	ASN
2	E	4130	ASN
2	E	4142	ASN
2	E	4728	HIS
2	E	4886	HIS
2	E	4984	ASN
2	E	4987	ASN
2	E	5003	HIS
1	F	25	HIS
2	G	57	ASN
2	G	111	HIS

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Mol	Chain	Res	Type
2	G	113	HIS
2	G	218	HIS
2	G	224	HIS
2	G	273	HIS
2	G	379	HIS
2	G	383	HIS
2	G	395	GLN
2	G	405	HIS
2	G	479	GLN
2	G	495	ASN
2	G	838	HIS
2	G	1035	ASN
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	1941	ASN
2	G	1973	GLN
2	G	2005	GLN
2	G	2127	GLN
2	G	3809	ASN
2	G	3889	GLN
2	G	3896	ASN
2	G	3946	GLN
2	G	3950	ASN
2	G	3960	GLN
2	G	3963	ASN
2	G	4120	ASN
2	G	4130	ASN
2	G	4142	ASN
2	G	4728	HIS
2	G	4886	HIS
2	G	4984	ASN
2	G	4987	ASN
2	G	5003	HIS
1	H	25	HIS
2	I	57	ASN
2	I	111	HIS
2	I	151	HIS
2	I	218	HIS

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Mol	Chain	Res	Type
2	I	224	HIS
2	I	273	HIS
2	I	308	HIS
2	I	379	HIS
2	I	383	HIS
2	I	395	GLN
2	I	405	HIS
2	I	479	GLN
2	I	495	ASN
2	I	838	HIS
2	I	1035	ASN
2	I	1158	ASN
2	I	1231	GLN
2	I	1598	GLN
2	I	1679	ASN
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	1941	ASN
2	I	1973	GLN
2	I	2005	GLN
2	I	2127	GLN
2	I	3809	ASN
2	I	3889	GLN
2	I	3896	ASN
2	I	3946	GLN
2	I	3950	ASN
2	I	3960	GLN
2	I	3963	ASN
2	I	4120	ASN
2	I	4130	ASN
2	I	4142	ASN
2	I	4728	HIS
2	I	4886	HIS
2	I	4984	ASN
2	I	4987	ASN
2	I	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	B	12
2	I	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	B	3613:UNK	C	3639:THR	N	44.41
1	I	3613:UNK	C	3639:THR	N	44.36
1	E	3613:UNK	C	3639:THR	N	44.35
1	G	3613:UNK	C	3639:THR	N	44.35

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3163:UNK	C	3170:UNK	N	16.42
1	E	3163:UNK	C	3170:UNK	N	16.36
1	G	3163:UNK	C	3170:UNK	N	16.35
1	I	3163:UNK	C	3170:UNK	N	16.29
1	G	3468:UNK	C	3511:UNK	N	14.86
1	E	3468:UNK	C	3511:UNK	N	14.84
1	I	3468:UNK	C	3511:UNK	N	14.84
1	B	3468:UNK	C	3511:UNK	N	14.79
1	I	3063:UNK	C	3134:UNK	N	14.53
1	G	3063:UNK	C	3134:UNK	N	14.50
1	G	2703:UNK	C	2734:ASN	N	14.49
1	E	3063:UNK	C	3134:UNK	N	14.48
1	I	2703:UNK	C	2734:ASN	N	14.48
1	B	3063:UNK	C	3134:UNK	N	14.46
1	B	2703:UNK	C	2734:ASN	N	14.44
1	E	2703:UNK	C	2734:ASN	N	14.34
1	B	3236:UNK	C	3241:UNK	N	13.22
1	G	3236:UNK	C	3241:UNK	N	13.20
1	E	3236:UNK	C	3241:UNK	N	13.17
1	I	3236:UNK	C	3241:UNK	N	13.16
1	I	1564:UNK	C	1573:MET	N	12.84
1	B	1564:UNK	C	1573:MET	N	12.82
1	E	1564:UNK	C	1573:MET	N	12.72
1	G	1564:UNK	C	1573:MET	N	12.61
1	B	2976:UNK	C	2995:UNK	N	12.18
1	E	2976:UNK	C	2995:UNK	N	12.15
1	I	2976:UNK	C	2995:UNK	N	12.07
1	G	2976:UNK	C	2995:UNK	N	12.06
1	G	3254:UNK	C	3261:UNK	N	8.57
1	I	3254:UNK	C	3261:UNK	N	8.57
1	B	3254:UNK	C	3261:UNK	N	8.56
1	E	3254:UNK	C	3261:UNK	N	8.53
1	E	1297:UNK	C	1430:UNK	N	5.79
1	I	1297:UNK	C	1430:UNK	N	5.74
1	G	1297:UNK	C	1430:UNK	N	5.65
1	B	1297:UNK	C	1430:UNK	N	5.48
1	B	2479:LEU	C	2487:UNK	N	3.92
1	E	2479:LEU	C	2487:UNK	N	3.92
1	I	2479:LEU	C	2487:UNK	N	3.89
1	G	2479:LEU	C	2487:UNK	N	3.81
1	G	2939:ARG	C	2942:UNK	N	3.63
1	I	2939:ARG	C	2942:UNK	N	3.56

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	2939:ARG	C	2942:UNK	N	3.53
1	E	2939:ARG	C	2942:UNK	N	3.53

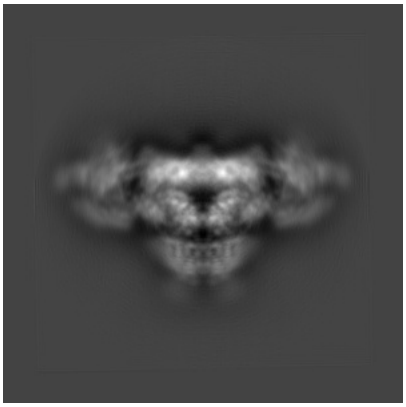
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22394. These allow visual inspection of the internal detail of the map and identification of artifacts.

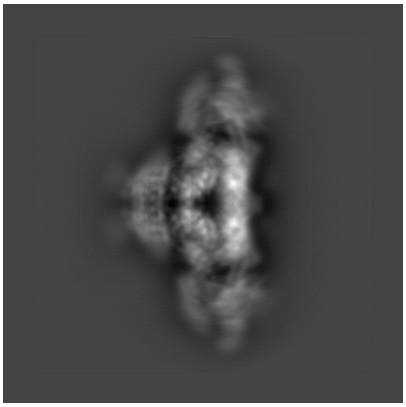
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

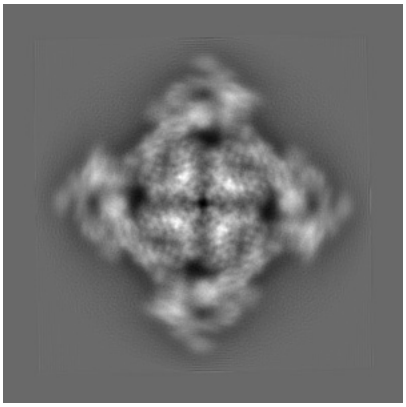
6.1.1 Primary map



X



Y

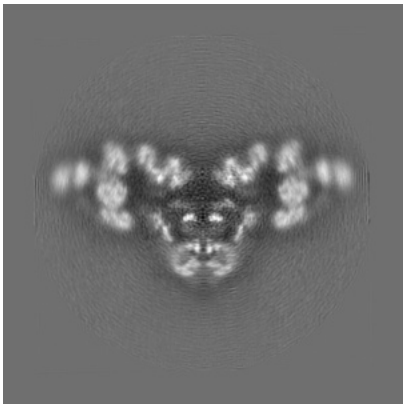


Z

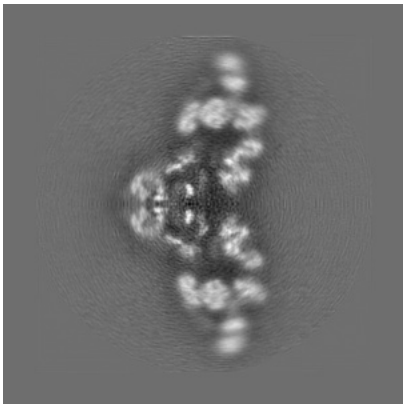
The images above show the map projected in three orthogonal directions.

6.2 Central slices

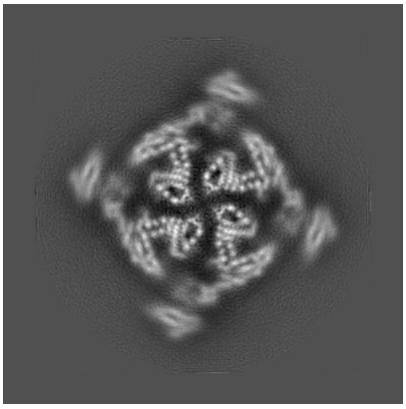
6.2.1 Primary map



X Index: 200



Y Index: 200

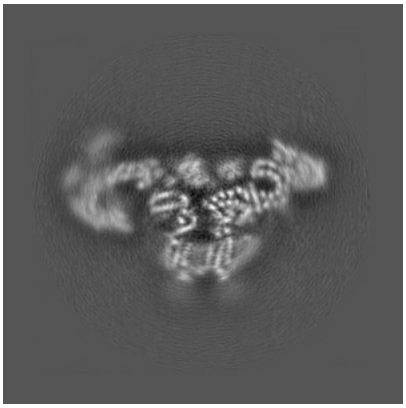


Z Index: 200

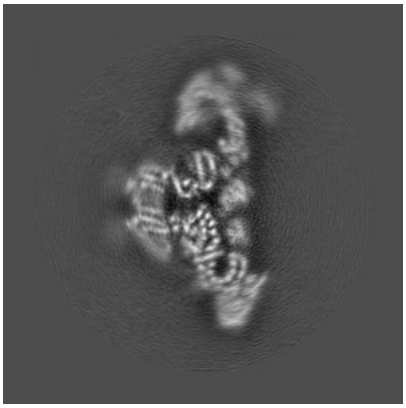
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

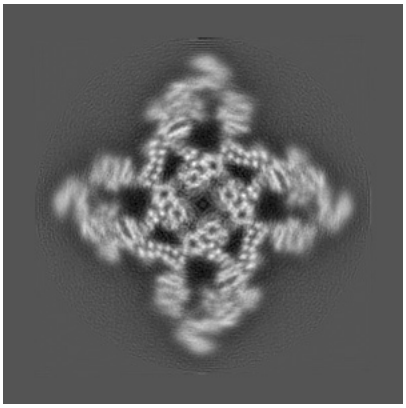
6.3.1 Primary map



X Index: 177



Y Index: 177



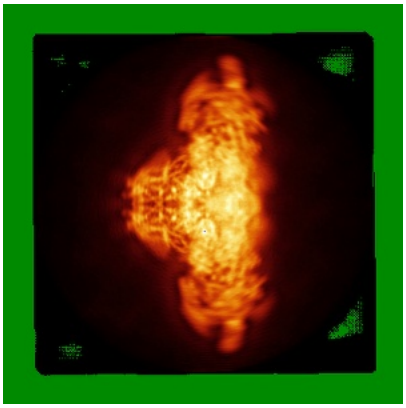
Z Index: 227

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

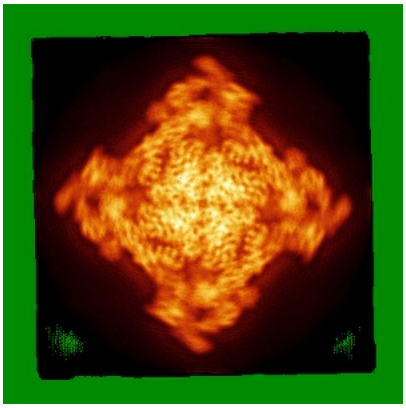
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X



Y



Z

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 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

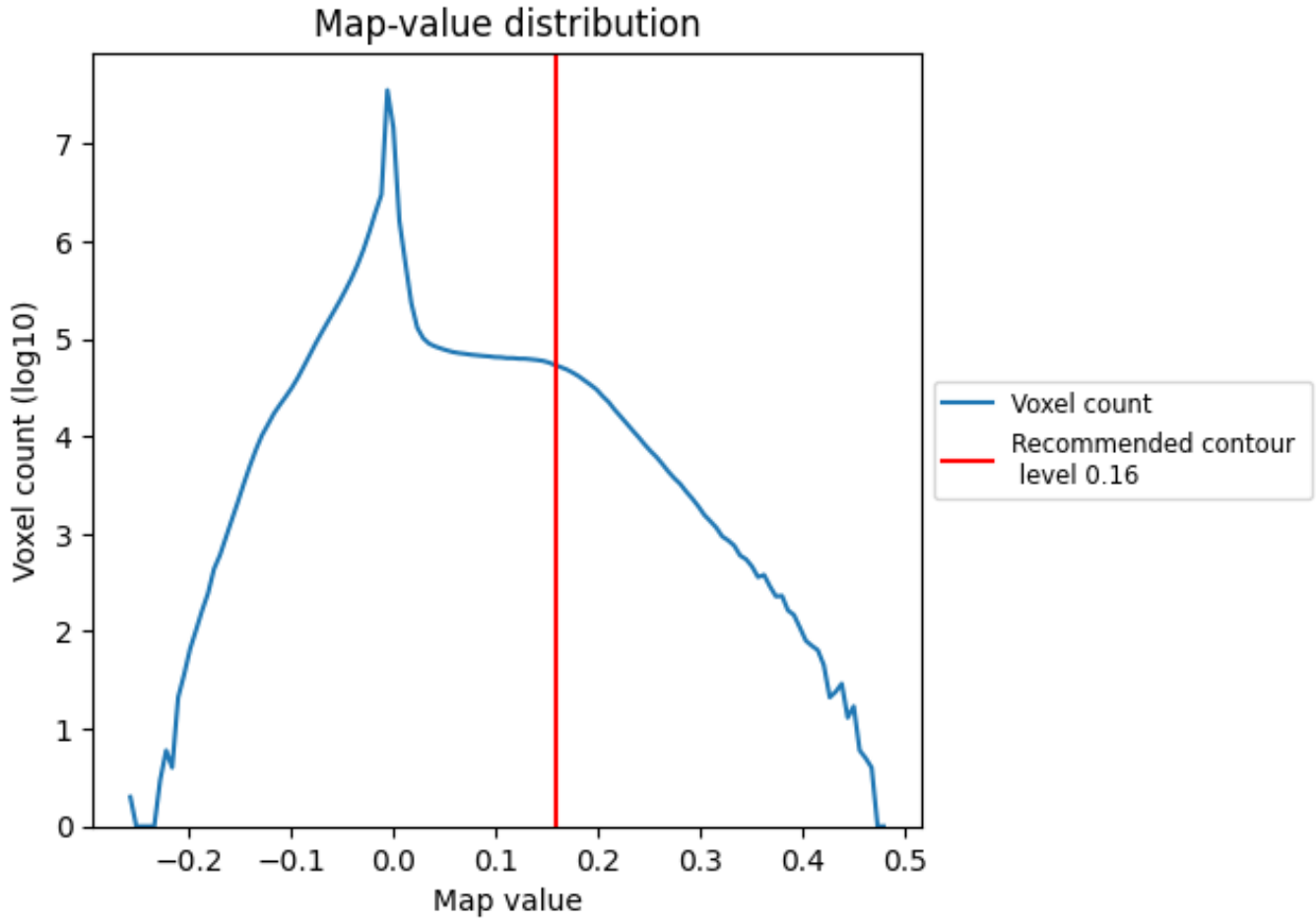
6.6 Mask visualisation (i)

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

7 Map analysis

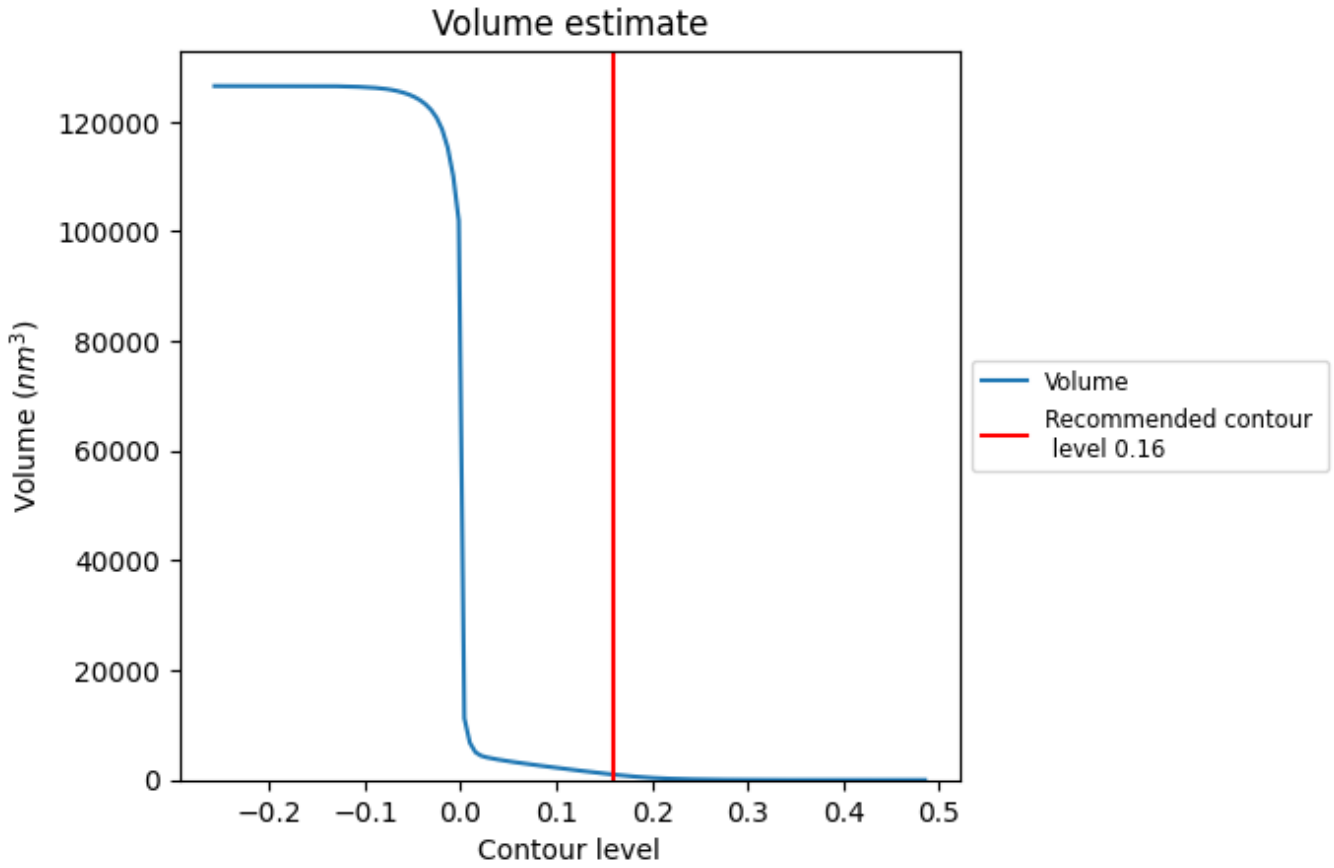
This section contains the results of statistical analysis of the map.

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.

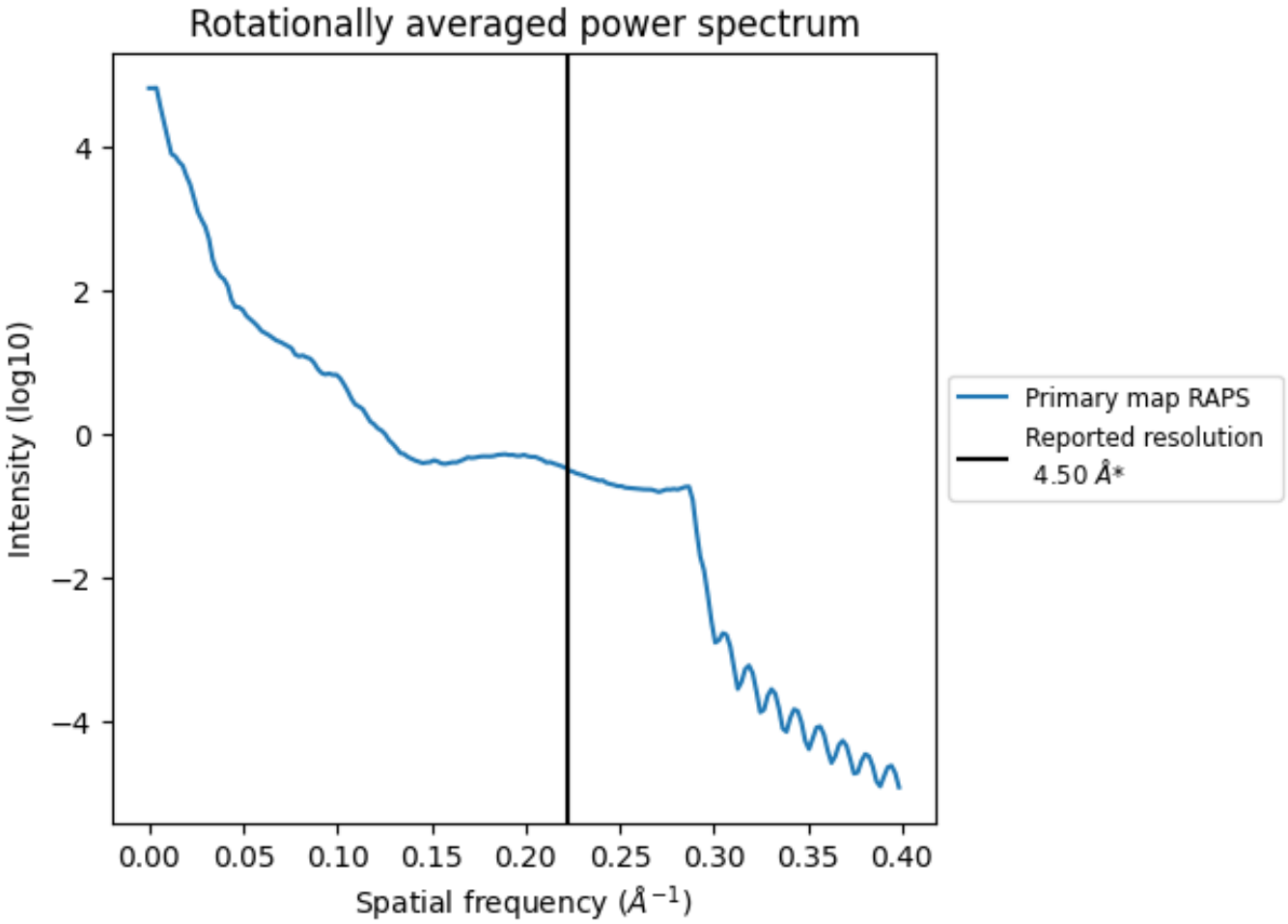
7.2 Volume estimate



The volume at the recommended contour level is 979 nm^3; this corresponds to an approximate mass of 884 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 0.222 Å^{-1}

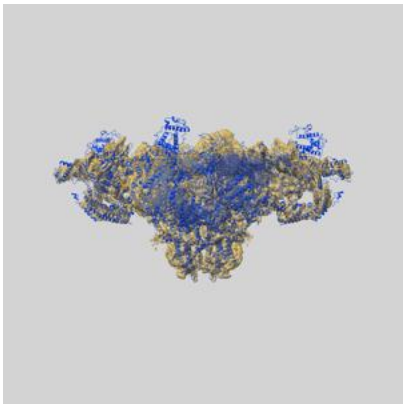
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

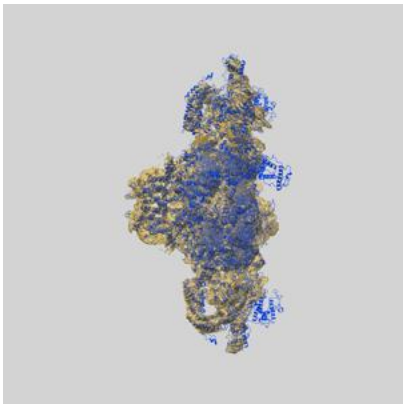
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22394 and PDB model 7JMH. Per-residue inclusion information can be found in section 3 on page 5.

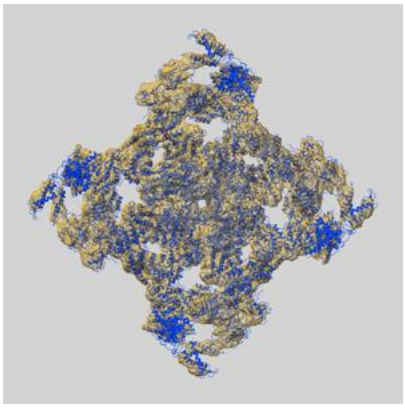
9.1 Map-model overlay



X



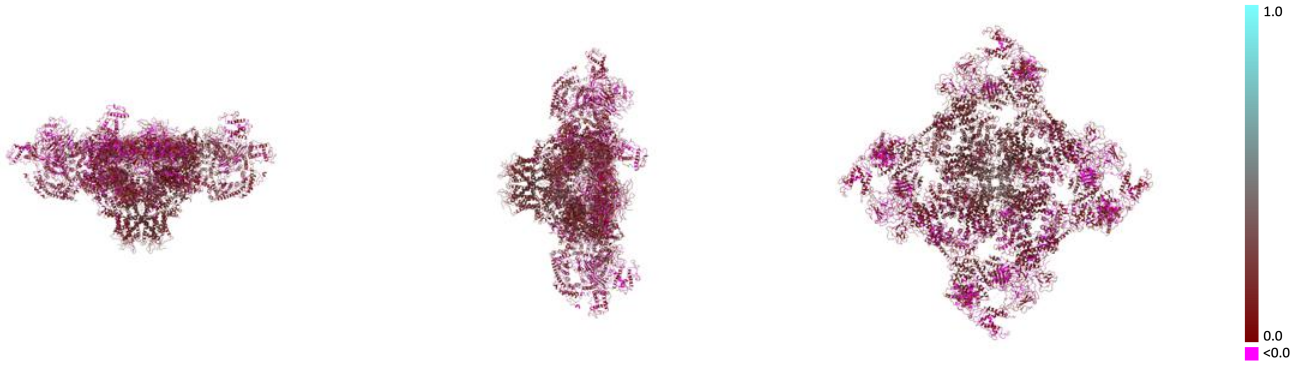
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

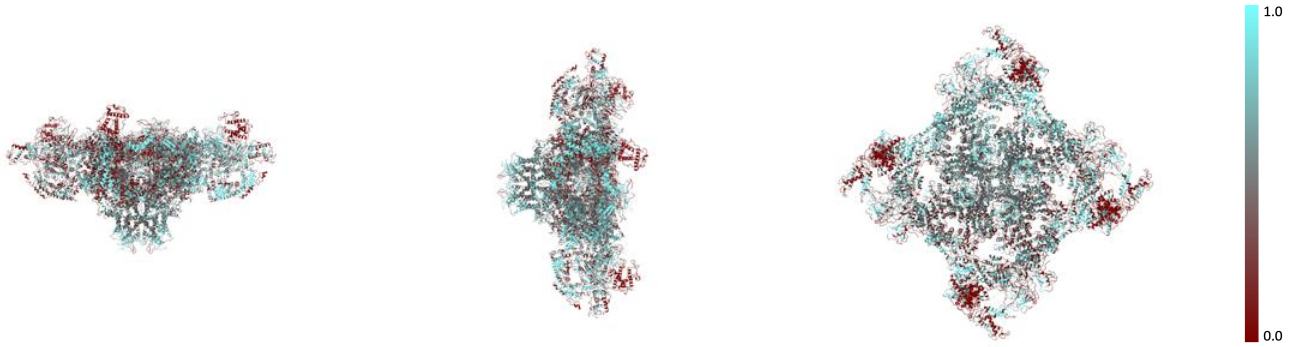
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

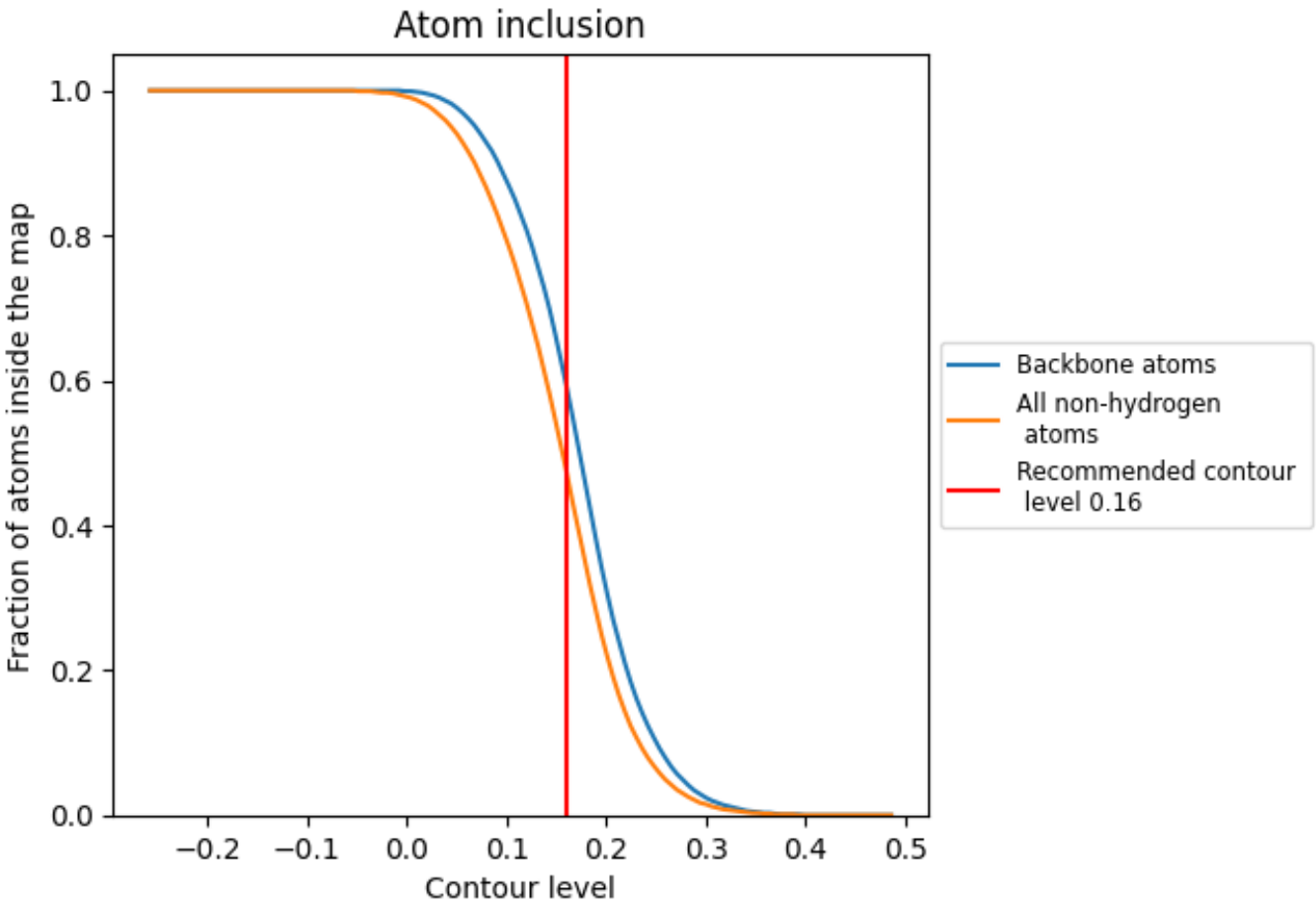
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4750	0.1320
A	0.5620	0.1390
B	0.5150	0.1680
E	0.4810	0.1330
F	0.4890	0.1070
G	0.4450	0.1070
H	0.4530	0.1190
I	0.4560	0.1230
J	0.4690	0.1180